

Graduate courses in Physics

# *Quantum Mechanics*

*applied to Atoms and Light*

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# Preface

This script represents a synthesis of several postgraduate courses given at the Institute of Physics of São Carlos (IFSC) of the University of São Paulo (USP). The courses are *Quantum Mechanics* (SFI5774), *Atomic and Molecular Physics* (SFI5814), *Quantum Mechanics B* (SFI5707), *Interaction of Light and Matter* (SFI5905), and *Atomic Optics* (SFI5887). The topics of the courses are, of course, closely intertwined. The purpose of this composite script is to emphasize the interconnection of topics and facilitate the understanding of how they are related. In part I we introduce the quantum mechanics, which represents the fundamental theory for the rest of the book. In the second part we focus on the structure of the atom. In the third and fourth part we study the properties of light, its interaction with individual atoms and atomic ensembles and how the interaction is influenced by cavities and surfaces. Finally, in part V we introduce the optics of matter wave.

The course is intended for masters and PhD students in physics. The script is a preliminary version continually being subject to corrections and modifications. Error notifications and suggestions for improvement are always welcome. The script incorporates exercises the solutions of which can be obtained from the author.

Information and announcements regarding the course will be published on the website:

<http://www.ifsc.usp.br/strotrium/> - > Teaching - > Semester

The student's assessment will be based on written tests and a seminar on a special topic chosen by the student. In the seminar the student will present the chosen topic in 15 minutes. He will also deliver a 4-page scientific paper in digital form. Possible topics are:

- Observation of super- and subradiant spontaneous emission of two ions (Exc. 21.2.5.2),
- Squeezed states (Sec. 3.8),
- The Jaynes-Cummings model (Sec. 15.2),
- Quantum projection noise (Sec. 16.3.2),
- Quantum gates (Sec. ??),
- The method of quantum Monte-Carlo wavefunction simulation (Sec. 16.1.2),
- The quantum Zeno effect (Sec. 16.3.1),
- Bloch equations: derivation and interpretation (Sec. 14.2),
- The quantum jumps, its history and observation (Sec. 16.1.2),
- Schrödinger's cat (Sec. 16.1.1),
- The Einstein-Podolski-Rosen hypothesis and its experimental falsification (Sec. ??),
- Elitzur and Vaidman bomb testing problem (Sec. ??),
- Topological phases and the Aharonov-Bohm effect (Sec. 16.4),
- Quantum non-demolition measurements (Sec. 16.3.3),
- Calculation of photoelectric effect from Fermi's golden rule (Exc. 6.4.5.7),
- Quantum correlations and the experiments of Young and Hanbury-Brown-Twiss (Sec. 15.3.1),
- The Hartree-Fock method (Sec. 10.3.3),
- Temporal evolution of a free particle described by a Gaussian wave packet,
- The WKB approximation (Sec. 6.3),
- Rydberg atoms (Sec. 8.4.4),



- The helium atom (Sec. 10.2),
- The quadratic and the dynamic Stark effect (Sec. 9.3),
- The blackbody radiation-induced Stark effect (Exc. 6.4.5.9),
- The method of combining atomic orbitals (LCAO) (Sec. 11.1.4),
- Ultracold molecules,
- Efimov states (Sec. 12.3.9),
- Bose-Einstein condensation (Chp. 26.9).

The following literature is recommended for preparation and further reading:

- Ph.W. Courteille, script on *Optical spectroscopy: A practical course* (2020)
- Ph.W. Courteille, script on *Electrodynamics: Electricity, magnetism, and radiation* (2020)
- Ph.W. Courteille, script on *Quantum mechanics applied to atomic and molecular physics* (2020)
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- H.J. Metcalf, P. van der Straten, *Laser Cooling and Trapping*, Graduate Texts in Contemporary Physics, Springer (1999)
- J. Weiner and P-T. Ho, *Light-Matter Interaction: Fundamentals and Applications*, Springer-Verlag, Berlin (2003)
- Ch.J. Foot, *Atomic physics*, (Oxford Master Series in Atomic, Optical and Laser Physics, 2005)
- R. Loudon, *The quantum theory of light*, Oxford Science Publications, Oxford (1973)
- Ch.C. Gerry and P.L. Knight, *Introductory Quantum Optics*, Cambridge University Press (2005)
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- M. Weissbluth, *Photon-Atom Interactions* (Academic Press, Boston, 1989)
- C. Cohen-Tannoudji, B. Diu, F. Laloe, *Quantum mechanics, vol. 1*, Wiley Interscience
- D.J. Griffiths, *Introduction to Quantum mechanics*, Pearson Education Limited (2014)
- L.I. Schiff, *Quantum mechanics*, McGraw-Hill Book Company (1968)
- J.J. Sakurai, J.J. Napolitano, *Modern Quantum Mechanics*, 2<sup>nd</sup> ed., Springer (2011)
- P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, (3<sup>rd</sup> ed. Oxford University (2001)

- I.N. Levine, *Quantum Chemistry*, Allyn and Bacon, 7<sup>th</sup> ed. Pearson (1983)
- H.A. Bethe, R. Jackiw, *Intermediate Quantum Mechanics*, 3<sup>rd</sup> ed. Taylor & Francis (1997)
- J.I. Steinfeld, *Molecules and Radiation*, The MIT Press, Cambridge (2005)
- A. Corney, *Atomic and Laser Spectroscopy*, Clarendon Press, Oxford (1977)
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**Part I**

**Quantum Mechanics**





# Chapter 1

## Antecedents of quantum mechanics

Developed at the beginning of the 20<sup>th</sup> century, quantum mechanics is today the most fundamental and abrageant theory in physics. Despite its long history and its incomparable success, it is far from being exhausted. Quantum information science has matured to a point to be able to trigger important technological progress, such that we are today at the verge of a new quantum revolution 2.0, from which we expect profound scientific, economic, and societal changes.

This chapter traces briefly the historical conditions and the discoveries that led to the invention of quantum mechanics.

### 1.1 The discovery of the atom

The fundamental idea of quantum mechanics is the assumption of the existence of entities that, reaching a limit, can no longer be subdivided. Examples are the mass of a body, the speed of an electron orbiting an atom, or the intensity of a beam of light. This idea was first uttered by *Leucippus* 500 years a.c. and his student *Democritus*, who imagined matter being made of smallest particles which they called *atoms*. These atoms move freely, collide, combine, and separate: 'There is nothing more than atoms and free space.' The microscopic atoms would have the same characteristics as the macroscopic objects they form when they combine, for example, color and shape. The idea of the atom resurfaced and was refined in the course of the 18<sup>th</sup> century (see Tab. 1.1 below). Today, we know that the basic idea was good, but the reality is a little more complicated.

At the end of the 19<sup>th</sup> century, the physical world seemed simple: matter and light was all that existed. Matter was made up of atoms and light was a wave. Therefore, to describe a real system, it was enough to calculate the trajectories of its elementary particles, the propagation of light and the way they interact. We now know that life is not as simple, and that atoms are also waves and light also behaves like particles.

Frictions between the old notions and new observations appeared in the late 19<sup>th</sup> century, such as the ultraviolet divergence of black-body radiation. The pioneer of the new ideas was *Max Planck* who, in 1905, with a little help from Einstein quantized the electromagnetic field, and therefore the light, into small harmonic oscillators. This was the starting point for the development of a new theory called quantum mechanics. Soon, this theory was applied to explain the photoelectric effect. The

Table 1.1: *Historical sketch of the quantization of matter*

500 a.c.	Democritus	invention of the atom
1800	Avogadro, Dalton	reinvention of the atom
1897	Thomson	charge transport, model of raisins in a cake
1909	Rutherford, Geiger, Marsden	$\alpha$ -scattering, charge localized in nuclei
1911	Rutherford	planetary model
1900	Bohr	quantized orbitals
1923	de Broglie	matter has characteristics of waves
1927	Davisson, Germer, Stern	electron and atoms diffraction

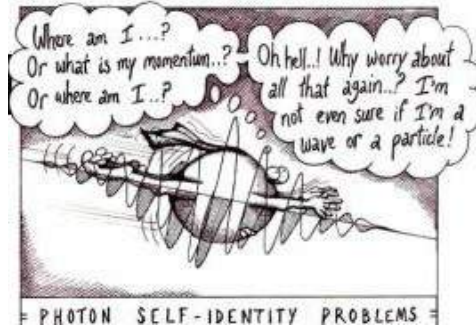


Figure 1.1: Particle-wave duality.

second important step was initialized by *Niels Bohr*, who quantized the hydrogen atom in 1913 into discrete excitation levels.

Table 1.2: *Historical sketch of the quantization of light*

1801	Young	light is diffracted like a wave
1860	Maxwell	unified theory of electrodynamics including light
1888	Hertz	detection of radio waves
~ 1890		accurate measurements of the black-body radiation spectrum
1900	Planck	quantum hypothesis: $E = h\nu$
1905	Einstein	photoelectric effect, light behaves like a particle

### 1.1.1 Democrit's model

'The principles of reality are atoms and emptiness while other things are mere opinions.' This is a quotation from the Greek philosopher *Democritus* 400 years before Christ and before Socrates. Together with his teacher Leucippus, he formed the first idea of indivisible particles: atoms.

Democritus' work only survived as second-hand accounts, the major part of it having been written down by *Aristotle*, who also, defending the idea of the contin-

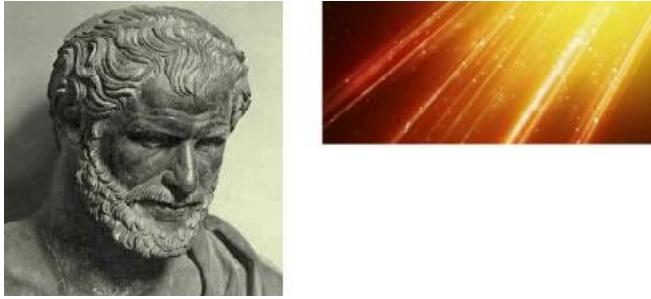


Figure 1.2: Democritus and dust in a sun ray.

uum, was the greatest critic of Democritus' theory. Aristotle said that the reasoning that guided Democritus to affirm the existence of atoms was as follows. For a body to change its shape, it is necessary that its parts can move. This presupposes an emptiness (or vacuum) in which the matter moves. But if matter were divided infinitely into ever smaller parts, it would lose its consistency. Nothing could be formed because nothing could arise from the ever more infinitely deep dilution of matter into emptiness. Hence, he concluded that the division of matter can not be infinite, that is, there is an indivisible limit: the atom. 'There is only atoms and emptiness', he said.

Observing dust particles in a whirling motion within a ray of sunlight, Democritus was led to the idea that atoms would behave in the same way, randomly colliding, some crowding, others dispersing, others never yet joining with another atom.

The consistency of clusters of atoms, which makes something look solid, liquid, gaseous, or animated (which is the state of the soul) would then be determined by the shape of the atoms involved and their spatial arrangement. In this sense, water atoms are smooth and slippery; the atoms of steel have shapes with sharp edges that hold them solidly together; the atoms of salt, as their taste shows, are harsh and pointed; the atoms of air are small and little connected, penetrating all other materials; and the atoms of soul and fire are spherical and very delicate.



Figure 1.3: Atoms of steel and air, atoms of the soul, and Bohr's atom model.

We know nowadays that Democritus' first theory of the structure of matter was very close to the truth: There really are indivisible particles called atoms composed of a nucleus and an electronic shell, and the space between the atomic nuclei is, in fact, quite empty.

The atomic hypothesis came to be reborn in the modern age with the scientists Boyle, Clausius, Maxwell, and Boltzmann due to their successful explanations of the properties of gases based on the so-called kinetic theory, where they assumed a gas being constituted of identical molecules that collided elastically with each other and with the walls of the recipient containing them. The discovery of the atom through the *laws of proportions* in chemistry and the establishment of Avogadro's number considerably strengthened the atomic hypothesis. The hypothesis was definitely consecrated with the various experiments that established the charge of the electron and the mass ratio between electrons and protons.

By the beginning of the 19<sup>th</sup> century the atomic nature of matter had definitely been established, and the basic composition of the atoms was already relatively well known. It was known, through experiments, that electrons could be removed from neutral atoms thus creating positively charged ions and that only a certain number of electrons could be removed from each atom. This number proved to be dependent on the atomic species and was called the atomic number  $Z$ . This information was fundamental for establishing the basic composition of atoms. The question that arose at this point concerned the dimensions and configurations of the atomic system. How would loads and masses be distributed in this entity?

### 1.1.2 Thomson's model and Rutherford's experiment

The internal structure of a body can be studied by throwing beams of small particles against it. The detection of the angular distribution of the scattered particles gives access to the structure factor of the body. In crystallography we throw X-rays into super-complicated molecules to learn the architecture e.g. of proteins. And in medicine, X-rays reveal the internal structure of the human body. Obviously, the scattering technique is an extremely powerful tool, used in many areas of modern physics.

In a series of experiments done before 1911, *Ernest Rutherford* analyzed the internal structure of gold atoms using  $\alpha$ -particles, i.e.,  $\text{He}^{2+}$  atoms. The experiments carried out by Geiger, Marsden, and Rutherford consisted of observing the deflection of particles from a collimated beam when scattered by a thin metallic sheet (gold of thickness  $\sim 1 \mu\text{m}$ ) carefully obtained by electroplating [see Fig. 1.4(cd)].

The atomic model proposed by *Joseph John Thomson* suggests a structure resembling a *pudding with raisins*: the electrons would be homogeneously distributed within an extended nucleus (size 0.1 nm) of positive charge thus compensating for the negative charge of the electrons. The  $\alpha$ -particles would penetrate the gold nucleus, perceived as almost homogeneous, but would suffer multiple deflections due to collisions with the disordered electrons within the nucleus. Since electrons are very light, the angle of deflection  $\theta$  would be small, even after many collisions. For this model we expect a Gaussian dependence of the particles' deflection angle given by the *scattering cross section* [see Fig. 1.4(a-b)],

$$\frac{d\sigma}{d\Omega} \propto e^{-\theta^2/\theta_0^2}, \quad (1.1)$$

where  $\theta_0$  is a small angle.

However, the measurements performed on this *Rutherford scattering* showed different results:

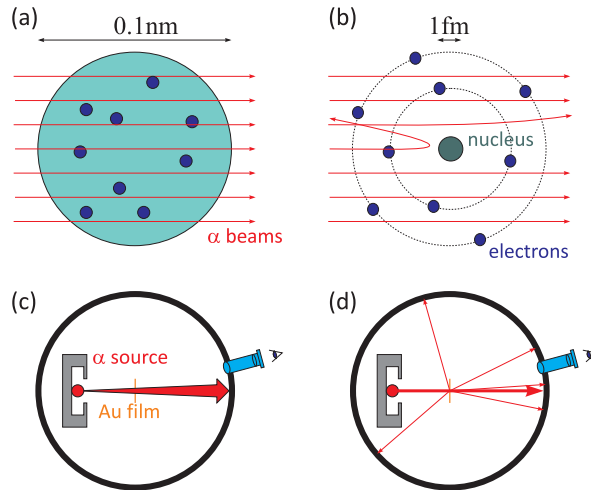


Figure 1.4: Comparison of Rutherford scattering by free electrons and electrons strongly bound to small nuclei. (a) Thomson's 'raisin-in-a-pudding' type atom; (b) Rutherford's 'planetary' atom. (c) Rutherford scattering by a raisin pudding atom and (d) by a planetary atom.

- For a fixed scattering angle, the amount of particles scattered into a solid angle element  $d\Omega$  is proportional to the thickness of the metal foil.
- For a given fixed angle and a given metal sheet the amount of scattered particles in  $d\Omega$  varies inversely with  $E_{kin}^2$ , where  $E_{kin}$  is the kinetic energy of the  $\alpha$ -particles.
- For a given energy and a given metal sheet, the number of particles scattered into  $d\Omega$  is proportional to  $(\sin \frac{\theta}{2})^{-4}$ .
- For a given energy and sheet thickness, the number of particles scattered into  $d\Omega$  in a given direction is proportional to  $Z_{tg}^2$ , where  $Z_{tg}$  is the atomic number of the element that constitutes the sheet.

The extremely rare deflection of  $\alpha$ -particles and their angular distribution can be understood by the assumption that the positive charge is concentrated in a very small volume ( $\sim 1$  fm, that is 10000 times less than the size of the atom itself). This volume is called the atomic nucleus, hence the denomination of *nuclear model*. Since most of the particles pass through the gold sheet without hindrance, there must be a large gap between the nuclei. The electrons, which move within a large (in comparison with the diameter of the nucleus) empty space (the vacuum) around the nucleus, shield the positive nuclear charge, so that the atom appears outwardly neutral.

We now derive Rutherford's scattering formula from the hypothesis of a point-like nucleus. Due to the repulsive action of the Coulomb force,

$$F = \frac{Z_{\alpha} Z_{tg} e^2}{4\pi\epsilon_0 r^2}, \quad (1.2)$$

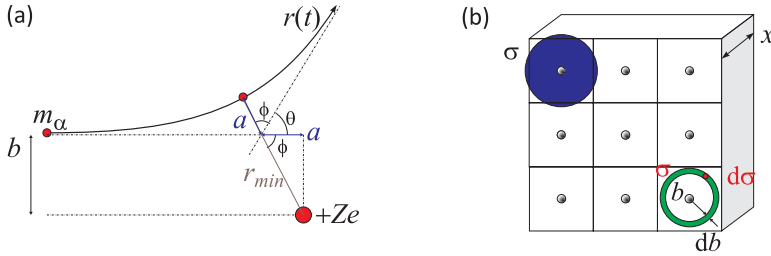


Figure 1.5: (a) Trajectory of an  $\alpha$ -particle. (b) Illustration of the scattering cross section.

we have for the trajectory of the  $\alpha$ -particle ( $Z_\alpha = 2$ ) a hyperbola [see Fig. 1.5(a)]. The large half-axis of the hyperbola can be determined from the following ansatz,

$$E_{\text{kin}} = \frac{Z_\alpha Z_{tg} e^2}{4\pi\epsilon_0} \frac{1}{2a}, \quad (1.3)$$

where  $2a$  is the minimum distance of the particle  $\alpha$ , when it collides with the nucleus in a central collision<sup>1</sup>. The distance  $a$  depends on the kinetic energy and can also be used for non-central collisions. The collision parameter  $b$  is the minimum distance of the  $\alpha$ -particle to the nucleus, if it continued to fly in a straight line. In fact the  $\alpha$ -particle will be deflected by an angle  $\theta$ . From the geometry of the hyperbola, as  $2\phi + \theta = 180^\circ$ , we obtain the following equation:

$$\tan \phi = \frac{b}{a} = \tan \left(90^\circ - \frac{\theta}{2}\right) = \cot \frac{\theta}{2}, \quad (1.4)$$

and therefore

$$\cot \frac{\theta}{2} = \frac{b}{a} = \frac{8\pi\epsilon_0 E_{\text{kin}} b}{Z_\alpha Z_{tg} e^2}, \quad (1.5)$$

replacing  $a$  with the formula (1.3). Taking the derivative of this latter formula, we obtain a relation between the width  $db$  of the hollow cone and the pertinent width  $d\theta$  of the deflection angle  $\theta$ ,

$$-\frac{1}{2 \sin^2 \frac{\theta}{2}} d\theta = \frac{8\pi\epsilon_0 E_{\text{kin}}}{Z_\alpha Z_{tg} e^2} db. \quad (1.6)$$

Let  $n_{tg} = \frac{N_{tg}}{V}$  be the density of the particles in the target ( $N_{tg}$  atoms per volume  $V$ ) and  $x$  the film thickness. Then  $\sigma = \frac{A}{N_{tg}} = \frac{V/x}{N_{tg}} = \frac{1}{n_{tg} x}$  is the average cross-section per atom sensed by the  $\alpha$ -particle on its way through the film. The probability  $P(\theta)d\theta$  for the  $\alpha$ -particle of being within a ring at distance  $b$  from the nucleus (whose area is  $2\pi b db$ ) and being scattered into the angle  $\theta$  is then given by,

$$P(\theta)d\theta = \frac{2\pi b db}{\sigma} = n_{tg} x 2\pi b db. \quad (1.7)$$

<sup>1</sup>In a central collision, when the  $\alpha$ -particle reaches the minimum distance  $2a$ , its initial kinetic energy,  $E_{\text{kin}}$  is fully converted into potential energy.

These particles, i.e.,  $dN$  of the  $N$  particles, are deflected into the hollow cone with the probability,

$$\begin{aligned} \frac{dN}{N} &= P(\theta)d\theta = n_{tg}x2\pi \frac{Z_\alpha Z_{tg}e^2}{8\pi\epsilon_0 E_{\text{kin}}} \cot \frac{\theta}{2} \cdot \frac{Z_\alpha Z_{tg}e^2}{8\pi\epsilon_0 E_{\text{kin}}} \cdot \frac{1}{2 \sin^2 \frac{\theta}{2}} d\theta \\ &= n_{tg}x \frac{Z_\alpha^2 Z_{tg}^2 e^4}{64\pi\epsilon_0^2 E_{\text{kin}}^2} \cdot \frac{\cos \frac{\theta}{2}}{\sin^3 \frac{\theta}{2}} d\theta, \end{aligned} \quad (1.8)$$

where we replaced the parameters  $b$  and  $db$  with the expressions (1.5) and (1.6). The solid angle of the cone can be expressed by,

$$d\Omega = 2\pi \sin \theta d\theta = 4\pi \sin \frac{\theta}{2} \cos \frac{\theta}{2} d\theta. \quad (1.9)$$

Thus, the number  $dN$  of particles scattered to the solid angle  $d\Omega$  remains,

$$\boxed{\frac{dN}{N} = n_{tg}x \frac{Z_\alpha^2 Z_{tg}^2 e^4}{256\pi^2 \epsilon_0^2 E_{\text{kin}}^2} \cdot \frac{1}{\sin^4 \frac{\theta}{2}} d\Omega}. \quad (1.10)$$

That is Rutherford's scattering formula. Often, the formula is expressed with the *differential* cross section  $\frac{d\sigma}{d\Omega}$ . We get,

$$\frac{dN}{N} = \frac{d\sigma}{\sigma} = n_{tg}x d\sigma, \quad (1.11)$$

and therefore

$$\frac{d\sigma}{d\Omega} = \frac{dN}{N n_{tg}x d\Omega} = \left( \frac{Z_\alpha Z_{tg}e^2}{4\pi\epsilon_0 \cdot 4E_{\text{kin}}} \right)^2 \frac{1}{\sin^4 \frac{\theta}{2}}. \quad (1.12)$$

Here, we have to make some comments:

- The angle  $\theta = 0$  is not defined, since there exists a minimum deflection angle  $\theta_{\text{min}}$ . This angle is reached, when the  $\alpha$ -particle moves at the distance  $b = b_{\text{max}}$  from the atom, that is, at the edge of the circular area of the cross section. For a greater collision parameter  $b$ , the  $\alpha$ -particle traverses the field of the next neighboring atom, and the deflection angle increases again. We have:

$$\sigma = \frac{A}{N_{tg}} = \pi b_{\text{max}}^2 \quad \text{and} \quad \frac{\theta_{\text{min}}}{2} \simeq \tan \frac{\theta_{\text{min}}}{2} = \frac{Z_\alpha Z_{tg}e^2}{8\pi\epsilon_0 E_{\text{kin}} \cdot b_{\text{max}}}, \quad (1.13)$$

simply by inverting the formula (1.5). For very large impact parameters, that is, when the  $\alpha$ -particle passes the atom outside its electronic layer, the electrons of the atom shield the charge of the nucleus, an effect called *screening*.

- For very high energies, the distribution of the nuclear charge over a finite volume influences the scattering, calling for corrections in the Rutherford formula. Moreover, at short internuclear distances, nuclear forces appear additionally to the electromagnetic interaction.



- The integral over the probability distribution  $P(\theta)d\theta$  is normalized,

$$\int_{\theta_{\min}}^{\pi} P(\theta)d\theta = 1 . \quad (1.14)$$

Similarly, we have for the surface integrals,

$$\int_{\theta \geq \theta_{\min}} \frac{d\sigma}{d\Omega} d\Omega = \sigma . \quad (1.15)$$

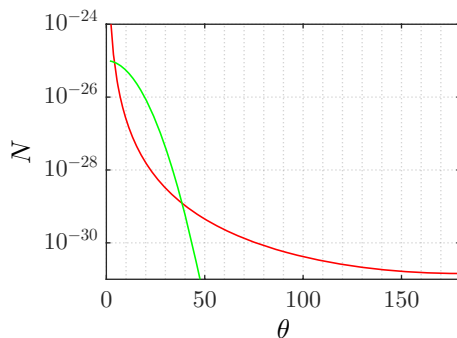


Figure 1.6: (code) Angular dependence of the cross-section corresponding to Thomson's (green) and Rutherford's (red) models.

Rutherford derived the formula (1.12) describing the scattering of  $\alpha$ -particles within classical physics. A derivation from the laws governing quantum mechanics using the *Born approximation* shows that Rutherford's formula describes scattering correctly in first order, and that purely quantum effects present only minor corrections. We will review the Rutherford scattering in Excs. 1.1.6.1 and 1.1.6.2 and discuss the screening effect in Exc. 1.1.6.3.

### 1.1.3 Emission of radiation in the planetary model

The *planetary model* proposed by Rutherford suggests electrons spinning around a positively charged nucleus in circular orbits<sup>2</sup>. This motion of electrons should obey the laws of Maxwell's electrodynamic theory. Let us now calculate some consequences of this picture.

We now treat the atom as a rotor where the negative particle, the electron, orbits the positive particle. The dipole moment is,

$$p_0 = -er . \quad (1.16)$$

<sup>2</sup>This type of model had already been proposed by Jean Perrin in 1901 and by Hantaro Nagaoka in 1903, around the same time when Thompson developed his model. The planetary model was later on rescued by John William Nicholson in 1911.

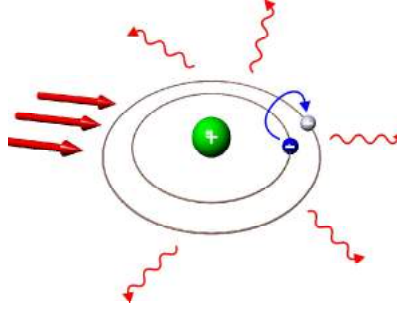


Figure 1.7: Light-induced transitions between orbits in the planetary model.

We calculate in the Exc. 1.1.6.4 the power emitted by the acceleration  $a = \omega^2 r$  of the electron on its circular trajectory,

$$P = \frac{\mu_0 \omega^4 p_0^2}{12\pi c} . \quad (1.17)$$

The initial energy of the electron spinning around the nucleus (for a hydrogen atom  $Z = 1$ ),

$$E = \frac{p^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 r} = \frac{m_e \omega^2 r^2}{2} - \frac{e^2}{4\pi\epsilon_0 r} , \quad (1.18)$$

is dissipated by radiation of the power (1.17), i.e.,

$$-P = \frac{dE}{dt} = m_e \omega^2 r \frac{dr}{dt} + \frac{e^2}{4\pi\epsilon_0 r^2} \frac{dr}{dt} = 2m_e \omega^2 r \frac{dr}{dt} . \quad (1.19)$$

The latter equation supposes an equilibrium between the centrifugal force and the Coulomb force,

$$m_e \omega^2 r = \frac{e^2}{4\pi\epsilon_0 r^2} , \quad (1.20)$$

allowing to link the revolution frequency  $\omega$  to the instantaneous radius of the orbit  $r(t)$ . Resolving the Eq. (1.19) by  $\dot{r}$  and replacing the power by the relation (1.17) and the frequency  $\omega$  by the relation (1.20), we obtain,

$$\frac{dr}{dt} = -\frac{P}{2m_e \omega^2 r} = -\frac{\mu_0 \omega^2 e^2}{24\pi m_e c} r = -\frac{e^4}{96\pi^2 \epsilon_0^2 m_e^2 c^3} \frac{1}{r^2} . \quad (1.21)$$

Integration of this equation gives,

$$t - t_0 = -\frac{32\pi^2 \epsilon_0^2 m_e^2 c^3}{e^4} [r^3 - r^3(t_0)] . \quad (1.22)$$

Now inserting  $t_0 = 0$  and assuming  $r(t_0) = a_B$ , the time  $\tau$  within which the loss of energy due to radiation emission decreases the radius of the electronic orbit to  $r = 0$ , is,

$$t = \tau = \frac{32\pi^2 \epsilon_0^2 m_e^2 c^3 a_B^3}{e^4} . \quad (1.23)$$

Insertion of the numerical values gives the decay time  $\tau \sim 10^{-10}$  s. This is the effect called *radiation collapse* of the classical atomic model.

### 1.1.4 Zeeman effect in the planetary model

The orbital motion of the electron generates a ring current  $I = e/T = e\omega/2\pi$ , which produces an *orbital magnetic moment* which, as shown in Exc. 1.1.6.5, can be calculated following the laws of electromagnetism,

$$\vec{\mu}_\ell = IA\hat{\mathbf{n}} = \frac{e\omega}{2\pi}\pi r^2\hat{\mathbf{n}}, \quad (1.24)$$

where  $A = \pi r^2$  is the area of the trajectory. Introducing the angular momentum  $\mathbf{L} = m_e\omega r^2\hat{\mathbf{n}}$  we get in vector notation,

$$\vec{\mu}_\ell = \frac{e}{2m_e}\mathbf{L}. \quad (1.25)$$

We now imagine this atom in the presence of a magnetic field  $\mathbf{B}$  oriented in the direction that we will call  $z$ . This results in a precession of the magnetic moment around the field (similar to the precession of a spinning top in the presence of a gravitational field) governed by the equation,

$$\frac{d\mathbf{L}}{dt} = \vec{\mu}_\ell \times \mathbf{B} = \frac{e}{2m_e}\mathbf{L} \times \mathbf{B} = -\Omega_L \times \mathbf{L},$$

with  $\Omega_L = \frac{e}{2m_e}\mathbf{B}$  representing the precession frequency and being called *Larmor frequency*. It is evident that the presence of the magnetic field considerably alters the state of the atom, even producing profound modifications in the frequency of the orbit of the electron  $\omega_0$  and therefore in the energetic state of the atom. This change is called *Zeeman effect*.

The Zeeman effect can be calculated by imagining that the field has an arbitrary direction with respect to  $\mathbf{L}$ . In this case, the equation describing the electronic motion as resulting from an equilibrium between the centrifugal force and the Coulomb force needs to be complemented by a Lorentz force,

$$m_e\ddot{\mathbf{r}} + m_e\omega_0^2\mathbf{r} = \mathbf{F}_L = -e\mathbf{v} \times \mathbf{B}. \quad (1.26)$$

where  $m\ddot{\mathbf{r}}$  is the centrifugal force due to the circular motion of the electron and  $m_e\omega_0^2\mathbf{r}$  the centripetal force due to the Coulomb attraction exerted by the nucleus. Assuming the direction of the magnetic field given by  $\mathbf{B} = B\hat{\mathbf{e}}_z$  with  $B = 2m_e\Omega_L/e$ , the equations of motion can be decomposed into,

$$\ddot{x} + \omega_0^2x + 2\Omega_L\dot{y} = 0 \quad (1.27)$$

$$\ddot{y} + \omega_0^2y - 2\Omega_L\dot{x} = 0$$

$$\ddot{z} + \omega_0^2z = 0.$$

The  $z$ -direction is not influenced. With the ansatz  $x = ae^{i\omega t}$  and  $y = be^{i\omega t}$  we obtain the system of equations,

$$a(\omega_0^2 - \omega^2) + 2i\Omega_L\omega b = 0 \quad (1.28)$$

$$b(\omega_0^2 - \omega^2) - 2i\Omega_L\omega a = 0,$$

which has a non-trivial solution for  $a$  and  $b$  only when the determinant of the coefficients of  $a$  and  $b$  vanishes:

$$0 = \begin{vmatrix} \omega_0^2 - \omega^2 & 2i\Omega_L\omega \\ -2i\Omega_L\omega & \omega_0^2 - \omega^2 \end{vmatrix} = \omega^4 - (2\omega_0^2 + 4\Omega_L^2)\omega^2 + \omega_0^4 . \quad (1.29)$$

We get,

$$\omega = \omega_{1,2} = \sqrt{\omega_0^2 + 2\Omega_L^2 \pm 2\Omega_L\sqrt{\omega_0^2 + \Omega_L^2}} = \omega_0 \pm \Omega_L + \frac{1}{2}\frac{\Omega_L^2}{\omega_0} + \dots , \quad (1.30)$$

or, as  $\Omega_L \ll \omega$ , we get  $\omega_{1,2} = \omega_0 \mp \Omega_L$ . The result is a splitting of the energy levels proportional to the magnetic field,

$$\Delta E = 2\hbar\Omega_L = \frac{\hbar e}{m_e}B = 2\mu_B B , \quad (1.31)$$

where the abbreviation  $\mu_B = e\hbar/2m_e \simeq 9.27 \cdot 10^{-24} \text{ JT}^{-1}$  is called the *magneton Bohr*.

Although the classical derivation shows quantitative deviations from experimental observations, it is quite interesting, as it illustrates several aspects which have a quantum mechanical equivalence.

**Example 1 (*Stern-Gerlach experiment*):** Among several historical experiments carried out to unravel the atomic structure, one of the most important is the experiment carried out by *Otto Stern* and *Walther Gerlach* in 1922 to measure the magnetic moment of atoms. The results of this experiment once again demonstrated the need for new concepts to explain the observations. Using Bohr's quantization rule,  $L = n\hbar$ , within the formula (1.25) we get,

$$\vec{\mu} = -\mu_B \frac{\mathbf{L}}{\hbar} .$$

In the presence of a magnetic field the dipole undergoes an interaction  $W = -\vec{\mu} \cdot \mathbf{B}$ , and therefore a feels a force,

$$\mathbf{F} = -\vec{\mu} \cdot \nabla \mathbf{B} .$$

By subjecting beams of atoms to the gradient of a magnetic field and detecting this force, Stern and Gerlach were able to measure the magnetic moment produced by the rotation of the electrons around the atomic nuclei.

### 1.1.5 Bohr's theory and its limitations

The classical model of the planetary atom provides a mechanical illustration of the microscopic world but fails to quantitatively explain experimental observations such as the discrete nature of atomic spectra.

The radiation emitted by hydrogen atoms is characterized by discrete, spectrally very thin lines. The observed lines are grouped in series named after Lyman, Ballmer and others,

$$\frac{1}{\lambda} = R_H \frac{\mu}{m_e} \left( \frac{1}{m^2} - \frac{1}{n^2} \right) , \quad (1.32)$$

where  $m$  and  $n$  are integers.  $R_H = (1/4\pi\epsilon)^2(m_e e^4/4\pi\hbar^3 c)$  is the Rydberg constant and  $\mu = m_e m_{at}/(m_e + m_{at})$  the reduced mass.

The discrete nature of spectral lines and the problem of the radiation collapse led *Niels Bohr* to formulate the following *postulates*:

1. There are specific stationary orbits, where electrons do not emit energy.
2. Each emission or absorption of radiation energy by electrons comes with a transition between stationary orbits. The radiation emitted during this transition is homogeneous.
3. The laws of mechanics can describe the dynamic equilibrium of electrons in stationary states, but fails to describe the transition of electrons *between* stationary orbits.

Thus, Bohr's model predicts the quantization of energy levels, known as *first quantization* of quantum mechanics. The radii of the possible orbits can be calculated from the postulate that the orbital angular momentum be quantized in units of  $\hbar$ , that is, the electrons form stationary de Broglie waves along the orbits<sup>3</sup>. We discuss Bohr's model in Excs. 1.1.6.6 and 1.1.6.7.

In the picture proposed by Bohr, the radiative decay happens as an abrupt transition of an electron between an outer (more energetic) orbit and an inner (less energetic) orbit. Since the energies of stationary orbits are very well defined, the emitted radiation is mono-energetic, i.e., the spectrum consists of discrete characteristic lines.

We note here that the picture of an abrupt transition of electrons between discrete states, called the *quantum jump*, did not receive Schrödinger's blessing. He rather imagined for electrons, within his theory of quantum wave mechanics, wave-shaped orbitals instead of planetary trajectories, thus avoiding the problem of radiation due to charge deceleration and the quantum jump concept. According to him, during a transition between electronic orbits, the energy is transformed into radiation *gradually*<sup>4</sup>.

## 1.1.6 Exercises

### 1.1.6.1 Ex: Analysis of Rutherford scattering

- a. What conclusions can be drawn from the observation that Rutherford's formula describes well the scattering of charged particles traveling through matter over a wide range of parameters?
- b. Why do we see a deviation from Rutherford's formula for large energies?
- c. The scattering of protons with energy  $E$  crossing a thin film of thorium is well described up to energies of  $E = 4.3$  MeV by Rutherford's formula. Estimate for this case the range of nuclear forces.
- d. For small scattering angles  $\theta$  we observe large deviations from Rutherford's formula.

<sup>3</sup>A generalization of Bohr's theory was provided by *Arnold Johannes Wilhelm Sommerfeld*. Assuming elliptical orbits for the electrons he managed to explain some features of the fine structure, provided the motion of the electron was treated relativistically. The basic premises were 1. stable orbits when the Coulomb attraction is balanced by the centrifugal force, 2. quantization of phase space  $\int r_q dq = n_q \hbar$ , and 3. quantization of angular momentum  $\int L d\theta = n_\theta \hbar$ .

<sup>4</sup>We note here, that quantum jumps were observed much later!

Explain why?

e. Assume the thorium atoms of item (c) to form a periodic crystal with the lattice constant  $d = 10a_B$ . At which minimum angle  $\theta$  Rutherford's formula loses its validity.

### 1.1.6.2 Ex: Rutherford scattering

a. A beam of  $\alpha$ -particles with energy  $E_{\text{kin}} = 3 \text{ MeV}$  and flux  $I = 5 \cdot 10^3 \text{ s}^{-1}$  impinges on a thick gold film  $x = 1 \text{ }\mu\text{m}$ . Using Rutherford's formula, calculate how many particles are scattered in  $\Delta t = 10$  minutes in the range of angles  $10^\circ \leq \theta \leq 30^\circ$ .

b. Now, the gold film is replaced with an aluminum film of the same thickness. How many  $\alpha$ -particles are scattered under equal circumstances?

### 1.1.6.3 Ex: Screening of electrons

Consider thin layer of charge  $-Z_{tq}e$  with radius  $R$ . This screening causes a scattering angle,

$$\tan \frac{\theta}{2} = \frac{D}{2b} \frac{\sqrt{1 - (b/R)^2}}{1 + D/2R},$$

with  $D \equiv \frac{3Ze^2}{m_2v^2/2}$  for  $b < R$ . Verify how the screening changes the differential cross section  $\frac{d\sigma}{d\Omega}$ .

### 1.1.6.4 Ex: Radiation of an oscillating dipole

Calculate the angular distribution of the power radiated by an oscillating electric or magnetic dipole from expressions for the emitted electric and magnetic fields found in literature.

### 1.1.6.5 Ex: Magnetic moments

a. Derive from the expression  $\vec{\mu}_L = \frac{1}{2} \int_{\mathbb{R}^3} \mathbf{r} \times \mathbf{j}(\mathbf{r}') d^3r'$  of classical electrodynamics and an appropriate parametrization of the current density  $\mathbf{j}$  the relation between the magnetic dipole moment  $\vec{\mu}$  due to the orbiting electron and the angular momentum  $\mathbf{L}$ .

b. The length of the angular momentum vector being given by  $|\mathbf{L}| = \hbar$ , calculate the magnetic moment for an electron and for a proton.

### 1.1.6.6 Ex: Bohr's atom

In 1913, Niels Bohr presented his atomic model adapting Rutherford's model to the quantization ideas proposed by Max Planck.

a. Impose the quantization rule for the angular momentum ( $L = n\hbar$ ) of an electron orbiting an atom of atomic number  $Z$  to find an expression for the radii of the allowed orbits.

b. According to Bohr's model, the transition between different orbits is accompanied by the emission (or absorption) of a photon. Determine the energy of a photon emitted during a transition between the first excited state and the ground state of a hydrogen atom.

c. Consider an electron trapped in an infinite one-dimensional box potential of width

- a. Determine an expression for the electronic energy levels.  
 d. What should be the width  $a$  of this potential, in terms of the Bohr radius, so to ensure that a photon emitted during a transition between the first excited state and the ground state equals that obtained in item (b)?

### 1.1.6.7 Ex: The hydrogen atom

The hydrogen atom can be seen as a point-like proton and an electron distributed over space with charge density  $\rho = Ae^{-2r/a_B}$  around the proton that is in the center. Here,  $A$  is a constant and  $r$  is the distance from the center.

- a. Calculate  $A$  considering the fact that the atom is electrically neutral.  
 b. Calculate the amplitude of the electric field at a radius  $r = a_B$ .

## 1.2 The discovery of the photon

The concept of the nature of light has a variable history. Newton proposed around  $\sim 1650$  a corpuscular model to explain Snellius' law on the refraction of a light beam penetrating a crystal. Around the same time Huygens found a wave-based interpretation. The two models predicted different speeds of light within the dense medium. Newton found, that the speed of light is greater in the medium than outside, while Huygens found the opposite <sup>5</sup>. In the late 1800's the wave nature of light was established through observations of interference effects confirming Huygens' hypothesis. At that time, the world appeared to be simple: Light was a wave and matter was composed of particles. However, some observations made were incompatible with this simplistic ideas, for example, the spectrum of blackbody radiation, the Compton effect, the specific heat of the solid, the radiation pressure, and the photoelectric effect. All these observations are readily understood by assuming a corpuscular nature of the light <sup>6</sup>.

Nowadays, knowing the theory of quantum mechanics, we know that both ideas have their range of validity and that the electromagnetic radiation is dual: In general, propagation and interference effects are best described by waves. However, when interacting with matter, light tends to localize into small particles called photons.

### 1.2.1 Radiation in a conductive cavity

In the age of lasers a classical treatment of the emission and absorption of light may seem an atavism. However, even with coherent and monochromatic radiation sources, the most commonly used physical picture is that of a classical optical field interacting with an atom or a molecule whose energetic structure is treated quantum mechanically. And even the atomic or molecular dipole is often treated like a classical oscillator. The exposition of such a dipole to simple boundary conditions prepares the analogous development of a quantum oscillator and provides a direct path to quantization of the radiation field.

<sup>5</sup>Note, until today there remain doubts about the correct value of the momentum of light in dielectric media [488].

<sup>6</sup>The corpuscular hypothesis is now called the second quantization of quantum theory or quantization of the electromagnetic field.

Even if we rarely do experiments by throwing light into a small hole in a metallic box, the electromagnetic fields obtained by solving Maxwell's equation are particularly simple for boundary conditions, where the fields disappear on the inner surfaces of the box. Before discussing the physics of radiation in a perfectly conducting cavity, we have to introduce some basic relations between electromagnetic amplitudes, stored energy, and intensity.

The electric field of a plane wave oscillating with frequency  $\omega$  and propagating through vacuum in the direction of propagation defined by the *wave vector*,

$$\mathbf{k} = \frac{2\pi}{\lambda} \hat{\mathbf{k}}, \quad (1.33)$$

can be written,

$$\mathbf{E} = \mathbf{E}_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)}, \quad (1.34)$$

where  $\mathbf{E}_0 = E_0 \hat{\mathbf{e}}$  consists of an amplitude  $E_0$  and a polarization  $\hat{\mathbf{e}}$ . Since the field  $\mathbf{E}_0$  is transverse to the direction of propagation, the polarization has two components perpendicular to  $\mathbf{k}$ . The magnetic induction field associated with the wave is,

$$B_0 = \frac{1}{c} E_0. \quad (1.35)$$

For a propagating wave  $\mathbf{E}$  and  $\mathbf{B}$  are in phase, while for a standing wave they are out of phase.

For a given cavity mode we can express the standing wave in this mode as,

$$\mathbf{E} = \mathbf{E}_0(\mathbf{r}) e^{-i\omega t}. \quad (1.36)$$

The energy of the electromagnetic field of a standing wave, averaged over one oscillation of the frequency  $\omega$  is,

$$\bar{U} = \frac{1}{2} \int \left( \frac{\varepsilon_0}{2} |\mathbf{E}|^2 + \frac{1}{2\mu_0} |\mathbf{B}|^2 \right) dV. \quad (1.37)$$

Now, the *energy density* of the oscillating electromagnetic field is given by,

$$\bar{u} = \frac{d\bar{U}}{dV} = \frac{1}{4} \left( \varepsilon_0 |\mathbf{E}|^2 + \frac{1}{\mu_0} |\mathbf{B}|^2 \right). \quad (1.38)$$

From the equation (1.35) we can see that the contributions of the electric and magnetic fields are equal. Therefore,

$$\bar{U} = \frac{1}{2} \int \varepsilon_0 |\mathbf{E}|^2 dV \quad \text{and} \quad \bar{u} = \frac{1}{2} \varepsilon_0 |\mathbf{E}|^2. \quad (1.39)$$

Another important quantity is the *flux of electromagnetic energy* through a surface. The *Poynting vector* describing this flux is defined by,

$$\mathbf{I} = \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B}. \quad (1.40)$$

Again using the equation (1.35), we find the value averaged over a time period,

$$\bar{I} = \frac{1}{2} \varepsilon_0 c |\mathbf{E}|^2. \quad (1.41)$$



This quantity, called *intensity*, describes the fact that the flux is a density of energy multiplied with the velocity of propagation in vacuum,

$$\bar{u}c = \frac{1}{2}\varepsilon_0c|\mathbf{E}|^2 = \bar{I} . \quad (1.42)$$

The intensity can also be written,

$$\bar{I} = \frac{1}{2}\sqrt{\frac{\varepsilon_0}{\mu_0}}|\mathbf{E}|^2 . \quad (1.43)$$

where the factor  $\sqrt{\mu_0/\varepsilon_0}$  is called *impedance of free space*, because it has the unit of a resistance and the last equation has the same form as the power dissipated in a resistor,

$$W = \frac{1}{2}\frac{V^2}{R} . \quad (1.44)$$

### 1.2.2 Black body radiation

We now want to calculate the energy density inside the cavity before using the result to describe the interaction between light and a sample of two-level atoms located inside the cavity. The basic idea is to say that the electrons inside the conducting surface of the cavity oscillate because of thermal motion. The oscillation generates a dipolar radiation leading to stationary waves developing within the cavity. As the walls of the cavity are conducting, the electric field  $\mathbf{E}$  must disappear inside the wall and on its surfaces. The task is now twofold: first count the number of possible standing waves, which satisfy the boundary conditions as a function of frequency; second, determine the energy for each wave and then calculate the spectral distribution of the energy within the cavity.

The equations describing the radiated energy in free space are,

$$\nabla^2\mathbf{E} = \frac{1}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2} \quad \text{and} \quad \nabla \cdot \mathbf{E} = 0 . \quad (1.45)$$

The stationary waves solutions separate into terms oscillating in time and in space.

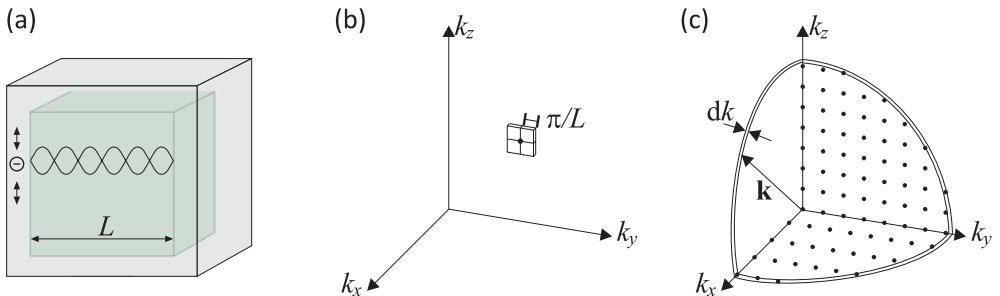


Figure 1.8: (a) Cavity in position space showing the thermal motion of the electrons inside the walls. (b and c) Density-of-states in a cavity in momentum space.

Now, respecting the boundary conditions for a three-dimensional box of length  $L$ , we

have for the components of  $\mathbf{E}$  <sup>7</sup>,

$$\begin{aligned} \mathbf{E}(\mathbf{r}, t) = e^{-i\omega t} [ & \hat{\mathbf{e}}_x \cos(k_x x) \sin(k_y y) \sin(k_z z) \\ & + \hat{\mathbf{e}}_y \sin(k_x x) \cos(k_y y) \sin(k_z z) \\ & + \hat{\mathbf{e}}_z \sin(k_x x) \sin(k_y y) \cos(k_z z) ] , \end{aligned} \quad (1.46)$$

with the components,

$$k_x = \frac{\pi n_x}{L} \quad \text{for} \quad n_x = 0, 1, 2, \dots \quad (1.47)$$

and similar for  $k_y$  and  $k_z$ . Note, that for each component  $E_{x,y,z}$  the transverse amplitudes disappear in 0 and  $L$ . By inserting this solution into Helmholtz's equation (1.45), we obtain,

$$k_x^2 + k_y^2 + k_z^2 = \frac{\omega^2}{c^2} . \quad (1.48)$$

The states  $k_{x,y,z}$  (enumerated by  $n_{x,y,z}$ ) form a three-dimensional orthogonal lattice of points in space  $\mathbf{k}$  separated by a distance along the axes  $k_x, k_y, k_z$  of  $\frac{\pi}{L}$ , as shown in Fig. 1.8. In principle, the number of states that can be placed within a sphere of radius  $k$  in the momentum space is,

$$N = \int_{\text{sphere}} dn_x dn_y dn_z . \quad (1.49)$$

However, the periodic boundary conditions for  $|\mathbf{k}|$  limit the components  $k_x, k_y, k_z$  to positive values ( $n \geq 0$ ), that is, the volume under consideration is limited to an octant. On the other hand, we must multiply the number of states by two because of the degeneracy of polarizations,

$$4N = \int_0^n 4\pi n^2 dn = \left(\frac{L}{\pi}\right)^3 \int_0^k 4\pi k^2 dk = \frac{4L^3}{\pi^2} \frac{k^3}{3} = \frac{4L^3 \omega^3}{3\pi^2 c^3} . \quad (1.50)$$

With this, we obtain the *mode density*,

$$\frac{N}{L^3} = \frac{\omega^3}{3\pi^2 c^3} . \quad (1.51)$$

The *spectral density of modes*  $\varrho$  can be given in several units,

$$\int \varrho(n) dn = \int \varrho(k) dk = \int \varrho(\omega) d\omega = \frac{N}{L^3} , \quad (1.52)$$

such that,

$$\boxed{\varrho(n) = \frac{\pi n^2}{L^3} \quad \text{or} \quad \varrho(k) = \frac{k^2}{\pi^2} \quad \text{or} \quad \varrho(\omega) = \frac{\omega^2}{\pi^2 c^3}} . \quad (1.53)$$

The density of oscillating modes within the cavity grows like the square of the frequency. Now, the mean energy per mode in a sample of oscillators in thermal equilibrium is, following the equipartition law, equal to,

$$\bar{E} = k_B T , \quad (1.54)$$

<sup>7</sup>See script on *Electrodynamics* (2020).

where  $k_B$  is the Boltzmann constant. We conclude that the *spectral energy density*  $u_{RJ}(\omega)$  in the cavity is,

$$\boxed{u_{RJ}(\omega)d\omega = k_B T \rho(\omega)d\omega = k_B T \frac{\omega^2}{\pi^2 c^3} d\omega} . \quad (1.55)$$

This law is known as the *Rayleigh-Jeans law of black-body radiation*. As seen in Fig. 1.9, this law suggests the physically impossible fact, called *ultraviolet catastrophe*, that the energy storage in the cavity grows without limits like the square of frequency.

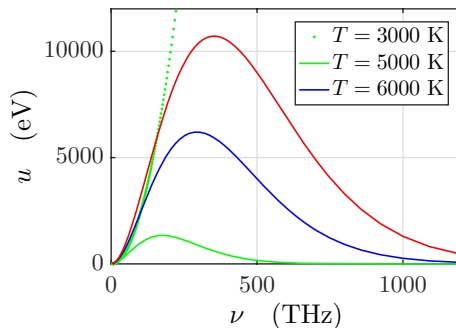


Figure 1.9: (code) Spectral energy density following Rayleigh-Jeans' and Planck's laws.

### 1.2.3 Planck's distribution of modes

We obtained the result (1.54) by multiplying the number of modes with the mean energy per mode. As there is no doubt about our method of counting the modes, the problem with the ultraviolet catastrophe can only root in the use of the equipartition principle for assigning energy to the oscillators.

Planck's idea to solve this problem was to first consider the probability distribution for exciting the modes (thermal states) for a sample of oscillators in thermal equilibrium at temperature  $T$ . This probability distribution  $p$  comes from mechanical statistics and can be written in terms of the *Boltzmann factor*,  $e^{-E_n/k_B T}$ , and the partition function  $q = \sum_{n=0}^{\infty} e^{-E_n/k_B T}$  as,

$$p_n = \frac{e^{-E_n/k_B T}}{q} . \quad (1.56)$$

Now Planck hypothesized that the energy be quantized, that is, it must be assigned in discrete portions, proportional to the frequency, such that,

$$\boxed{E_n = n\hbar\omega} , \quad (1.57)$$

where  $n = 0, 1, 2, \dots$  and the proportionality constant  $\hbar$  is called *Planck's constant*. With the abbreviation  $Z \equiv e^{-\hbar\omega/k_B T}$  and using the rule  $\sum_{n=0}^{\infty} Z^n = (1 - Z)^{-1}$ , we

find the average number,

$$\bar{n} = \sum_n n p_n = (1 - Z) \sum_n n Z^n = (1 - Z) Z \frac{\partial}{\partial Z} \sum_n Z^n = \frac{Z}{1 - Z} = \frac{1}{e^{\hbar\omega/k_B T} - 1} . \quad (1.58)$$

The probability of occupancy of state  $n$  is,

$$p_n = (1 - Z) Z^n = \frac{\bar{n}^n}{(1 + \bar{n})^{1+n}} , \quad (1.59)$$

and the average energy is,

$$\bar{E} = \sum_n E_n p_n = \sum_n n \hbar\omega e^{-n\hbar\omega/k_B T} = \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} , \quad (1.60)$$

in contrast to the initial assumption (1.55).

Finally, we obtain Planck's expression for the energy density inside the cavity by substituting  $\bar{\epsilon}$  for the factor  $k_B T$  in Rayleigh-Jeans' law (1.54),

$$u(\omega) d\omega = \bar{E} \varrho(\omega) d\omega = \frac{\omega^2}{\pi^2 c^3} \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} d\omega . \quad (1.61)$$

This result, drawn in Fig. 1.9, is much more satisfactory, because now the energy density has an upper bound, and coincides with the results of experiments. Note, that for high temperatures or low excitation energies,  $\hbar\omega \ll k_B T$ , Planck's distribution converges to that of Rayleigh-Jeans',  $u(\omega) \rightarrow u_{RJ}(\omega)$ .

Note that the form of the expression for the energy depends on the parametrization and must be derived respecting  $u(\omega) d\omega = u(\lambda) d\lambda$ , etc.. Often the blackbody radiation is expressed in terms of the *spectral radiance*,

$$L(\omega) \equiv \frac{c}{4\pi} u(\omega) , \quad (1.62)$$

which can be understood as the (isotropic) energy flux into all directions of space.

Solve the Excs. 1.2.10.1 to 1.2.10.7.

## 1.2.4 The corpuscular nature of the photon

### 1.2.4.1 The photoelectric effect

Light incident on a metallic surface can expel electrons. For this to occur, the light must have a *minimum frequency*. If the frequency is below this value, there is no point in increasing the light intensity: the electrons won't be expelled. The main experimental observations are: 1. Electrons are ejected without apparent delay, i.e. it is not necessary (and it doesn't help) to accumulate a certain amount of energy. 2. Higher light intensities increase the number of electrons, but not their kinetic energy after expulsion. 3. Red light does not eject electrons, even at high intensities. 4. Weak ultraviolet light only ejects few electrons, but with high kinetic energy.

These observations challenge the classical electromagnetic model according to which the Lorentz acceleration of the electrons should be proportional to the field

*amplitude*. The observations were explained by Einstein's theory of the *photoelectric effect*, which assumes the light to be quantized (unlike Planck, who preferred to quantize the process of light absorption),

$$E = h\nu . \quad (1.63)$$

Assuming a fixed exit work  $A$  for the extraction of an electron, we can measure the constant  $h$ :

$$h\nu = A + \frac{mv^2}{2} = A + eV \quad \rightarrow \quad h = \frac{eV}{\nu - \nu_g} . \quad (1.64)$$

The energy of the fastest electrons is measured through the decelerating voltage by varying  $\nu$  and  $I$ . We will discuss the photoelectric effect quantitatively later in the Exc. 6.4.5.7.

#### 1.2.4.2 Bremsstrahlung and the Franck-Hertz experiment

*Bremsstrahlung* is, in a way, the inverse process of the photoelectric effect. Here, electrons are accelerated toward a cathode. Finding a target they are rapidly decelerated, a process in which they emit a continuous spectrum of X-rays (in addition to characteristic lines attributed to electronic transitions in the target atoms). For any given kinetic energy the spectra have a red threshold corresponding to photons that receive the entire energy of the electron.

In the *Franck-Hertz experiment* free electrons produced in a plasma are accelerated by a strong electric field. Having traveled a sufficiently long distance they have acquired enough kinetic energy to excite electronic transitions in the atoms of the plasma. When an excitation occurs, the electron suddenly loses all its energy and must be accelerated again, starting from rest, before it can excite another atom.

#### 1.2.4.3 Radiative pressure and Compton scattering

When light is scattered from a particle, it transfers momentum to it called *photonic recoil*. This effect, known as *radiation pressure*, occurs for example in *Compton scattering*.

X-rays scattered by the electrons of a carbon target are red-shifted by an amount, which increases with the scattering angle. This is the *Compton effect*. The data are understood assuming a corpuscular nature of light and applying the laws of conservation of energy and momentum to the collision processes between photons and electrons. The scattered photon sees its energy reduced and therefore its wavelength increased.

In a material where there are free electrons, this effect will occur at all photon energies. In other materials, it is only observed with high energy photons. For high energy photons, exceeding the atomic binding energy, the electrons can be considered free such that, in the scattering process, the photon is able to eject the electron from its atom. The photon receives the remaining energy and is deviated, such that the overall momentum of the system is conserved. The loss of energy for the photon results in a spectral shift to the red during its passage through the material.

Photons of visible light, on the other hand, do not have enough energy to eject bound electrons. In this case, the mass in the Compton formula must be replaced by

the atomic mass, such that the spectral displacement becomes much smaller. This limit, which involves bound electrons, is that of Thomson and Rayleigh scattering.

The relevance of this effect lies in the fact that it shows that light exhibits properties commonly attributed to corpuscles, since Thomson's scattering model, based on the classical theory of charged particles accelerated by electromagnetic fields, can not explain any spectral shift.

### 1.2.5 Einstein's transitions rates

Bohr's atom model explained for the first, time how light interacts with matter: Atoms have discrete excitation levels. They absorb and emit energy packets  $\hbar\omega$ . Unfortunately, Bohr's model can not predict transition rates. Here, Einstein helped out by developing a useful theory (see Fig. 1.10).



Figure 1.10: Bohr model and Einstein rate diagram.

We consider a two-level atom or a sample of atoms within a conducting cavity. We have  $N_1$  atoms in the lower energy state  $E_1$  and  $N_2$  in the upper state  $E_2$ . Light interacts with these atoms through stimulated resonant absorption and emission. The rates,  $B_{12}u(\omega)$  and  $B_{21}u(\omega)$  are proportional to the energy spectral density  $u(\omega)$  of the cavity modes. The central idea of Einstein is to postulate that atoms in the higher state can emit light spontaneously at a rate  $A_{21}$ , which depends only on the density of modes of the cavity, i.e. the volume of the cavity, but not the energy of the field of radiation. With the Einstein coefficients we can formulate valid rate equations in situations, where the spectral distribution of the radiation is wider than the spectral width of the atomic transition and where the spectral distribution of the light flux from the source,  $\bar{I}(\omega)$ , is weak compared to the saturation intensity of the atomic transition. Even if modern light sources generally have very narrow and intense spectral emission bands, Einstein's coefficients are often used in the spectroscopic literature to characterize the light-matter interaction with atoms and molecules.

The Einstein rate equations describe the energy flux between atoms and the optical modes of the cavity,

$$\begin{aligned} \frac{dN_1}{dt} = -\frac{dN_2}{dt} &= -R_{1\rightarrow 2} + R_{2\rightarrow 1} + S_{2\rightarrow 1} \\ &= -N_1 B_{12} u(\omega) + N_2 B_{21} u(\omega) + N_2 A_{21} . \end{aligned} \quad (1.65)$$

$R_{1\rightarrow 2}$  is the *absorption rate*,  $R_{2\rightarrow 1}$  the *stimulated emission rate* and  $S_{2\rightarrow 1}$  the *spontaneous emission rate*. The assumption of a third type of transition, called spontaneous emission, is necessary, if  $B_{12} = B_{21}$  but  $N_1 > N_2$  in thermal equilibrium. In thermal equilibrium we have the condition of stationarity,  $\frac{dN_1}{dt} = -\frac{dN_2}{dt} = 0$  for a given energy

density value  $u(\omega) = u_{th}(\omega)$ , such that,

$$u_{th}(\omega) = \frac{A_{21}}{\left(\frac{N_1}{N_2}\right) B_{12} - B_{21}} . \quad (1.66)$$

The *Boltzmann distribution law* controlling the distribution of the number of atoms in the lower and upper states is given by,

$$\frac{N_1}{N_2} = \frac{g_1}{g_2} e^{-(E_1 - E_2)/k_B T} , \quad (1.67)$$

where  $g_{1,2}$  are the degeneracies of the lower and upper states and  $E_2 - E_1 = \hbar\omega_0$ . We find,

$$u_{th}(\omega) = \frac{A_{21}}{\frac{g_1}{g_2} e^{\hbar\omega_0/k_B T} B_{12} - B_{21}} . \quad (1.68)$$

But this result must be consistent with the Planck's distribution (1.61). Therefore, by comparing this equation with the equation (1.68), it must be,

$$\frac{g_1 B_{12}}{g_2 B_{21}} = 1 . \quad (1.69)$$

and also,

$$\frac{A_{21}}{B_{21}} = \frac{\hbar\omega_0^3}{\pi^2 c^3} . \quad (1.70)$$

This equation shows that, once we know one of the three transition rates, we can always calculate the others.

It is useful to compare the rate  $A_{21}$  with  $B_{21}$  from the equation (1.68) inserting the equation (1.69),

$$\frac{A_{21}}{B_{21} u_{th}(\omega)} = e^{\hbar\omega_0/k_B T} - 1 . \quad (1.71)$$

This expression shows that, when  $\hbar(\omega_2 - \omega_1) \gg k_B T$ , that is, for optical, UV, or X-ray frequencies, spontaneous emission dominates. But in low-frequency regimes, that is, IR, microwave, or radio waves, stimulated emission is more important. Note that even when stimulated emission dominates, spontaneous emission is always present and plays an important role, for example, in processes ultimately limiting the emission bandwidth of lasers.

## 1.2.6 Absorption spectrum for a single atom

Every light source has a certain spectral width. Conventional light sources, such as incandescent bulbs or plasmas have relatively broad emission bands compared to atomic or molecular absorbers, at least when the latter ones are studied in dilute gases. Even when we use pure spectral sources, such as a laser tuned to the peak of a resonance, the transition line always exhibits an intrinsic width associated with the interruption of the phase evolution of the excited state. Phase interruptions such as spontaneous or stimulated emission and collisions are common examples of line broadening mechanisms. The emission or absorption of radiation occurs within a

frequency distribution centered about  $\omega_0 \equiv \omega_2 - \omega_1$ , and we must account for this spectral distribution in our calculation of the energy transfer.

The total power  $P$  absorbed by a two-level atom with resonance frequency  $\omega_0$  from a radiation field with the spectral intensity distribution  $I(\omega)$  with the total intensity of the laser beam  $\bar{I} = \int I(\omega)d\omega$  can be expressed as the integral,

$$P = \int \sigma(\omega)I(\omega)d\omega, \quad (1.72)$$

with the frequency-dependent optical cross section <sup>8</sup>,

$$\sigma(\omega) = \frac{g_2}{g_1} \lambda^2 \frac{\Gamma}{2\pi} \frac{\frac{1}{4}\Gamma}{(\omega - \omega_0)^2 + \frac{1}{4}\Gamma^2} = \frac{g_2}{g_1} \lambda^2 \frac{\Gamma}{4} \mathcal{L}_\Gamma(\omega - \omega_0). \quad (1.73)$$

where we defined the Lorentzian profile as,

$$\mathcal{L}_\beta(\Delta) \equiv \frac{\beta}{2\pi} \frac{1}{\Delta^2 + (\beta/2)^2} \quad \text{with} \quad \int_{-\infty}^{\infty} \mathcal{L}_\beta(\Delta)d\Delta = 1. \quad (1.74)$$

**Example 2 (Limiting cases):** Let us analyze the two limiting cases when either one of the spectral distributions  $I(\omega)$  or  $\sigma(\omega)$  is much narrower than the other.

For a *narrow laser*, we may assume a  $\delta$ -peaked spectral intensity distribution,

$$I(\omega) = \bar{I}\delta(\omega - \omega_L). \quad (1.75)$$

When it drives a *broad transition* described by an optical cross section given by (1.73), the scattered power is,

$$P = \bar{I}\sigma(\omega_L). \quad (1.76)$$

For a *narrow transition*, we may substitute the Lorentzian in (1.73) by a Dirac  $\delta$ -function,

$$\sigma(\omega) \xrightarrow{\Gamma \rightarrow 0} \frac{g_2}{g_1} \lambda^2 \frac{\Gamma}{4} \delta(\Delta). \quad (1.77)$$

When it is driven by a *broad laser*, for which we assume a spectral intensity distribution,

$$I(\omega) = \bar{I}\mathcal{L}_\beta(\omega - \omega_L) \quad \text{with} \quad \bar{I} = \int I(\omega)d\omega = \frac{I(\omega_L)}{\mathcal{L}_\beta(0)} = \frac{\pi\beta}{2}I(\omega_L) \quad (1.78)$$

we obtain for the scattered power,

$$P = \int \frac{g_2}{g_1} \lambda^2 \frac{\Gamma}{4} \delta(\omega - \omega_0) \bar{I} \mathcal{L}_\beta(\omega - \omega_L) d\omega = \frac{g_2}{g_1} \lambda^2 \frac{\Gamma}{4} \bar{I} \mathcal{L}_\beta(\omega_0 - \omega_L). \quad (1.79)$$

---

<sup>8</sup>At low saturation.



### 1.2.6.1 Broad laser driving a broad transition

Until now we assumed a fixed laser frequency  $\omega_L$  (with finite emission bandwidth) driving a fixed resonance frequency  $\omega_0$ . What we call *absorption spectrum* is what we obtain when we tune either the laser frequency or when we (somehow) vary the resonance frequency, such that  $\Delta \equiv \omega_L - \omega_0$  is ramped. Assuming Lorentzian profiles with finite linewidths for both,  $\bar{I}$  and  $\sigma$ , we get,

$$\begin{aligned} P(\Delta) &= P(\omega_L - \omega_0) = \int \sigma(\omega) I(\omega) d\omega = \int \frac{g_2 \lambda^2 \Gamma}{g_1 4} \mathcal{L}_\Gamma(\omega - \omega_L) \bar{I} \mathcal{L}_\beta(\omega - \omega_0) d\omega \\ &= \frac{g_2 \lambda^2 \Gamma}{g_1 4} \bar{I} \int \mathcal{L}_\Gamma(\omega' + \omega_0 - \omega_L) \mathcal{L}_\beta(\omega') d\omega' . \end{aligned} \quad (1.80)$$

That is, the absorption spectrum is obtained as a convolution of both profiles,

$$P(\Delta) = \frac{g_2 \lambda^2 \Gamma \bar{I}}{g_1 4} (\mathcal{L}_\Gamma \star \mathcal{L}_\beta)(\Delta) . \quad (1.81)$$

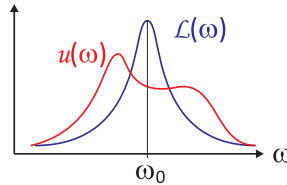


Figure 1.11: Absorption spectrum (blue) and spectral energy distribution of the source (red).

This result reproduces the two limiting cases discussed in the above example, since for narrow transitions,  $\Gamma \rightarrow 0$ , that is  $\mathcal{L}_\Gamma \rightarrow \delta$ , we recover the results (1.79), and for narrow lasers,  $\beta \rightarrow 0$ , that is,  $\mathcal{L}_\beta \rightarrow \delta$ , we recover (1.76). Obviously, this formula holds for other line profiles e.g. when the resonance is broadened by some perturbations<sup>9</sup>.

### 1.2.6.2 Two-level atom in a blackbody radiation field

When considering a two-level atom interacting with a blackbody a radiation field, we describe the spectral intensity distribution by (1.61),

$$\begin{aligned} I(\omega) &= \frac{\omega^2}{\pi^2 c^2} \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1} \\ \text{with } \bar{I} &= \int I(\omega) d\omega = \frac{\hbar}{\pi^2 c^2} \left( \frac{k_B T}{\hbar} \right)^4 \int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{\pi^2}{15 c^2 \hbar^3} (k_B T)^4 . \end{aligned} \quad (1.82)$$

<sup>9</sup>Let us here remind the following identities holding for Lorentzian and Gaussian line profiles:

$$(\mathcal{L}_\gamma \star \mathcal{L}_\beta)(\Delta) = \mathcal{L}_{\gamma+\beta}(\Delta) \quad \text{and} \quad (\mathcal{G}_\Gamma \star \mathcal{G}_\beta)(\Delta) = \mathcal{G}_{\sqrt{\gamma^2+\beta^2}}(\Delta) .$$

Since the width of the transition is negligibly small in comparison with the blackbody spectrum,  $\Gamma \rightarrow 0$ , we may evaluate the scattered power as,

$$P = \int \frac{g_2}{g_1} \frac{\lambda^2 \Gamma}{4} \mathcal{L}_\Gamma(\omega - \omega_0) \frac{\omega^2}{\pi^2 c^2} \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1} d\omega \quad (1.83)$$

$$\xrightarrow{\Gamma \rightarrow 0} \frac{g_2}{g_1} \frac{\lambda^2 \Gamma}{4} \frac{\omega_0^2}{\pi^2 c^2} \frac{\hbar \omega_0}{e^{\hbar \omega_0 / k_B T} - 1} .$$

### 1.2.7 Absorption in a gas

Let us now generalize the results to a gas of two-level atoms. As long as the transition linewidth is narrow [case (1.77)], the power is removed from the system only by spontaneous emission; absorption only converts radiation into atomic excitation which, subsequently, can be returned to the radiation field by stimulated emission. At steady-state the Einstein rate equation (1.65) reads,

$$0 = -N_1 B_{12} u(\omega_0) + N_2 B_{21} u(\omega_0) + N_2 A_{21} . \quad (1.84)$$

Using the result (1.69), we can write the amount of power removed from the system by spontaneous emission as,

$$P = N_2 A_{21} \hbar \omega_0 = u(\omega_0) B_{12} (N_1 - \frac{g_1}{g_2} N_2) \hbar \omega_0 . \quad (1.85)$$

On the other hand, the power absorbed from the radiation field  $u(\omega_0)$ , by atoms whose transition is described by the cross section (1.73), is given by,

$$P = \int (N_1 - \frac{g_1}{g_2} N_2) \sigma(\omega) I(\omega) d\omega . \quad (1.86)$$

Remembering  $I(\omega) = cu(\omega)$  and assuming a large radiation spectrum,  $I(\omega) \simeq I(\omega_0)$ , a comparison of equations (1.85) and (1.86) yields,

$$\boxed{B_{12} = \frac{c}{\hbar \omega_0} \int \sigma(\omega) d\omega} . \quad (1.87)$$

#### 1.2.7.1 Lambert-Beer law

The absorption probability distribution is convoluted with the spectral energy distribution of the light source,  $u(\omega) = d\bar{u}/d\omega$ , which in turn is related to the energy *density* via,  $\bar{U} = V\bar{u}$ , where  $V$  is the mode volume of the light field. Assuming that light propagates toward  $z$  and converting the time dependence into a spatial dependence, we have on one hand,

$$P = -\frac{dU}{dt} = -\frac{d\bar{u}}{dt} \Delta V = -c \frac{d\bar{u}}{dz} \Delta V = -\frac{d\bar{I}}{dz} \Delta V . \quad (1.88)$$

On the other hand, assuming a narrow laser,  $I(\omega) = \bar{I} \delta(\omega - \omega_L)$ , we get,

$$P = \int (N_1 - \frac{g_1}{g_2} N_2) \sigma(\omega) I(\omega) d\omega = \bar{I} (N_1 - \frac{g_1}{g_2} N_2) \sigma(\omega_L) , \quad (1.89)$$

Now comparing both results,

$$\frac{d\bar{I}}{\bar{I}} = -\frac{N_1 - \frac{g_1}{g_2}N_2}{\Delta V}\sigma(\omega_L)dz \simeq -n\sigma(\omega_L)dz, \quad (1.90)$$

The solution of this differential equation is,

$$\boxed{\bar{I} = \bar{I}_0 e^{-\sigma(\omega_L)nz}}. \quad (1.91)$$

Here,  $z$  is the total distance, over which absorption takes place. The last equation is the *Lambert-Beer law* for light absorption. It is very useful for measuring atomic densities in gas cells or of atomic beams [466, 440, 715]. Solve the Excs. 1.2.10.9 to 1.2.10.11.

### 1.2.8 Saturation

Strong driving of a transition leads to its saturation and causes line broadening. To see this we go back to Einstein's rate equations in steady-state (1.65) additionally simplifying by assuming  $g_1 = 1 = g_2$ , such that  $B_{12} = B_{21}$ . Resolving these equations by  $N_1$  and  $N_2$  and using  $N_1 + N_2 = N$  and  $N_1 - N_2 \equiv \Delta N$ , we get,

$$N_1 = N \frac{B_{21}u(\omega) + A_{21}}{2B_{21}u(\omega) + A_{21}} \quad \text{and} \quad N_2 = N \frac{B_{12}u(\omega)}{2B_{21}u(\omega) + A_{21}}. \quad (1.92)$$

For vanishing pump rate we expect,  $N_1 \xrightarrow{u \rightarrow 0} N$  and  $N_2 \xrightarrow{u \rightarrow 0} 0$ . In contrast, when the pump rate becomes much larger than the relaxation rates,  $N_1, N_2 \xrightarrow{u \rightarrow \infty} \frac{1}{2}$ . This means that the absorption coefficient  $\alpha = \sigma(N_1 - N_2)$  goes to zero, and the medium becomes completely transparent,

$$\Delta N = N \frac{A_{21}}{2B_{21}u(\omega) + A_{21}} = \frac{N}{1 + s(\omega)}. \quad (1.93)$$

The *saturation parameter*

$$s(\omega) \equiv \frac{2B_{12}u(\omega)}{A_{21}} \quad (1.94)$$

represents the ratio of pumping rate to the relaxation rate. The pump rate due to a monochromatic wave with intensity  $\bar{I}$  is obtained by comparing (1.85) with (1.89),

$$B_{12}u(\omega) = \frac{\sigma(\omega)\bar{I}}{\hbar\omega}. \quad (1.95)$$

We obtain for the saturation parameter,

$$s(\omega) = \frac{2\sigma(\omega)\bar{I}}{\hbar\omega A_{21}}. \quad (1.96)$$

According to (1.85) and (1.93) the power absorbed per unit volume on the transition by atoms with the populations  $N_{1,2}$  in a radiation field with a broad spectral profile and spectral energy density  $u(\omega)$  is,

$$P = \hbar\omega B_{12}u(\omega)\Delta N = \hbar\omega B_{12}u(\omega) \frac{N}{1 + s(\omega)}. \quad (1.97)$$

With (1.94) this can be written as,

$$P = \hbar\omega \frac{A_{21}}{2} \frac{N}{1 + s(\omega)^{-1}} . \quad (1.98)$$

Let us now remember that the absorption cross section (1.73) of a homogeneously broadened line is Lorentzian. This means that the saturation parameter itself becomes Lorentzian. We can assume that the relaxation rate  $A_{21}$  is independent of  $\omega$  within the frequency range of the line profile,

$$s(\omega) = s(\omega_0) \frac{(\Gamma/2)^2}{\Delta^2 + (\Gamma/2)^2} . \quad (1.99)$$

Substituting this into (1.98) yields the frequency dependence of the absorbed radiation power per unit frequency interval  $d\omega$ ,

$$P = \hbar\omega \frac{A_{21}N}{2} \frac{s(\omega_0)(\Gamma/2)^2}{(\omega - \omega_0)^2 + (\Gamma/2)^2 [1 + s(\omega_0)]} = N\bar{I}\sigma(\omega_0) \frac{(\Gamma/2)^2}{\Delta^2 + (\gamma_s/2)^2} , \quad (1.100)$$

where we introduced the increased halfwidth of the Lorentzian profile,

$$\gamma_s \equiv \Gamma \sqrt{1 + s(\omega_0)} . \quad (1.101)$$

Apparently, the halfwidth of the saturation-broadened line increases with the resonant saturation parameter  $s(\omega_0)$ . If according to (1.94) the induced transition rate at resonance equals the total relaxation rate  $A_{21}/2$ , the resonant saturation parameter becomes  $s(\omega_0) = 1$ , which increases the linewidth by a factor  $\sqrt{2}$ , compared to the unsaturated linewidth  $\Gamma$  for weak radiation fields. Starting from (1.100) we can define a *saturated* absorption cross section,

$$\sigma_s(\omega) = \sigma_s(\omega_0) \frac{(\gamma_s/2)^2}{\Delta^2 + (\gamma_s/2)^2} = \sigma(\omega_0) \frac{(\Gamma/2)^2}{\Delta^2 + (\gamma_s/2)^2} = \sigma(\omega) \frac{1}{1 + s(\omega)} , \quad (1.102)$$

where the unsaturated absorption profile is,

$$\sigma(\omega) = \sigma(\omega_0) \frac{(\gamma/2)^2}{\Delta^2 + (\gamma/2)^2} . \quad (1.103)$$

This shows that the saturation decreases the absorption coefficient by the factor  $1 + s(\omega)$ . At the line center, this factor has its maximum value  $1 + s(\omega_0)$ , while it decreases to 1 for increasing  $|\Delta|$ , see (1.101), see Fig. 1.12. This is the reason why the line broadens.

From (1.96) we see, that unity saturation,  $s(\omega_0) = 1$ , corresponds to a light intensity of,

$$\bar{I}_{sat} \equiv \frac{\hbar\omega}{2\sigma(\omega_0)} \Gamma = \frac{2\pi^2 c \hbar}{3\lambda^2} \Gamma . \quad (1.104)$$

This intensity is called *saturation intensity*. Taking account of the degeneracies  $g_j$  of the levels the saturation intensity becomes <sup>10</sup>,

$$I_{sat} = \frac{g_1}{g_2} \frac{2\pi^2 c \hbar}{3\lambda_0^3} \Gamma . \quad (1.105)$$

<sup>10</sup>Some authors define the saturation for  $s = 2$ , as happens when  $\Omega = \Gamma$ .

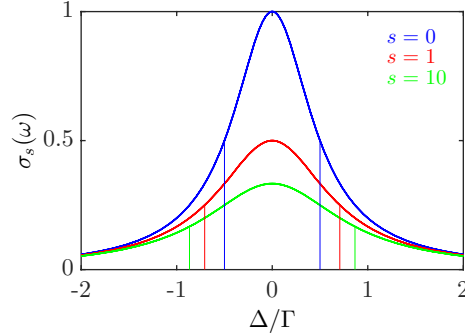


Figure 1.12: (code) Optical cross section at various saturation parameters.

Finally, we note that the resonant saturation parameter is basically a measure for the ratio between the stimulated population transfer rate, given by the Rabi frequency  $\Omega$  and the spontaneous decay rate  $\Gamma$ ,

$$s(\omega_0) = \frac{2\Omega^2}{\Gamma^2} . \quad (1.106)$$

We thus obtain the important relationship between laser intensity and Rabi frequency,

$$\Omega^2 = \sigma(\omega_0) \frac{\bar{I}}{\hbar\omega_0} \Gamma . \quad (1.107)$$

### 1.2.9 Specific heat of solids

The *Debye model* applies Planck's law on the distribution of energy in electromagnetic radiation, which treats radiation as a gas of *photons*, to the energy distribution of atomic vibrations in a solid, treating them as a gas of *phonons* in a box (the box being the solid). Most of the steps of the calculation are identical, as both are examples of a massless bosonic gas with linear dispersion relation.

According to the equipartition theorem, every atom has 3 degrees of freedom due to its translational motion. Thus, in a crystal lattice with  $N$  atoms, we expect the total energy  $E = 3Nk_B T$  and the *specific heat* should be, following the *Dulong-Petit law*,

$$C_V = \left( \frac{\partial E}{\partial T} \right)_V = 3Nk_B , \quad (1.108)$$

for all solids regardless of temperature.

It was observed, however, that the specific heat of solids decreases like  $C_V \propto T^3$  as  $T$  approaches zero. It was Einstein's idea to apply Planck's formula by treating the  $N$  atoms as three-dimensional harmonic oscillators vibrating in a lattice. The discrete energies  $n\hbar\omega$  are identified with quasi-particles called *phonons*. The quantum nature of atoms does not matter, they just provide the medium supporting the phonons. Following the Bose-Einstein statistics, we must replace,

$$k_B T \rightarrow \hbar\omega / (e^{\hbar\omega/k_B T} - 1) , \quad (1.109)$$

such that the derivative of the energy,

$$C_V = \left( \frac{\partial}{\partial T} \frac{3Nk_B \hbar \omega}{e^{\hbar \omega / k_B T} - 1} \right)_V = 3Nk_B \left( \frac{\hbar \omega}{k_B T} \right)^2 \frac{e^{\hbar \omega / k_B T}}{(e^{\hbar \omega / k_B T} - 1)^2}, \quad (1.110)$$

gives the specific heat. The disappearance of the specific heat at low temperatures,

$$C_V \simeq \frac{3N(\hbar \omega)^2}{k_B T^2} e^{-\hbar \omega / (k_B T)}, \quad (1.111)$$

which is related to the finite localization energy of harmonic oscillators, does not describe experimental observations very well, and the model had to be refined by Debye, later on.

### 1.2.9.1 Debye model for the specific heat

While Einstein assumed monochromatic lattice vibrations, Debye's approach was to allow a *spectrum* of vibrational frequencies. With the density of states,

$$\rho(\nu) d\nu = (4\pi V v^3) \nu^2 d\nu, \quad (1.112)$$

where  $v$  is the velocity of sound propagation, the formula is totally equivalent to the density-of-states for photons in a cavity. Assuming that there is an upper bound  $\nu_m$  for the vibrational frequencies, we normalize as  $3N_0 = \int_0^{\nu_m} \rho(\nu) d\nu$ . The energy now is <sup>11</sup>,

$$E = \int_0^{\nu_m} \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1} \frac{4\pi V}{v^3} \nu d\nu = 9Nk_B \frac{T^4}{\theta^3} \int_0^{\theta/T} \frac{x^3 dx}{e^x - 1}. \quad (1.113)$$

The *Debye temperature*  $\theta = h\nu_m/k_B$  is characteristic for the metal. The derivative is then,

$$C_V = 9Nk_B \left[ 4 \left( \frac{T}{\theta} \right)^3 \int_0^{\theta/T} \frac{x^3 dx}{e^x - 1} - \frac{\theta}{T} \frac{1}{e^{\theta/T} - 1} \right]. \quad (1.114)$$

At low temperatures this formula reproduces the *Debye law*,

$$C_V = \frac{12\pi^4}{5} Nk_B (T/\theta)^3. \quad (1.115)$$

## 1.2.10 Exercises

### 1.2.10.1 Ex: Resistance of vacuum

Show that  $\sqrt{\mu_0/\epsilon_0}$  has the dimension of a resistance and the value of 376.7  $\Omega$ .

### 1.2.10.2 Ex: The laws of Planck and Rayleigh-Jeans

Show that Planck's law reproduces the Rayleigh-Jeans law in the low-frequency limit.

<sup>11</sup>The fact that the electron gas also has a heat capacity is neglected.

**1.2.10.3 Ex: The laws of Wien and Stefan-Boltzmann**

- Derive the parametrization of Planck's law in terms of frequency  $\nu$  and wavelength  $\lambda$ .
- Derive the law of *Stefan-Boltzmann* according to which the total power radiated per unit surface area of a black body across all wavelengths (also known as the blackbody radiant emittance) is given by  $\sigma T^4$ , where  $\sigma \equiv \pi^2 k_B^4 / 60c^2 \hbar^3$  is called the Stefan-Boltzmann constant.
- Derive *Wien's displacement law* according to which the maximum emission of a blackbody spectrum occurs at  $\lambda_{\max} T = 2.898 \times 10^{-3}$  Km in the wavelength parametrization and  $\nu_{\max} / T = 0.0588$  THz/K in the frequency parametrization. Determine the frequency of the maximum emission for the 2.7 K background radiation of the universe.

**1.2.10.4 Ex: Radiometric thermometry**

Modern radiometric thermometers measure the blackbody radiation emitted by a hot body. Calculate the variation of the blackbody radiant emittance of a person having fever ( $40^\circ$  instead of  $37^\circ$  body temperature). How much does the maximum emission wavelength change? In which spectral range should the thermometer be sensitive?

**1.2.10.5 Ex: Photons in a resonator**

- The light power emitted by a laser ( $\lambda = 633$  nm) be  $P = 1$  nW. How many photons does the laser emit per second? How many laser photons are in a mode volume of  $L = 10$  cm length?
- How many photons on average are inside an optical cavity having the same mode volume at ambient temperature, when there is no incident light?

**1.2.10.6 Ex: Number of modes in a cavity**

- How many modes do fit into a cubical box of 10 cm size for a frequency interval of 1000 Hz centered at a wavelength of 500 nm?
- How many photons are in the box supposing it has a temperature of  $T = 300$  K, respectively,  $T = 6000$  K?

**1.2.10.7 Ex: Number of photons emitted from lasers and blackbodies**

- Calculate the total number of photons per area per unit time emitted by a blackbody at temperature  $T$ .
- The linewidth of a helium-neon laser is  $\Delta\nu = 1000$  Hz. The operating wavelength is  $\lambda = 632.8$  nm, the power is  $P = 1$  mW, and the beam size  $w_0 = 1$  mm. How many photons are emitted per second?
- What would be the temperature of a blackbody radiator emitting the same number of photons from an equal area and over the same frequency interval as the laser?

**1.2.10.8 Ex: Number of photons per radiation mode**

Assume the isotropic emission of a pulsed flashlamp with spectral bandwidth  $\Delta\lambda = 100$  nm around  $\lambda = 400$  nm amounts to  $P_0 = 100$  W peak power out of a volume of  $1 \text{ cm}^3$ . Calculate the spectral power density  $u(\nu)$  and the spectral intensity  $I(\nu)$  through a spherical surface  $r = 2$  cm away from the center of the emitting sphere. How many photons per mode are contained in the radiation field?

**1.2.10.9 Ex: Atoms in an optical cavity**

- Consider a closed optical cavity at  $T = 600^\circ\text{C}$ . The cavity has the shape of a  $L = 1$  m-long and  $d = 3$  cm-diameter tube. Calculate the total energy of the black-body radiation inside the cavity.
- Inside the cavity there is a gas with strontium atoms (1 fundamental level and 3 degenerate excited levels,  $\lambda = 461$  nm). Using the expression (1.61), assuming thermal equilibrium, calculate the number of excited atoms for a partial pressure of the strontium gas of  $10^{-3}$  mbar.
- Calculate the optical density for a laser in resonance with the transition traversing the cavity along the symmetry axis.

**1.2.10.10 Ex: Sodium atoms in an optical cavity**

A sodium atom is placed in a cavity of volume  $V = 1 \text{ cm}^3$  with walls at the temperature  $T$ , producing a thermal radiation field with spectral energy density  $\bar{u}(\nu)$ . At what temperature  $T$  are the spontaneous and induced transition probabilities equal

- for the transition  $3P \rightarrow 3S$  with the transition wavelength  $\lambda = 589$  nm and the excited state lifetime  $\tau_{3P} = 16$  ns;
- for the hyperfine transition  $3S$  ( $F = 3 \rightarrow F = 2$ ) with the transition frequency  $\nu = 1772$  MHz and the excited state lifetime  $\tau_{3F} \simeq 1$  s?

**1.2.10.11 Ex: Applying the Lambert-Beer law**

The beam of a monochromatic laser passes through an absorbing atomic vapor with path length  $L = 5$  cm. If the laser frequency is tuned to the center of an absorbing transition  $|i\rangle \rightarrow |k\rangle$  with absorption cross section  $\sigma_0 = 10^{-14} \text{ cm}^2$ , the attenuation of the transmitted intensity is 10%. Calculate the atomic density  $n_i$  in the absorbing level  $|i\rangle$ .

**1.3 Further reading**

et al., [\[DOI\]](#)





# Chapter 2

## Foundations and mathematical tools

In this chapter, we will introduce step by step the formalism of quantum mechanics by gradually increasing the degree of abstraction. Applications of the formalism will be shown in consecutive chapters.

### 2.1 Basic notions

The aim of this section is to give 'feeling' for the new concepts introduced and used by quantum mechanics. We will first motivate the fundamental quantum equations of motion by linking them to classical dispersion relations and then spend some time to discuss the probabilistic concept proposed by Max Born.

#### 2.1.1 Dispersion relation and Schrödinger equation

A fundamental problem in physics is the issue of the propagation of physical entities. On one hand, we have the light, whose propagation in the vacuum is described by the dispersion relation  $\omega = ck$  or,

$$\omega^2 - c^2k^2 = 0 . \quad (2.1)$$

Since light is a wave, in the most general form, assuming the validity of the superposition principle, it can be described by a wave packet,  $A(\mathbf{r}, t) = \int e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} a(\mathbf{k}) d^3k$ . It is easy to verify that the *wave equation*,

$$\frac{\partial^2}{\partial t^2} A - c^2 \nabla^2 A = 0 , \quad (2.2)$$

reproduces the dispersion relation.

On the other hand, we have slow massive particles possessing kinetic energy,

$$E = \frac{p^2}{2m} . \quad (2.3)$$

With the hypothesis of de Broglie that even a massive particle has wave quality, we can try an *ansatz*<sup>1</sup> of a wave equation satisfying the dispersion relation (2.3). From

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<sup>1</sup>Trial, working hypothesis.

Planck's formula,  $E = \hbar\omega$ , and the formula of *Louis de Broglie*,  $\mathbf{p} = \hbar\mathbf{k}$ , describing the particle by a wave packet  $\psi(\mathbf{r}, t) = \int e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} \varphi(\mathbf{k}) d^3k$  not subject to external forces, it is easy to verify that the equation,

$$i\hbar \frac{\partial}{\partial t} \psi = \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \psi, \quad (2.4)$$

reproduces the dispersion relation. If the particle is subject to a potential, its total energy is  $E = \mathbf{p}^2/2m + V(\mathbf{r}, t)$ . This dispersion relation corresponds to the famous *Schrödinger equation*,

$$i\hbar \frac{\partial}{\partial t} \psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right) \psi. \quad (2.5)$$

### 2.1.2 Relativistic particle waves

Despite the similarities between light particles and material particles, there are notable differences: The photon is a relativistic particle with no rest mass. How can we establish a relationship between such different objects?

To clarify this relationship we now consider particles that are similar to light in the sense that they have high velocities, that is, relativistic particles. From the relativistic principle of the equivalence of mass and energy, we obtain for a massive particle  $E^2 = m^2c^4 + c^2p^2$  or,

$$\omega^2 - c^2k^2 = \frac{m^2c^4}{\hbar^2}. \quad (2.6)$$

This dispersion relation can be obtained from the differential equation,

$$\frac{\partial^2}{\partial t^2} A - c^2 \nabla^2 A = -\frac{m^2c^4}{\hbar^2} A, \quad (2.7)$$

inserting, for example, the already proposed wave packet  $A(\mathbf{r}, t) = \int e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} a(\mathbf{k}) d^3k$ , supposed not to be subject to external forces. The equation (2.7) is a wave equation called *Klein-Gordon equation*. For particles without rest mass, as in the case of photons, the equation is reduced to the wave equation of light (2.2).

Now, making the transition to non-relativistic velocities,  $v \ll c$ , we can expand the dispersion relation,

$$E = \sqrt{m^2c^4 + c^2m^2v^2} = mc^2 \left( 1 + \frac{v^2}{2c^2} + \dots \right) \quad \text{or} \quad \hbar\omega \simeq mc^2 + \frac{\hbar^2k^2}{2m}. \quad (2.8)$$

In analogy with the Klein-Gordon equation we can derive the approximate dispersion relation (2.8) from a wave equation,

$$i\hbar \frac{\partial}{\partial t} A = \left( mc^2 - \frac{\hbar^2}{2m} \nabla^2 \right) A. \quad (2.9)$$

With the transformation  $\psi = e^{-imc^2t/\hbar} A$ , we rediscover the Schrödinger equation (2.4),

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi \quad (2.10)$$

as the non-relativistic limit of the Klein-Gordon equation.

It is interesting to note that in all cases discussed, obviously the dispersion relations and the differential equations can be interconverted by the substitutions,

$$E \longrightarrow i\hbar \frac{\partial}{\partial t} \quad \text{and} \quad \mathbf{p} \longrightarrow -i\hbar \nabla . \quad (2.11)$$

We will discuss this later in the context of Ehrenfest's theorem in Secs. 2.1.6, 2.1.7, and 2.4.6.

### 2.1.3 Born's interpretation

The first part of this script is devoted to *individual particles* or systems of distinguishable *massive particles*, and we will only turn our attention to *light* and *indistinguishable particles* when discussing the (second) *quantization of fields*.

According to our current conviction, the complete reality (neglecting relativistic effects) on any system is contained in the Schrödinger equation (2.5). That statement does not make us smarter without having to explaining the meaning of the *wave-function*  $\psi$ . In an attempt to marry the concepts of particles and waves, *Max Born* proposed in 1926 the interpretation of the quantity

$$\int_V |\psi(\mathbf{r}, t)|^2 d^3r \quad (2.12)$$

as probability of finding the particle inside the volume  $V$ .

If  $|\psi(\mathbf{r}, t)|^2$  has the meaning of a *probability density* or *probability distribution*, the square of the wavefunction must be integrable,

$$\|\psi(\mathbf{r}, t)\|^2 \equiv \int_{\mathbb{R}^3} |\psi(\mathbf{r}, t)|^2 d^3r < \infty . \quad (2.13)$$

This allows us to proceed to a *normalization* of the wave function,

$$\tilde{\psi}(\mathbf{r}, t) \equiv \frac{\psi(\mathbf{r}, t)}{\sqrt{\int_{\mathbb{R}^3} |\psi(\mathbf{r}, t)|^2 d^3r}} , \quad (2.14)$$

such that  $\|\tilde{\psi}(\mathbf{r}, t)\| = 1$ .

### 2.1.4 Continuity equation

In quantum mechanics we associate the wavefunction that describes a quantum system to a *probability wave*. As the Schrödinger equation describes a time evolution, in order to be useful, the wavefunction must allow for probability flows. We define the probability density and the probability flow by,

$$\begin{aligned} \rho(\mathbf{r}, t) &\equiv \psi^*(\mathbf{r}, t)\psi(\mathbf{r}, t) , \\ \mathbf{j}(\mathbf{r}, t) &\equiv \frac{\hbar}{2mi} [\psi^*(\mathbf{r}, t)\nabla\psi(\mathbf{r}, t) - \psi(\mathbf{r}, t)\nabla\psi^*(\mathbf{r}, t)] . \end{aligned} \quad (2.15)$$

Starting from the Schrödinger equation we can easily derive the *continuity equation* (see Exc. 2.1.8.1),

$$\dot{\rho}(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0, \quad (2.16)$$

or in the integral form,

$$-\frac{d}{dt} \int_V \rho d^3r = \int_V \nabla \cdot \mathbf{j} d^3r = \oint_{\partial V} \mathbf{j} \cdot d\mathbf{S}, \quad (2.17)$$

using Gauß' law. With  $I \equiv \int_S \mathbf{j} \cdot d\mathbf{S}$ , the *probability current* which flows through the surface  $S$  delimiting the *probability charge*  $Q \equiv \int_V \rho(\mathbf{r}, t) d^3r$ , we obtain,

$$-\dot{Q} = I. \quad (2.18)$$

The continuity equation is obviously similar to that of electromagnetism.

### 2.1.5 Distributions in space and time

So far we only spoke of spatial distributions,  $\psi(\mathbf{r}, t)$ . But we could also consider velocity or moment distributions. In classical mechanics, a particle has a well-defined position and velocity. Knowing the position and velocity, Newton's equations allow predicting its coordinates at future times. Let us now investigate whether the Schrödinger equation allows this as well.

The more general solution of the Schrödinger equation can be written as a superposition of plane waves  $e^{i(\mathbf{r} \cdot \mathbf{k} - \omega t)}$  with frequencies  $\omega = \mathbf{p}^2/2m\hbar$  and wave vectors  $\mathbf{k} = \mathbf{p}/\hbar$ . Each plane wave has an individual amplitude  $\varphi(\mathbf{p})$ , such that,

$$\psi(\mathbf{r}, t) = \frac{1}{h^{3/2}} \int d^3p \varphi(\mathbf{p}) e^{i(\mathbf{r} \cdot \mathbf{k} - \omega t)} = \int d^3p \frac{1}{h^{3/2}} \varphi(\mathbf{p}) e^{i(\mathbf{r} \cdot \mathbf{p}/\hbar - \mathbf{p}^2 t/2m\hbar)}, \quad (2.19)$$

with  $h \equiv 2\pi\hbar$ . At time  $t = 0$ , this expansion is nothing more than a Fourier transform,

$$\psi(\mathbf{r}, 0) = \frac{1}{h^{3/2}} \int d^3p \varphi(\mathbf{p}) e^{i\mathbf{r} \cdot \mathbf{k}}, \quad (2.20)$$

that we can reverse,

$$\varphi(\mathbf{p}) = \frac{1}{h^{3/2}} \int d^3r \psi(\mathbf{r}, 0) e^{-i\mathbf{r} \cdot \mathbf{k}}. \quad (2.21)$$

In the absence of forces the momentum distribution becomes stationary. We can now use the momentum distribution  $\varphi(\mathbf{p})$  as coefficients of the expansion of the temporal wavefunction  $\psi(\mathbf{r}, t)$ , as shown above. Thus, the expansion represents a general solution of the time-dependent Schrödinger equation. The magnitude  $|\varphi(\mathbf{p})|^2$  is the probability density in *momentum space*.

**Example 3 (Normalization of the wave function in momentum space):** It is easy to show that the probability density in momentum space is also normalized:

$$\begin{aligned} \int |\varphi(\mathbf{p})|^2 d^3p &= \frac{1}{h^3} \int d^3p \int d^3r \psi^*(\mathbf{r}) e^{i\mathbf{r} \cdot \mathbf{k}} \int d^3r' \psi(\mathbf{r}') e^{-i\mathbf{r}' \cdot \mathbf{k}} \\ &= \int d^3r \int d^3r' \psi^*(\mathbf{r}) \psi(\mathbf{r}') \frac{1}{(2\pi)^3} \int d^3k e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \\ &= \int d^3r \int d^3r' \psi^*(\mathbf{r}) \psi(\mathbf{r}') \delta^3(\mathbf{r} - \mathbf{r}') = \int |\psi(\mathbf{r})|^2 d^3r = 1, \end{aligned}$$

knowing that the Fourier transform of a plane wave is nothing more than the Dirac distribution.

Since the probability distributions  $|\psi(\mathbf{r})|^2$  and  $|\varphi(\mathbf{p})|^2$  are interconnected by Fourier transform, we already know that we can not localize <sup>2</sup> both simultaneously. If one is well localized, the other is necessarily delocalized. Do the Exc. 2.1.8.2.

### 2.1.6 Eigenvalues

We have already seen that the position and momentum distributions of a particle are spread. We calculate the mean values of these distributions, denoted by  $\langle \mathbf{r} \rangle$  and  $\langle \mathbf{p} \rangle$ , as *first moments* of the respective distributions:

$$\langle \mathbf{r} \rangle = \int d^3r |\psi(\mathbf{r}, t)|^2 \mathbf{r} \quad \text{and} \quad \langle \mathbf{p} \rangle = \int d^3p |\varphi(\mathbf{p}, t)|^2 \mathbf{p} . \quad (2.22)$$

Using the expansions (2.19) and (2.20), we can calculate,

$$\begin{aligned} \langle \mathbf{p} \rangle &= \int \varphi^*(\mathbf{p}) \mathbf{p} \varphi(\mathbf{p}) d^3p = \int \frac{1}{h^{3/2}} \int \psi^*(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3r \mathbf{p} \varphi(\mathbf{p}) d^3p \\ &= \frac{1}{h^{3/2}} \int \psi^*(\mathbf{r}) \int \varphi(\mathbf{p}) \mathbf{p} e^{i\mathbf{k}\cdot\mathbf{r}} d^3p d^3r \\ &= \frac{1}{h^{3/2}} \int \psi^*(\mathbf{r}) \frac{\hbar}{i} \nabla \int \varphi(\mathbf{p}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3p d^3r = \int \psi^*(\mathbf{r}) \frac{\hbar}{i} \nabla \psi(\mathbf{r}) d^3r . \end{aligned}$$

This calculation shows that the expectation value, called *eigenvalue*, of the momentum can be expressed through an operator  $\hat{p} \equiv (\hbar/i) \nabla$  acting on the wavefunction <sup>3,4</sup>.

More generally, we can compute the eigenvalue of a function in  $\mathbf{r}$  and  $\mathbf{p}$  via,

$$\langle f(\mathbf{r}, \mathbf{p}) \rangle = \int d^3r \psi^*(\mathbf{r}) f(\mathbf{r}, \hat{\mathbf{p}}) \psi(\mathbf{r}) . \quad (2.23)$$

However, it is important to note that the operators  $\hat{\mathbf{r}}$  and  $\hat{\mathbf{p}}$  do not necessarily commute.

**Example 4 (Non-commutation of space and momentum):** Considering a one-dimensional motion, we verify,

$$\hat{p}_x x \psi = \frac{\hbar}{i} \frac{d}{dx} x \psi = \frac{\hbar}{i} \psi + x \frac{\hbar}{i} \frac{d}{dx} \psi \neq x \frac{\hbar}{i} \frac{d}{dx} \psi = x \hat{p}_x \psi .$$

<sup>2</sup>Localize: Restrict the distribution volume indefinitely.

<sup>3</sup>From now on, the hat over a physical magnitude will denote quantum operators.

<sup>4</sup>We note here that the rules  $\langle \psi | \hat{x} | \psi \rangle \leftrightarrow \langle \phi | -\frac{\hbar}{i} \nabla_p | \phi \rangle$  and  $\langle \psi | \frac{\hbar}{i} \nabla_r | \psi \rangle \leftrightarrow \langle \phi | \hat{p} | \phi \rangle$  from the Fourier transformation are useful for numerical simulations of the Schrödinger equation: Instead of calculating the spatial derivative  $\left(\frac{\hbar}{i} \nabla\right)^2$  of the wavefunction, one makes a Fast Fourier Transform (FFT) to momentum space, multiplies with  $\mathbf{p}$ , and transforms back.

### 2.1.7 Temporal evolution of eigenvalues

We now consider the temporal evolution of the position of a particle. We will use in the following the partial integration rule  $\int_V \psi \nabla \xi = \oint_{\partial V} \psi \xi - \int_V \nabla \psi \xi = - \int_V (\nabla \psi) \xi$ , assuming that at least one of the functions,  $\psi$  or  $\xi$ , disappears at the edge of the volume, which can be guaranteed by choosing the volume large enough. To begin with, we will concentrate on the  $x$ -component of the position, the time derivative of which is computed using the continuity equation (2.16),

$$\frac{d}{dt} \langle x \rangle = \int d^3r \frac{d}{dt} |\psi|^2 x = - \int d^3r x \nabla \cdot \mathbf{j} = - \int d^3r \mathbf{j} \cdot \nabla x = \int d^3r \mathbf{j} \cdot \nabla x, \quad (2.24)$$

Generalizing to three dimensions, we can write,

$$\begin{aligned} \frac{d}{dt} \langle m\mathbf{r} \rangle &= m \int d^3r \mathbf{j} = m \int d^3r \frac{\hbar}{2mi} [\psi^* \nabla \psi - \psi \nabla \psi^*] \\ &= \frac{1}{2} \int d^3r [\psi^* \hat{\mathbf{p}} \psi + \psi \hat{\mathbf{p}} \psi^*] = \int d^3r \psi^* \hat{\mathbf{p}} \psi = \langle \hat{\mathbf{p}} \rangle, \end{aligned} \quad (2.25)$$

since the eigenvalue of  $\hat{\mathbf{p}}$  is a real quantity.

Now, we define the abbreviation:

$$\hat{H} \equiv -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t), \quad (2.26)$$

called the *Hamilton operator* or *Hamiltonian* and we calculate the second derivative of the position using the Schrödinger equation (2.5),

$$\frac{d}{dt} \langle \hat{\mathbf{p}} \rangle = \int d^3r \left[ \left( \frac{1}{i\hbar} \hat{H} \psi \right)^* \hat{\mathbf{p}} \psi + \psi^* \hat{\mathbf{p}} \frac{1}{i\hbar} \hat{H} \psi \right] = \frac{i}{\hbar} \int d^3r \psi^* (\hat{H} \hat{\mathbf{p}} - \hat{\mathbf{p}} \hat{H}) \psi = \frac{i}{\hbar} \langle [\hat{H}, \hat{\mathbf{p}}] \rangle, \quad (2.27)$$

introducing the *commutator*  $[\hat{a}, \hat{b}] \equiv \hat{a}\hat{b} - \hat{b}\hat{a}$  as an abbreviation. After that,

$$\frac{i}{\hbar} \langle [\hat{H}, \hat{\mathbf{p}}] \rangle = \frac{i}{\hbar} \langle [\hat{V}, \hat{\mathbf{p}}] \rangle = \frac{i}{\hbar} \int d^3r \psi^* \left[ \hat{V} \frac{\hbar}{i} \nabla \psi - \frac{\hbar}{i} \nabla (V\psi) \right] = - \int d^3r \psi^* \psi \nabla V = \langle \hat{\mathbf{F}} \rangle. \quad (2.28)$$

In summary, we found a law,

$$\langle \hat{\mathbf{F}} \rangle = \frac{d^2}{dt^2} \langle m\hat{\mathbf{r}} \rangle, \quad (2.29)$$

much like the *Newton law*, but instead of applying to localized particles, the law applies to the eigenvalues of probability distributions. Similar laws can be derived for angular momentum and energy conservation.

The observation made by *Paul Ehrenfest*, that in quantum mechanics the mean values follow the same laws of classical mechanics, is called *Ehrenfest's theorem*.

## 2.1.8 Exercises

### 2.1.8.1 Ex: Conservation of probability

Demonstrate the conservation of local probability through the definitions of probability densities,  $\rho(\mathbf{r}, t)$ , and probability current  $\mathbf{j}(\mathbf{r}, t)$ .

### 2.1.8.2 Ex: Fourier theorem

The spatial distribution of a particle is given by a Gaussian function with the width  $\Delta x$ . Calculate the momentum distribution and its width  $\Delta p$ . Just consider one spatial dimension. Show that  $\Delta x \Delta p = \hbar$  using the *rms* definition for the widths.

## 2.2 Postulates of quantum mechanics

In this section we will introduce the fundamentals and main methods of quantum mechanics. We will learn what are observables and get to know the postulates which establish the foundation of quantum mechanics, as well as Heisenberg's famous principle of uncertainty.

### 2.2.1 Superposition principle (1. postulate)

A physical system can be found in several states. For example, a particle may be at rest or in motion, an atom may be excited or deexcited. In quantum mechanics, every possible state is described by a *wavefunction*  $\psi$ . Wavefunctions can be functions of various types of coordinates, for example, of position  $\psi = \psi(\mathbf{r})$ , of momentum  $\psi = \psi(\mathbf{p})$ , or of energy  $\psi = \psi(E)$ . The choice of the coordinates is called *representation*.

One peculiarity of quantum systems is that they may be in a *superposition of states*. That is, if  $\psi_1, \psi_2, \dots, \psi_k$  are possible states with amplitudes  $c_k$ , automatically the functions,

$$\psi = \sum_k c_k \psi_k \quad \text{or} \quad \psi = \int dk c(k) \phi(k) \quad (2.30)$$

are possible states as well. This is called *superposition principle*, and means, for example, that a particle may be *simultaneously* in several places or that an atom may be *at the same time* excited and deexcited.

There are systems that can only exist in a *restricted number* of states, such as the two-level atom. Others may exist in an *infinite number* of states or even in a *continuous distribution* of states.

### 2.2.2 Interpretation of the wave function (2. postulate)

A *state function* (or wavefunction) characterizes a system of which we may calculate various properties. The function can adopt complex values devoid of immediate physical interpretation. In fact, the wavefunction is above all a mathematical construct. On the other hand, the norm  $|\psi|^2$  has the meaning of a probability of the system to be in the state  $\psi$ . This is the famous interpretation of *Max Born* of the wave function (see Sec. 2.1.3).

If  $\psi_k$  with  $k = 1, 2, \dots$  are all possible states of a system, the interpretation as a probability requires,

$$\sum_k |\psi_k|^2 = 1 . \quad (2.31)$$

Analogically, for a continuous distribution, for example, in spatial representation,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 . \quad (2.32)$$



That is, the probability needs *normalization*.

### 2.2.3 Dirac bra-ket notation and vector representation

In order to distinguish more easily the amplitudes (which are complex numbers) and the wavefunctions we will now use the Bra-Ket notation introduced by *Paul Dirac*. The functions are represented by *kets*,

$$|\psi\rangle = \sum_k c_k |k\rangle . \quad (2.33)$$

The complex transpositions of these states are represented by *bras*,

$$\langle\psi| = |\psi\rangle^\dagger = \sum_k c_k^* \langle k| . \quad (2.34)$$

But the notation has other advantages. For example, let us suppose that we know the three possible states of a system,  $|1\rangle$ ,  $|2\rangle$ , and  $|3\rangle$ , which are linearly independent. Then we can define the states as vectors:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} , \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} , \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} . \quad (2.35)$$

These three states can be interpreted as the basis of a *vector space* representing the system. Now, each wavefunction can be expanded on this basis and expressed by a vector. An arbitrary ket state of this system will then be,

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} . \quad (2.36)$$

The corresponding bra state will be,

$$\langle\psi| = (c_1^* \quad c_2^* \quad c_3^*) . \quad (2.37)$$

Now we can easily calculate the probability for a system to be in a state  $|\psi\rangle$ ,

$$||\psi\rangle|^2 = \langle\psi|\psi\rangle = (c_1^* \quad c_2^* \quad c_3^*) \cdot \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = |c_1|^2 + |c_2|^2 + |c_3|^2 . \quad (2.38)$$

### 2.2.4 Observables (3. postulate)

The only way to get information about a system is to *measure* the values of characteristic quantities of the system, e.g. energy or linear momentum. In classical mechanics we have learned that a system can be completely characterized by a set of measurable physical quantities. For example, the motion of a rigid body of mass  $m$  and inertial moment  $\mathbf{I}$  is defined by its position  $\mathbf{r}$ , its moment  $\mathbf{p}$ , and its angular momentum  $\mathbf{L}$ . In quantum mechanics we describe observable physical quantities by *operators* acting on

the *Hilbert space* of wavefunctions,  $|\psi\rangle \mapsto \hat{\mathbf{p}}|\psi\rangle$ , where  $\hat{\mathbf{p}}$  would be the operator of the linear momentum. To better distinguish the observables, we decorate their symbols with a hat. We will see more ahead (see Sec. 2.3.5) that every quantum system is completely described by a complete set of observables.

To find the current values  $a_\psi$  of any *observable*  $\hat{A}$  in a specific situation given by a wave function  $\psi$ , we need to solve an equation of eigenvalues,

$$\hat{A}|\psi\rangle = a_\psi|\psi\rangle . \quad (2.39)$$

We can rewrite the equation as  $a_\psi = \langle\psi|\hat{A}|\psi\rangle$ . The values  $a_n$  are real numbers, if the observable is a *Hermitian operator*, that is,

$$\hat{A} = \hat{A}^\dagger \implies a_\psi = a_\psi^* . \quad (2.40)$$

We leave proof of this for the Exc. 2.2.9.1.

Thus, we postulate the substitution of the *dynamic variables* characterizing a classical system by abstract objects called operators. These operators can be understood as mathematical prescriptions, e.g., differential operators acting on a state of the system. The expectation value of any operator  $\hat{A}$  characterizing a system in a state  $|\psi\rangle$  is  $a_\psi \equiv \langle\hat{A}\rangle_\psi \equiv \langle\psi|\hat{A}|\psi\rangle/\langle\psi|\psi\rangle$ . Such operators are specific for a system, but independent of its state. The dynamical variables for a specific state are obtained as eigenvalues of the respective variable in that specific state. The temporal evolution of the operators or of the states is governed by equations of motion (see Sec. 2.4)<sup>5</sup>.

## 2.2.5 Representation of operators as matrices

In the same way as we already represented wavefunctions by vectors, we can also represent operators by matrices,

$$\hat{A} \equiv \sum_{i,j} |i\rangle a_{ij} \langle j| = \begin{pmatrix} & \vdots & \\ \dots & a_{ij} & \dots \\ & \vdots & \end{pmatrix} = \begin{pmatrix} & \vdots & \\ \dots & \langle j|\hat{A}|i\rangle & \dots \\ & \vdots & \end{pmatrix} . \quad (2.41)$$

To extract components from a matrix we do,  $\langle i|\hat{A}|j\rangle$ , for example,

$$\langle 1|\hat{A}|1\rangle = (1 \quad 0 \quad \dots) \cdot \hat{A} \cdot \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix} = a_{11} . \quad (2.42)$$

*Projectors* are particular operators defined by,

$$\hat{P}_k \equiv |k\rangle\langle k| = \begin{pmatrix} 0 & \vdots & 0 \\ \dots & 1 & \dots \\ 0 & \vdots & 0 \end{pmatrix} . \quad (2.43)$$

---

<sup>5</sup>Note that there are theoretical attempts to generalize the concept of observables to non-Hermitian operators [57, 58] only displaying  $\mathcal{PT}$ -symmetry.

The eigenvalue of a projector,  $\langle \hat{P}_k \rangle = \langle \psi | \hat{P}_k | \psi \rangle = |\langle k | \psi \rangle|^2$ , is nothing more than the probability of finding a system, whose general state is  $|\psi\rangle$ , in the particular state, since expanding as done in (2.33), we have,

$$\langle \hat{P}_k \rangle = \sum_{m,n} c_m^* c_n \langle m | k \rangle \langle k | n \rangle = |c_k|^2 . \quad (2.44)$$

Using the matrix formalism we can define other interesting operators and verify their properties,

$$\boxed{\begin{array}{l} |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad , \quad |2\rangle\langle 2| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad , \\ |1\rangle\langle 2| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \hat{\sigma}^- \quad , \quad |2\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \hat{\sigma}^+ \end{array}} . \quad (2.45)$$

The rising and lowering operators,

$$\hat{\sigma}^\pm = \frac{1}{2}(\hat{\sigma}_x \pm i\hat{\sigma}_y) , \quad (2.46)$$

are also called *Pauli spin matrices*, because they were introduced by *Wolfgang Pauli*. The vector,

$$\hat{\vec{\sigma}} \equiv \begin{pmatrix} \hat{\sigma}_x \\ \hat{\sigma}_y \\ \hat{\sigma}_z \end{pmatrix} = \begin{pmatrix} \hat{\sigma}^+ + \hat{\sigma}^- \\ i(\hat{\sigma}^+ - \hat{\sigma}^-) \\ [\hat{\sigma}^-, \hat{\sigma}^+] \end{pmatrix} \quad (2.47)$$

is called *Pauli vector* and the vector

$$\vec{\rho} \equiv \begin{pmatrix} \langle \hat{\sigma}_x \rangle \\ \langle \hat{\sigma}_y \rangle \\ \langle \hat{\sigma}_z \rangle \end{pmatrix} \quad (2.48)$$

is called *Bloch vector*<sup>6,7</sup>. The eigenvalue of the Bloch vector has a fixed length (see Exc. 2.2.9.2). An important property of the Pauli matrices is their behavior under commutation and anti-commutation,

$$\begin{aligned} [\hat{\sigma}_k, \hat{\sigma}_m]_- &\equiv \hat{\sigma}_k \hat{\sigma}_m - \hat{\sigma}_m \hat{\sigma}_k = i\epsilon_{kmn} \hat{\sigma}_n \\ [\hat{\sigma}_k, \hat{\sigma}_m]_+ &\equiv \hat{\sigma}_k \hat{\sigma}_m + \hat{\sigma}_m \hat{\sigma}_k = 2\delta_{km} . \end{aligned} \quad (2.49)$$

The representation of physical quantities by matrices allows the description of quantum superposition states. The purpose of Exc. 2.2.9.3 is to illustrate this at the example of a particle passing through a double slit.

<sup>6</sup>The Bloch vector is widely used in describing the interaction of a two-level system with a light field.

<sup>7</sup>Schrödinger invented the *wave mechanics* when he derived his wave equation from the dispersion relation for massive particles. Heisenberg invented a mechanics (detailed in later sections), which he called *mechanics of matrices*. Later, he showed the formal equivalence of both theories.

### 2.2.6 Correspondence principle (4. postulate)

Operators do not necessarily commute. We have already seen in Sec. 2.1.6, that in one dimension the position and the momentum operators do not commute. We can generalize to three dimensions via,

$$[\hat{p}_j, \hat{x}_k] = -i\hbar\delta_{jk} \quad \text{and} \quad [\hat{p}_j, \hat{p}_k] = 0 = [\hat{x}_j, \hat{x}_k], \quad (2.50)$$

which is easily verified by replacing the operators with  $\hat{x}_k = x_k$  and  $\hat{p}_k = \frac{\hbar}{i}\nabla$  and allowing the commutators to act on a wavefunction  $\psi(x)$ .

Conversely, quantum mechanics follows from classical mechanics with the prescription <sup>8</sup>,  $A(q_k, p_k, t) \rightarrow A(\hat{q}_k, \hat{p}_k, t) = \hat{A}$ . Letting the smallest amount of energy possible go to zero,  $\hbar \rightarrow 0$ , the commutator disappears, the energy spectrum becomes continuous, and we recover classical mechanics.

### 2.2.7 Schrödinger equation and quantum measurements (5. postulate)

The time evolution is given by the Schrödinger equation,

$$\boxed{i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle}. \quad (2.51)$$

A closed system, disconnected from the rest of the world (we will now call the rest of the world *reservoir*) is not subject to dissipation, i.e., it does not lose energy to the reservoir. Such a system is always described by a hermitian Hamiltonian. Unfortunately, this system also does not allow information leakage, that is, we can not measure the system. This is reflected in the fact that the Schrödinger equation does not allow to describe the process of a *quantum measurement*. This is because before the measurement, the system can be in several states or even in a superposition of states, while after the measurement we know exactly the state. This amounts to a reduction of entropy, which is not allowed in a closed system.

The famous *postulate of state reduction* or *projection of the wavefunction* formulated by *John von Neumann* describes the quantum measurement process as a sequence of two distinct steps <sup>9</sup>. In a first step, the measuring apparatus projects the measured operator  $\hat{A}$  on an eigenvector basis. That is, if the measurement is compatible with the operator <sup>10</sup>, we obtain a distribution of probability amplitudes of the results,

$$\hat{A} \rightsquigarrow \langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \langle \psi | \hat{A} | \sum_k c_k |k\rangle = \sum_k a_k c_k \langle \psi |k\rangle = \sum_k a_k |c_k|^2, \quad (2.52)$$

with  $\langle \psi | \psi \rangle = \sum_k |a_k|^2 = 1$ . Therefore, we can understand  $|\langle k | \psi \rangle|^2$  as the probability of the system to be in the eigenstate  $|k\rangle$ . In other words, this first step of the measurement process removes in an irreversible manner all coherences from the observable,  $\hat{A} \rightsquigarrow \sum_k |k\rangle \langle k | \hat{A} |k\rangle \langle k|$ .

<sup>8</sup>Considering the Weyl order.

<sup>9</sup>For simplicity, we only consider pure state, here.

<sup>10</sup>To understand the meaning of *compatible*, we must establish a more complete theory of measurement including the reservoir in the quantum description.

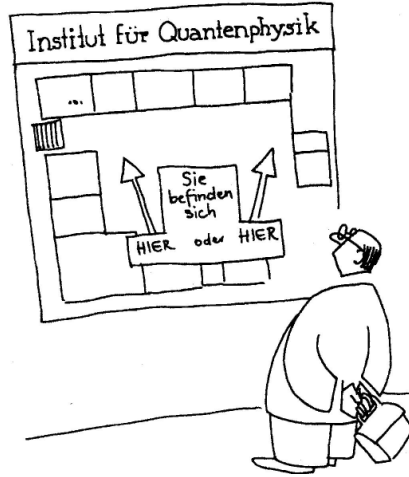


Figure 2.1: Superposition.

In a second step, the observing scientist will *read* the measuring device and note the result, which will necessarily be one of the possible  $a_k$ ,

$$\langle \hat{A} \rangle \rightsquigarrow a_k . \quad (2.53)$$

If the state is stationary, it will never change any more. That is, each subsequent measurement will yield the same result. The Exc. 2.2.9.4 illustrates the process of quantum measurement at the example of a measurement of the excitation energy of a two-level atom.

## 2.2.8 Stationary Schrödinger equation

The general form of the Schrödinger equation in one dimension is,

$$\hat{H}\Psi(t, x) = i\hbar \frac{\partial}{\partial t} \Psi(t, x) , \quad (2.54)$$

with  $\hat{H} \equiv \frac{\hat{p}^2}{2m} + V(x, t)$  and  $\hat{p} \equiv -i\hbar \frac{\partial}{\partial x}$ . If the potential is independent of time,  $V(x, t) = V(x)$ , we can do the following ansatz,  $\Psi(x, t) \equiv \psi(x)f(t)$ . Insertion into the Schrödinger equation yields,

$$\frac{1}{\psi(x)} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi(x) = \frac{i\hbar}{f(t)} \frac{d}{dt} f(t) = \text{const.} \equiv E . \quad (2.55)$$

The solution of the right-hand side of the equation is  $i\hbar(\ln f - \ln f_0) = E(t - t_0)$ . Hence,

$$f(t) = f(0)e^{-iE(t-t_0)/\hbar} . \quad (2.56)$$

Obviously,  $|\Psi(x, t)|^2 = |\psi(x)|^2$ .

Now, we can see that the stationary Schrödinger equation,

$$\hat{H}\psi(x) = E\psi(x) , \quad (2.57)$$

is nothing more than an eigenvalue equation. This means that the Schrödinger wave mechanics is equivalent to the mechanics of the Heisenberg matrices. The Excs. 2.2.9.5 and 2.2.9.6 are first simple calculations of the eigenvalues and eigenvectors of a two-level system.

## 2.2.9 Exercises

### 2.2.9.1 Ex: Reality of eigenvalues

Show that the eigenvalues of an observable are real.

### 2.2.9.2 Ex: Normalization of the Bloch vector

Calculate the expectation value of the length of the Pauli vector and the length of the Bloch vector (2.47).

### 2.2.9.3 Ex: Quantum superposition

Discuss how matrices can describe the creation of superposition states at the example of a particle passing through a double slit. Identify the slits with the states  $\langle 1| = (1 \ 0)$  and  $\langle 2| = (0 \ 1)$  and construct an observable for the position of the particle. How this observable must behave in the classical limit?

### 2.2.9.4 Ex: Quantum measurement

Explain the idea of quantum measurement at the example of a measurement of the excitation energy of a two-level atom.

### 2.2.9.5 Ex: Two-level atom

Consider a two-level atom. The Hamiltonian is given by,

$$\hat{H} = \begin{pmatrix} 0 & 0 \\ 0 & \hbar\omega_0 \end{pmatrix} .$$

Using the stationary Schrödinger equation, calculate the eigenvalues and eigenvectors.

### 2.2.9.6 Ex: The ammonium molecule

Consider the two states  $|1\rangle$  and  $|2\rangle$  of the ammonium molecule outlined in the figure. Suppose they are orthonormal,  $\langle i|j\rangle = \delta_{ij}$ , and that only these two states are accessible to the system, so that we can describe it using the basis formed by  $|1\rangle$  and  $|2\rangle$ . On this basis the Hamiltonian  $\hat{H}$  of the system is given by,

$$\hat{H} = \begin{pmatrix} E_0 & -E_1 \\ -E_1 & E_0 \end{pmatrix} .$$

- If the system is initially in state  $|1\rangle$ , will it remain in that state at a later time? How about if the initial state is  $|2\rangle$ ?
- Obtain the eigenvalues  $E_I$  and  $E_{II}$  and the respective eigenvectors  $|I\rangle$  and  $|II\rangle$  of

$\hat{H}$ , expressing them in terms of  $|1\rangle$  and  $|2\rangle$ .

c. What is the probability of measuring an energy  $E_I$  in the following state,

$$|\psi\rangle = \frac{1}{\sqrt{5}}|1\rangle - \frac{2}{\sqrt{5}}|2\rangle ?$$

d. Based on the above result, we can predict at least one possible electromagnetic radiation emission frequency for an ammonia sample. What is this frequency?

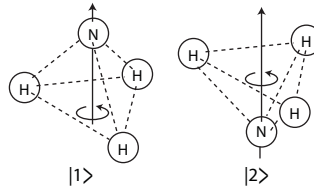


Figure 2.2: The two states of the ammonia molecule.

## 2.3 Abstract formalism of quantum mechanics

The formal development of quantum mechanics will be the subject of this section. We will learn how to find a complete set of observables characterizing a system, discuss the role of symmetries in quantum mechanics and show how to switch between several representations of the same system.

### 2.3.1 Lie algebra

The quantum mechanical operators form a *Lie algebra*  $\mathcal{L}^2$ . This means that  $\mathcal{L}^2$  is at the same time a complex and linear *vector space* with respect to addition and scalar multiplication and a *non-commutative ring* with scalar internal product. In particular,  $\mathcal{L}^2$  is unitary, normalized, and complete and acts on a *Hilbert space* of quantum states,

$$\begin{aligned} (\hat{A} + \hat{B})|\psi\rangle &= \hat{A}|\psi\rangle + \hat{B}|\psi\rangle, \\ (\alpha\hat{A})|\psi\rangle &= \alpha(\hat{A}|\psi\rangle), \\ (\hat{A}\hat{B})|\psi\rangle &= \hat{A}(\hat{B}|\psi\rangle). \end{aligned} \tag{2.58}$$

The properties of the Hilbert space are,

$$\begin{aligned} \hat{A}|\psi + \varphi\rangle &= \hat{A}|\psi\rangle + \hat{A}|\varphi\rangle, \\ \hat{A}|a\psi\rangle &= a\hat{A}|\psi\rangle. \end{aligned} \tag{2.59}$$

For a *Hermitian operator*,  $\hat{A} = \hat{A}^\dagger$ , we have  $\langle\psi|\hat{A}|\psi\rangle = \langle\hat{A}\psi|\psi\rangle$  or  $\langle\hat{A}\rangle \equiv \langle\psi|\hat{A}|\psi\rangle = \langle\hat{A}\rangle^*$ , using the Dirac bra-ket notation,

$$\langle\psi|\dagger \equiv |\psi\rangle. \tag{2.60}$$

There are identity and nullity operators,

$$\hat{1}|\psi\rangle = |\psi\rangle \quad \text{and} \quad \hat{0}|\psi\rangle = 0 . \quad (2.61)$$

We define the *(anti-)commutator* as,

$$[\hat{A}, \hat{B}]_{\mp} \equiv \hat{A}\hat{B} \pm \hat{B}\hat{A} , \quad (2.62)$$

which can be  $\neq 0$ . The sum of two Hermitian operators is Hermitian, but the product is not, since,

$$(\hat{A} + \hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger = \hat{A} + \hat{B} \quad \text{but} \quad (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A} \neq \hat{A}\hat{B} . \quad (2.63)$$

On the other hand, the following relations of Hermitian operators are always Hermitian,

$$\hat{A}\hat{B} + \hat{B}\hat{A} \quad \text{and} \quad i(\hat{A}\hat{B} - \hat{B}\hat{A}) . \quad (2.64)$$

We define the *scalar product* as,

$$\langle\psi|\varphi\rangle . \quad (2.65)$$

Two states are called *orthogonal*, if  $\langle\psi|\varphi\rangle = 0$ . The norm is written as,

$$|\psi|^2 = \langle\psi|\psi\rangle , \quad (2.66)$$

the deviation is,

$$\Delta A \equiv \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2} . \quad (2.67)$$

A *unitary operator* is defined by  $\hat{A}^{-1} = \hat{A}^\dagger$ .

### 2.3.2 Complete bases

If it is impossible to find a set of amplitudes  $c_n$ ,

$$\nexists\{c_n\} \quad \text{such that} \quad \sum_n c_n |n\rangle = 0 , \quad (2.68)$$

the functions are called *linearly independent*. A set of linearly independent functions may form a *basis*. The space opened by a set of linearly independent functions is called *Hilbert space*.

An operator  $\hat{A}$  is completely characterized by its *eigenvalues* and *eigenfunctions*. If a set of eigenfunctions  $|n\rangle$  is *complete*, every allowed state of the system can be expanded in these eigenfunctions,

$$|\psi\rangle = \sum_n c_n |n\rangle \quad \text{and} \quad \hat{A}|n\rangle = a_n |n\rangle . \quad (2.69)$$

To calculate properties of a specific system, we often want to find a matrix representation for the operator  $\hat{A}$ . For this, we solve the stationary Schrödinger equation,



that is, we calculate the eigenvalues and *eigenvectors*. When all eigenvalues are different,  $a_n \neq a_m$ , we know that the corresponding eigenvectors are orthogonal,  $\langle n|m \rangle = 0$ ,

$$\begin{aligned} \hat{A}|n\rangle &= a_n|n\rangle \quad , \quad \hat{A}|m\rangle = a_m|m\rangle \quad , \quad \forall\{n, m\} \ a_n \neq a_m \quad (2.70) \\ \implies \forall\{n, m\} \ \langle n|m \rangle &= \delta_{m,n} \ . \end{aligned}$$

Exc. 2.3.9.1 asks for demonstrating this.

Frequently, for example, in the case of a particle confined to a potential, there exist discrete eigenvalues (for  $E < 0$ ) simultaneously with continuous eigenvalues (for  $E > 0$ ). Assuming  $\langle m|m' \rangle = \delta_{m,m'}$ ,  $\langle m|\mathbf{k} \rangle = 0$  and  $\langle \mathbf{k}|\mathbf{k}' \rangle = \delta^{(3)}(\mathbf{k} - \mathbf{k}')$ , with a complete base,

$$\sum_m |m\rangle\langle m| + \int d^3k |\mathbf{k}\rangle\langle \mathbf{k}| = \hat{\mathbf{1}} \ , \quad (2.71)$$

an arbitrary vector can be expanded on an orthogonal basis,

$$|\psi\rangle = \sum_m |m\rangle\langle m|\psi\rangle + \int d^3k |\mathbf{k}\rangle\langle \mathbf{k}|\psi\rangle \ . \quad (2.72)$$

This also applies to observables,

$$\hat{A} = \sum_{m,n} |m\rangle\langle m|\hat{A}|n\rangle\langle n| + \int d^3k d^3l |\mathbf{k}\rangle\langle \mathbf{k}|\hat{A}|\mathbf{l}\rangle\langle \mathbf{l}| \ , \quad (2.73)$$

and functions of observables,

$$f(\hat{A}) = \sum_{m,n} |m\rangle f(\langle m|\hat{A}|n\rangle)\langle n| + \int d^3k d^3l |\mathbf{k}\rangle f(\langle \mathbf{k}|\hat{A}|\mathbf{l}\rangle)\langle \mathbf{l}| \ . \quad (2.74)$$

### 2.3.3 Degeneracy

The eigenvectors form a natural basis for the Hilbert space. However, a problem arises in the case of *degeneracy*, that is, when some eigenvalues are equal,  $a_n = a_m$ . In this case, the eigenvectors that correspond to degenerate eigenvalues are not completely defined, and we have to construct a basis verifying that all constructed eigenvectors are orthogonal. For this, there exists the method of *orthogonalization by Schmidt*, which works like this: We assume that we have already solved the eigenvalue equation, that we found a degenerate eigenvalue,  $\hat{A}|a_k\rangle = a|a_k\rangle$  for every  $k = 1, \dots, g_k$ , where  $g_k$  is the degree of degeneracy, and that we also found a complete basis of eigenvalues  $|a_m\rangle$ , but which is not orthogonal, that is,  $\exists\{m, n\}$  with  $\langle a_n|a_m \rangle \neq 0$ . The task is to build another basis  $|b_m\rangle$  satisfying  $\langle b_n|b_m \rangle = \delta_{n,m}$ .

The first vector of the orthogonal base can be chosen freely, e.g.,

$$|b_1\rangle \equiv |a_1\rangle \ . \quad (2.75)$$

Since the basis  $\{|a_k\rangle\}$  is assumed to be complete, the second vector is necessarily a linear combination of vectors  $|a_k\rangle$ , that is,  $|b_2\rangle = |a_2\rangle + \lambda|b_1\rangle$ . With the condition  $\langle b_1|b_2\rangle = 0 = \langle b_1|a_2\rangle + \lambda\langle b_1|b_1\rangle$  we can determine the parameter  $\lambda$ , and obtain for the second vector,

$$|b_2\rangle \equiv |a_2\rangle - |b_1\rangle \frac{\langle b_1|a_2\rangle}{\langle b_1|b_1\rangle} \ . \quad (2.76)$$

In the same way, we can derive for a third vector,  $|b_3\rangle = |a_3\rangle + \mu|b_1\rangle + \nu|b_2\rangle$ , the conditions,  $\langle b_1|b_3\rangle = 0 = \langle b_1|a_3\rangle + \mu\langle b_1|b_1\rangle$  and  $\langle b_2|b_3\rangle = 0 = \langle b_2|a_3\rangle + \nu\langle b_2|b_2\rangle$ , and obtain,

$$|b_3\rangle \equiv |a_3\rangle - |b_1\rangle \frac{\langle b_1|a_3\rangle}{\langle b_1|b_1\rangle} - |b_2\rangle \frac{\langle b_2|a_3\rangle}{\langle b_2|b_2\rangle} . \quad (2.77)$$

An overall way of writing this down is,

$$|b_k\rangle \equiv \left( 1 - \frac{|b_1\rangle\langle b_1|}{\langle b_1|b_1\rangle} - \frac{|b_2\rangle\langle b_2|}{\langle b_2|b_2\rangle} - \dots - \frac{|b_{k-1}\rangle\langle b_{k-1}|}{\langle b_{k-1}|b_{k-1}\rangle} \right) |a_k\rangle . \quad (2.78)$$

In the Exc. 2.3.9.2 we practice the orthogonalization of a set of three linearly independent but non-orthogonal vectors, and in the Exc. 2.3.9.3 we find an orthogonal basis for a partially degenerate three-level system.

### 2.3.4 Bases as unitary operators

One way to formulate the eigenvalue problem is as follows: Let  $|n\rangle$  be an orthonormal basis with the respective eigenvalues  $a_n$  of an operator  $\hat{A}$ :

$$\hat{A}|n\rangle = a_n|n\rangle \quad \text{with} \quad \langle n|m\rangle = \delta_{mn} . \quad (2.79)$$

We construct the matrices,

$$U \equiv (|1\rangle \quad |2\rangle \quad \dots) \quad \text{and} \quad \hat{E} \equiv \begin{pmatrix} a_1 & 0 & \dots \\ 0 & a_2 & \\ \vdots & & \ddots \end{pmatrix} . \quad (2.80)$$

With the definition of  $U^\dagger$  we have,

$$U^\dagger = \begin{pmatrix} \langle 1| \\ \langle 2| \\ \vdots \end{pmatrix} \quad \text{and} \quad U^\dagger U = \begin{pmatrix} \langle 1|1\rangle & \langle 1|2\rangle & \dots \\ \langle 2|1\rangle & \langle 2|2\rangle & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} = \hat{\mathbf{1}} . \quad (2.81)$$

Therefore,

$$\begin{aligned} U^\dagger U = \hat{\mathbf{1}} &\implies U^\dagger U U^{-1} = \hat{\mathbf{1}} U^{-1} \implies U^\dagger = U^{-1} \\ U^\dagger U = \hat{\mathbf{1}} &\implies U U^\dagger U U^{-1} = U \hat{\mathbf{1}} U^{-1} \implies U U^\dagger = \hat{\mathbf{1}} . \end{aligned} \quad (2.82)$$

Also,

$$\hat{A}|n\rangle = \hat{E}|n\rangle \quad \text{and} \quad \hat{A}U = U\hat{E} . \quad (2.83)$$

That is, by knowing the unitary matrix (or *transformation matrix*)  $U$ , we can solve the eigenvalue problem simply by  $\hat{E} = U^{-1}\hat{A}U$ .

Note, that this does not apply to a non-orthonormal basis. In this case, we need to do a Schmidt orthogonalization and use the condition  $\det U = 1$ . We apply the technique detailed in this section to solve Excs. 2.3.9.4, 2.3.9.5, and 2.3.9.6.

### 2.3.5 Complete set of commuting operators

Even for simple systems, we can ask various types of questions (measurements). Considering, for example, a particle flying freely in space, we can gather its position or its velocity. Let  $a$  be the result of a measurement of the observable  $\hat{A}$ , that is,  $a = \langle \psi_a | \hat{A} | \psi_a \rangle$ . Due to the measurement we know that the system is in the state  $|\psi_a\rangle$ . Immediately after this first measurement we perform another measurement of *another* observable  $\hat{B}$  giving  $\langle \psi_a | \hat{B} | \psi_a \rangle$ . The result of this measurement can only yield an eigenstate,  $b = \langle \psi_a | \hat{B} | \psi_a \rangle$ , if the operators commute,  $[\hat{A}, \hat{B}] = 0$ . That is, *if two operators  $\hat{A}$  and  $\hat{B}$  commute, and if  $|\psi\rangle$  is an eigenvector of  $\hat{A}$ , then  $\hat{B}|\psi\rangle$  is also an eigenvector of  $\hat{A}$  with the same eigenvalue:*

$$\begin{aligned} [\hat{A}, \hat{B}] = 0 \quad , \quad a = \langle \psi | \hat{A} | \psi \rangle \\ \implies \hat{A}(\hat{B}|\psi\rangle) = a(\hat{B}|\psi\rangle) \quad \text{and} \quad \langle \psi | \hat{B} | \psi \rangle \in \mathbb{R} . \end{aligned} \quad (2.84)$$

In addition, we observe that, if two operators commute, the orthonormal basis constructed for one of the operators is also orthonormal for the other. That is, *if two operators  $\hat{A}$  and  $\hat{B}$  commute and if  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are two eigenvectors of  $\hat{A}$  with different eigenvalues, then the matrix element  $\langle \psi_1 | \hat{B} | \psi_2 \rangle$  is equal to zero:*

$$\begin{aligned} [\hat{A}, \hat{B}] = 0 \quad , \quad a_1 = \langle \psi_1 | \hat{A} | \psi_1 \rangle \neq \langle \psi_2 | \hat{A} | \psi_2 \rangle = a_2 \\ \implies \langle \psi_1 | \hat{B} | \psi_2 \rangle = 0 . \end{aligned} \quad (2.85)$$

Finally, we affirm that, *if two operators  $\hat{A}$  and  $\hat{B}$  commute, we can construct an orthonormal basis  $\{|\psi_{a,b}\rangle\}$  with common eigenvectors of  $\hat{A}$  and  $\hat{B}$ :*

$$\begin{aligned} [\hat{A}, \hat{B}] = 0 \\ \implies \exists \{|\psi_{a,b}\rangle\} \quad \text{tal que} \quad \hat{A}|\psi_{a,b}\rangle = a|\psi_{a,b}\rangle \quad \text{and} \quad \hat{B}|\psi_{a,b}\rangle = b|\psi_{a,b}\rangle . \end{aligned} \quad (2.86)$$

The statements (2.84) to (2.86) are verified in Exc. 2.3.9.7.

The fact that commuting operators have a common system of eigenvectors authorizing sharp eigenvalues can be used to construct and characterize a state.

**Example 5 (Measuring momenta in orthogonal directions):** For example, the obvious solutions of the eigenvalue equations,

$$\hat{p}_x |\psi_{p_x}\rangle = \frac{\hbar}{i} \frac{d}{dx} |\psi_{p_x}\rangle = p_x |\psi_{p_x}\rangle \quad \text{and} \quad \hat{p}_y |\psi_{p_y}\rangle = \frac{\hbar}{i} \frac{d}{dy} |\psi_{p_y}\rangle = p_y |\psi_{p_y}\rangle$$

are the plane waves  $e^{ip_x x/\hbar}$  and  $e^{ip_y y/\hbar}$ . Therefore, the total state of the particle can be described by,

$$|\psi_{p_x, p_y, p_z}\rangle = |\psi_{p_x}\rangle |\psi_{p_y}\rangle = e^{(i/\hbar)(p_x x + p_y y)} f(z) .$$

However, these eigenfunctions are infinitely degenerate, since the linear momentum in  $z$ -direction is not specified. A third operator  $\hat{p}_z |\psi\rangle = p_z |\psi\rangle$  commutes with the others,

$$[\hat{p}_k, \hat{p}_m] = 0 .$$

Hence,

$$|\psi_{p_x, p_y, p_z}\rangle = e^{(i/\hbar)(p_x x + p_y y + p_z z)} ,$$

is a possible state of the system.

On the other hand, choosing  $\hat{p}_z^2 = -\hbar^2 \frac{\partial^2}{\partial z^2}$  as the third operator, giving the eigenvalues  $p_z^2$ , the state would have been,

$$|\psi_{p_x, p_y, p_z^2}\rangle = e^{(i/\hbar)(p_x x + p_y y)} \cos \frac{p_z z}{\hbar} \quad \text{or} \quad |\psi_{p_x, p_y, p_z^2}\rangle = e^{(i/\hbar)(p_x x + p_y y)} \sin \frac{p_z z}{\hbar}. \quad (2.87)$$

Therefore, there are two solutions with the same eigenvalues,  $p_x$ ,  $p_y$ ,  $p_z^2$ . To lift this degeneracy, we need to introduce yet another observable. This observable can be, for example, the *parity*  $\hat{P}$ , that is, the behavior of the wave function upon mirroring  $z \rightarrow -z$  in the  $x$ - $y$  plane. The fact that the set of operators  $p_x$ ,  $p_y$ ,  $p_z$  on one hand and  $p_x$ ,  $p_y$ ,  $p_z^2$ ,  $\hat{P}$  on the other are equivalent, shows that the required number of observables for a complete characterization depends on their judicious choice.

Also, the number needed for a *complete set of commuting operators* (CSCO) depends on the number of *degrees of freedom* and the symmetry of the system. In the case of the free particle in one dimension it is enough to consider one observable only, for example,  $\hat{x}$  or  $\hat{p}$ . In three dimensions, we already need at least three commuting observables. In Exc. 2.3.9.8 we will try to find a CSCO for a matrix with partially degenerate eigenvalues.

### 2.3.6 Uncertainty relation

We have already learned that observables that do not commute can not be measured with arbitrary precision. This principle can be quantified as follows: If  $\hat{A}$  and  $\hat{B}$  are two observables, then,

$$\Delta \hat{A} \Delta \hat{B} \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|. \quad (2.88)$$

This is Heisenberg's famous *uncertainty principle*. For example,  $[\hat{p}, \hat{x}] = -i\hbar$ , and hence,  $\Delta p \Delta x \geq \hbar/2$ . We will see later (see Sec. 4.3.1), that  $[\hat{l}_x, \hat{l}_y] = i\hbar \hat{l}_z$  such that  $\Delta l_x \Delta l_y \geq \hbar |\langle l_z \rangle|/2$ . More difficult to show, since time has no simple quantum operator, is  $\Delta E \Delta t \geq \hbar/2$ . In the Exc. 2.3.9.9 we will show the *Schwartz inequality*, and in the Exc. 2.3.9.10 we ask for a formal derivation of Heisenberg's uncertainty principle.

### 2.3.7 Representations

#### 2.3.7.1 Spatial representation

A Hilbert space can be discrete or, as in the case of the momentum of a free particle, continuous. In this latter case, the eigenvalues are continuously distributed, since the equation,

$$-i\hbar \nabla_{\mathbf{r}} \psi(\mathbf{r}) = \mathbf{p} \psi(\mathbf{r}), \quad (2.89)$$

has solutions for each value of  $E$ . The eigenfunctions are  $\psi(\mathbf{r}) = a e^{i\mathbf{p} \cdot \mathbf{r}/\hbar}$ . Eq. (2.89) clearly has the form of an eigenvalue equation, for which we have already introduced the Heisenberg matrix formalism. The question now is how these descriptions combine.

Observables that do not commute correspond to expansions on different bases and generate alternative representations. For example, we can represent quantum mechanics in *position space* or *linear momentum space*. If  $|\mathbf{r}\rangle$  is a basis of the space of the particles' state,

$$\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle \quad , \quad \langle \mathbf{r}'|\mathbf{r}\rangle = \delta^3(\mathbf{r}' - \mathbf{r}) \quad , \quad \int_{\mathbb{R}^3} |\mathbf{r}\rangle \langle \mathbf{r}| d^3r = \hat{\mathbf{1}} \quad , \quad (2.90)$$

we can expand the position operator on a position basis as,

$$\hat{\mathbf{r}} = \int_{\mathbb{R}^3} \mathbf{r}|\mathbf{r}\rangle \langle \mathbf{r}| d^3r \quad , \quad (2.91)$$

and any state vector as,

$$|\psi(t)\rangle = \int_{\mathbb{R}^3} |\mathbf{r}\rangle \psi(t, \mathbf{r}) d^3r \quad . \quad (2.92)$$

The quantities  $\langle \mathbf{r}|\psi(t)\rangle = \psi(t, \mathbf{r})$  Schrödinger wave functions. We can also say that the wavefunctions are the coordinates of the state in the particular base  $|\mathbf{r}\rangle$ . Consequently,

$$\begin{aligned} \langle \mathbf{r}|\hat{\mathbf{r}}|\mathbf{r}'\rangle &= \mathbf{r}\delta^3(\mathbf{r} - \mathbf{r}') \\ \langle \mathbf{r}|f(\hat{\mathbf{r}})|\mathbf{r}'\rangle &= f(\mathbf{r})\delta^3(\mathbf{r} - \mathbf{r}') \quad . \end{aligned} \quad (2.93)$$

It is also true that,

$$\langle \mathbf{r}|\hat{A}|\psi(t)\rangle = \int_{\mathbb{R}^3} A(\mathbf{r}, \mathbf{r}') \psi(t, \mathbf{r}') d^3r' \quad , \quad (2.94)$$

where the quantity  $A(\mathbf{r}, \mathbf{r}') \equiv \langle \mathbf{r}|\hat{A}|\mathbf{r}'\rangle$  is called *kernel* of the operator. The transition from Heisenberg's abstract mechanics to Schrödinger's wave mechanics is done by the substitutions  $|\psi(t)\rangle \rightarrow \psi(t, \mathbf{r})$  and  $\hat{A} \rightarrow A(\mathbf{r}, \mathbf{r}')$ .

### 2.3.7.2 Momentum representation

The uncertainty relation is symmetric in  $\hat{\mathbf{r}}$  and  $\hat{\mathbf{p}}$ . Nothing prevents us from choosing as a basis,

$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle \quad , \quad \langle \mathbf{p}'|\mathbf{p}\rangle = \delta^3(\mathbf{p}' - \mathbf{p}) \quad , \quad \int_{\mathbb{R}^3} |\mathbf{p}\rangle \langle \mathbf{p}| d^3p = \hat{\mathbf{1}} \quad , \quad (2.95)$$

in which we can expand the momentum operator on a momentum basis as,

$$\hat{\mathbf{p}} = \int_{\mathbb{R}^3} \mathbf{p}|\mathbf{p}\rangle \langle \mathbf{p}| d^3p \quad , \quad (2.96)$$

with the wavefunctions,

$$|\psi(t)\rangle = \int_{\mathbb{R}^3} |\mathbf{p}\rangle \varphi(\mathbf{p}, t) d^3p \quad , \quad (2.97)$$

where  $\langle \mathbf{p} | \psi(t) \rangle = \varphi(t, \mathbf{p})$ . The formulas are analogous to the ones in the spatial representation. In particular, in the momentum representation the position operator is  $\mathbf{r} = i\hbar \nabla_{\mathbf{p}}$ .

The representations follow from one another by Fourier transformation. Since  $-i\hbar \nabla_{\mathbf{r}} \langle \mathbf{r} | \mathbf{p} \rangle = \mathbf{p} \langle \mathbf{r} | \mathbf{p} \rangle$ , we know,

$$\boxed{\langle \mathbf{r} | \mathbf{p} \rangle = \frac{1}{h^{3/2}} \exp\left(\frac{i}{\hbar} \mathbf{r} \cdot \mathbf{p}\right)}, \quad (2.98)$$

where the prefactor  $h^{-3/2}$  is introduced to take account of the unit of the states <sup>11</sup>.  $\psi$  and  $\varphi$  are different representations of the same quantum state related by,

$$\begin{aligned} \langle \mathbf{r} | \psi(t) \rangle &= \int_{\mathbb{R}^3} \langle \mathbf{r} | \mathbf{p} \rangle \langle \mathbf{p} | \psi(t) \rangle d^3 p = \frac{1}{h^{3/2}} \int_{\mathbb{R}^3} e^{i\mathbf{r} \cdot \mathbf{p} / \hbar} \varphi(\mathbf{p}, t) d^3 p = \psi(\mathbf{r}, t) \\ \langle \mathbf{p} | \psi(t) \rangle &= \int_{\mathbb{R}^3} \langle \mathbf{p} | \mathbf{r} \rangle \langle \mathbf{r} | \psi(t) \rangle d^3 r = \frac{1}{h^{3/2}} \int_{\mathbb{R}^3} e^{-i\mathbf{r} \cdot \mathbf{p} / \hbar} \psi(\mathbf{r}, t) d^3 r = \varphi(\mathbf{p}, t). \end{aligned} \quad (2.99)$$

Normalization ensures that  $\psi = \mathcal{F}^{-1} \mathcal{F} \psi$  with the relation,

$$\delta(x) = \lim_{t \rightarrow \infty} \frac{1}{2\pi} \int_{-t}^t e^{ikx} dk. \quad (2.100)$$

Using the wavevector  $\hbar \mathbf{k} = \mathbf{p}$  we can also write,

$$\psi(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{i\mathbf{r} \cdot \mathbf{k}} \tilde{\varphi}(\mathbf{k}) d^3 k \quad \text{and} \quad \tilde{\varphi}(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-i\mathbf{r} \cdot \mathbf{k}} \psi(\mathbf{r}) d^3 r, \quad (2.101)$$

defining the function  $\tilde{\varphi}(\mathbf{k}) \equiv h^{3/2} \varphi(\mathbf{p})$ . Applying the Fourier transform to functions of operator we can calculate,

$$\begin{aligned} \langle \mathbf{r} | G(\hat{\mathbf{p}}) | \mathbf{r}' \rangle &= \int d^3 p \langle \mathbf{r} | G(\hat{\mathbf{p}}) | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}' \rangle = \int d^3 p G(\mathbf{p}) \langle \mathbf{r} | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}' \rangle \\ &= \frac{1}{h^3} \int d^3 p G(\mathbf{p}) e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} = \frac{1}{h^3} (\mathcal{F}G)(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (2.102)$$

In Exc. 2.3.9.11 we will show  $\langle \mathbf{r} | \hat{\mathbf{p}} | \psi \rangle = (\hbar/i) \nabla_{\mathbf{r}} \langle \mathbf{r} | \psi \rangle$ , thus justifying that we can understand an operator as a rule to determine what happens to a function. For example, the rule  $\hat{p}_x$  asks for a derivation of the wavefunction by  $x$ .

## 2.3.8 Spanning a Hilbert space with several degrees of freedom

All systems analyzed up to this point were characterized by a single degree of freedom (e.g., energy, momentum, or angular momentum), which could have a continuous or discrete spectrum. Even when we treated systems exhibiting various degrees of freedom (motion of a particle in 3D space, electron orbitals in the hydrogen atom), we always found a way to separate the degrees of freedom into orthogonal Hilbert

<sup>11</sup>Note that the units of the wavefunctions are defined by normalization:  $\langle \mathbf{r}' | \mathbf{r} \rangle = \delta^3(\mathbf{r} - \mathbf{r}')$ . Introducing the parenthesis [...] to extract the unit of a physical quantity, we find,  $[[\mathbf{r}]] = [\psi(\mathbf{r})] = [r^{-3/2}]$  and  $[[\mathbf{p}]] = [\varphi(\mathbf{p})] = [p^{-3/2}]$ . We do not assign a unit to the abstract state  $|\psi\rangle$ , that is,  $[[\psi]] = 1$ .

spaces, which allowed us to treat the dynamics of the degrees of freedom separately. In this chapter, we will establish the theoretical foundations allowing us to analyze systems, where degrees of freedom can not be separated because they are entangled or interact. In particular, we will consider the system of two spins and the coupling of angular momenta in general.

### 2.3.8.1 Projection and internal sum

A *projector* is an operator which *reduces* the domain of an operator, originally acting on a Hilbert space  $\mathcal{H}$  to the *subspace* defined by the projector. We consider an operator  $\hat{A}$  with the matrix representation,

$$\hat{A} \equiv \sum_{\substack{i,j \\ |i\rangle, |j\rangle \in \mathcal{H}}} |i\rangle A_{ij} \langle j| = \begin{pmatrix} & \vdots & \\ \dots & A_{ij} & \dots \\ & \vdots & \end{pmatrix}, \quad (2.103)$$

acting on wavefunctions  $|\psi\rangle \in \mathcal{H}$  which can be expanded on a basis  $|i\rangle$  of  $\mathcal{H}$ . Now, we consider a subspace  $\mathcal{R} \subset \mathcal{H}$  defined by the base  $|k\rangle$ . Then the projector  $\hat{P}_{\mathcal{R}}$  can be represented by,

$$\hat{P}_{\mathcal{R}} \equiv \sum_{\substack{k \\ |k\rangle \in \mathcal{R}}} |k\rangle \langle k| = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \begin{pmatrix} 1 & \\ & \dots & \\ & & 1 \end{pmatrix} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (2.104)$$

Applied to the operator  $\hat{A}$ ,

$$\hat{A}_{\mathcal{R}} \equiv \hat{P}_{\mathcal{R}} \hat{A} = \hat{P}_{\mathcal{R}} \hat{A}_{\mathcal{R}} = \sum_{k,l} |k\rangle A_{kl} \langle l| = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \begin{pmatrix} \vdots & \\ \dots & A_{kl} & \dots \\ \vdots & \end{pmatrix} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (2.105)$$

Applied to a state  $|i\rangle$ ,

$$|\psi\rangle_{\mathcal{R}} = \hat{P}_{\mathcal{R}} |\psi\rangle = \hat{P}_{\mathcal{R}} |\psi\rangle_{\mathcal{R}} = \sum_k c_k |k\rangle = \begin{pmatrix} 0 \\ \vdots \\ c_k \\ \vdots \\ 0 \end{pmatrix}. \quad (2.106)$$

We study an example in the [2.3.9.12](#)

Consequently, we can understand the Hilbert space as the sum of its subspaces,

$$\hat{A} = \bigoplus_{\mathcal{R}} \hat{A}_{\mathcal{R}} \quad \text{and} \quad \bigoplus_{\mathcal{R}} \hat{P}_{\mathcal{R}} = \mathbb{I}. \quad (2.107)$$

The dimensions of the subspaces are additive,

$$\dim \hat{A} = \sum_{\mathcal{R}} \dim \hat{A}_{\mathcal{R}} .$$

**Example 6 (Projection for a three-level atom):** The Hamiltonian of a three-level atom with excitation of two transitions is given by,

$$\hat{H} = \begin{pmatrix} \omega_1 & \Omega_{12} & 0 \\ \Omega_{12} & \omega_2 & \Omega_{23} \\ 0 & \Omega_{23} & \omega_3 \end{pmatrix} .$$

The projector,

$$\hat{P} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

reduces the Hamiltonian to a two-level transition,

$$\hat{H}_{\mathcal{R}} = \begin{pmatrix} \omega_1 & \Omega_{12} & 0 \\ \Omega_{12} & \omega_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} .$$

Obviously, the concatenation (2.107) only serves to increase the Hilbert space of a given degree of freedom described by a given observable, e.g., when we add one more level of energy to the spectrum of an atom described by a Hamiltonian. If, in contrast, we want to add another degree of freedom, we need the external sum or external product discussed below.

### 2.3.8.2 Tensorial product

We have previously worked with systems exhibiting more than one degree of freedom and therefore having to be characterized by more than one observable with its spectrum of eigenstates. One example are the electronic orbitals of the hydrogen atom  $|n\ell m\rangle$ , which need three quantum numbers to be labeled unambiguously. Obviously, each quantum number increases the dimensionality of the Hilbert space. Another example is the system  $|\alpha\beta\rangle$  of two particles with spin  $\frac{1}{2}$ , each spin being defined on its respective space,

$$|\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = (\alpha_i)_i \in \mathcal{H}_A \quad \text{and} \quad |\beta\rangle = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = (\beta_k)_k \in \mathcal{H}_B . \quad (2.108)$$

The combined state is,

$$|\alpha\beta\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B \quad \text{with} \quad \dim \mathcal{H}_A \otimes \mathcal{H}_B = \dim \mathcal{H}_A \dim \mathcal{H}_B . \quad (2.109)$$

The symbol  $\otimes$  denotes the *outer tensorial product* of two vectors (states)<sup>12</sup>. Now, in order to represent the multidimensional space  $\mathcal{H}_A \otimes \mathcal{H}_B$  by a matrix, we use the fact

<sup>12</sup>The tensorial product of two states should not be confused with other definitions of products, such as the inner (or scalar) product of two states,

$$\langle \alpha | \beta \rangle \equiv \alpha_1 \beta_1 + \alpha_2 \beta_2 ,$$



that it is isomorphic to the space  $\mathcal{H}_I \otimes \mathcal{H}_{A \otimes B}$ , that is, we proceed to a reorganization of the quantum numbers identifying,

$$|\gamma\rangle \equiv |\alpha\rangle|\beta\rangle = |\alpha\rangle \otimes |\beta\rangle = |\alpha\beta\rangle = \begin{pmatrix} \alpha_1|\beta\rangle \\ \alpha_2|\beta\rangle \end{pmatrix} = \begin{pmatrix} \alpha_1\beta_1 \\ \alpha_1\beta_2 \\ \alpha_2\beta_1 \\ \alpha_2\beta_2 \end{pmatrix} = (\gamma_m)_m \in \mathcal{H}_A \otimes \mathcal{H}_B, \quad (2.110)$$

where  $m = 1, 2, 3, 4$  is identified with  $(i, k) = (1, 1), (1, 2), (2, 1), (2, 2)$ . The new vector is element of the 4-dimensional vector space  $\mathcal{H}_A \otimes \mathcal{H}_B$ . If  $\{|\alpha\rangle_i\}$  and  $\{|\beta\rangle_k\}$  are bases in their respective spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , then  $\{|\gamma\rangle_m\}$  is a basis of the product space  $\mathcal{H}_A \otimes \mathcal{H}_B$ .

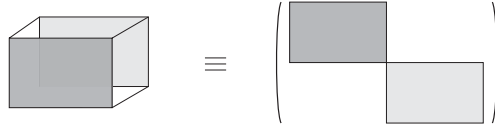


Figure 2.3: Illustration of the isomorphism between  $\mathcal{H}_A \otimes \mathcal{H}_B$  and  $\mathcal{H}_I \otimes \mathcal{H}_{A \otimes B}$  for matrices of rank 2.

For observables we proceed in the same way: The external product of two commutators spans a Hilbert product space with the dimension corresponding to product of the dimensions of the sub-spaces. Assuming that,

$$\hat{A} \equiv \sum_{i,j} |i\rangle A_{ij} \langle j| \quad \text{and} \quad \hat{B} \equiv \sum_{k,l} |k\rangle B_{kl} \langle l|. \quad (2.111)$$

then

$$\hat{A} \otimes \hat{B} \equiv \sum_{(ik)(jl)} |ik\rangle A_{ij} B_{kl} \langle jl|, \quad (2.112)$$

such that

$$\dim \hat{A} \otimes \hat{B} = \dim \hat{A} \dim \hat{B}.$$

the outer product,

$$|\alpha\rangle\langle\beta| \equiv \begin{pmatrix} \alpha_1\beta_1 & \alpha_1\beta_2 \\ \alpha_2\beta_1 & \alpha_2\beta_2 \end{pmatrix}$$

$$\begin{pmatrix} A_{11} \\ A_{12} \\ A_{21} \\ A_{22} \end{pmatrix} \begin{pmatrix} B_{11} \\ B_{12} \\ B_{21} \\ B_{22} \end{pmatrix}^\dagger = \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{11}B_{21} & A_{11}B_{22} \\ A_{12}B_{11} & A_{12}B_{12} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{21}B_{21} & A_{21}B_{22} \\ A_{22}B_{11} & A_{22}B_{12} & A_{22}B_{21} & A_{22}B_{22} \end{pmatrix},$$

the exterior (cross) product,

$$|\alpha\rangle \times |\beta\rangle = \begin{pmatrix} \alpha_2\beta_3 - \alpha_3\beta_2 \\ \alpha_3\beta_1 - \alpha_1\beta_3 \\ \alpha_1\beta_2 - \alpha_2\beta_1 \end{pmatrix},$$

nor the point-wise or *Hadamard product*,

$$\hat{A} \circ \hat{B} \equiv \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \circ \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = \begin{pmatrix} A_{11}B_{11} & A_{12}B_{12} \\ A_{21}B_{21} & A_{22}B_{22} \end{pmatrix}.$$

For example,  $|i\rangle\langle j| \otimes |k\rangle\langle l| = |ik\rangle\langle jl|$ .

For two two-dimensional operators  $\hat{A}$  and  $\hat{B}$ , the *tensorial external product* is defined by,

$$\hat{A} \otimes \hat{B} = \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{pmatrix}, \quad (2.113)$$

and can be decomposed as,

$$\hat{A} \otimes \hat{B} = (\hat{A} \otimes \mathbb{I})(\mathbb{I} \otimes \hat{B}) = \begin{pmatrix} A_{11} & & A_{12} & \\ & A_{11} & & \\ A_{21} & & A_{22} & \\ & A_{21} & & A_{22} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & & \\ B_{21} & B_{22} & & \\ & & B_{11} & B_{12} \\ & & B_{21} & B_{22} \end{pmatrix}. \quad (2.114)$$

The concept (2.112) can be generalized to more degrees of freedom like,

$$\hat{A} \otimes \hat{B} \otimes \hat{C} \equiv \sum_{(ikm)(jln)} |ikm\rangle A_{ij} B_{kl} C_{mn} \langle jln|, \quad (2.115)$$

Obviously, the external product is associative  $(\hat{A} \otimes \hat{B}) \otimes C = \hat{A} \otimes (\hat{B} \otimes C)$ , but does not commute, even though the operators acting on different spaces do commute,  $[\hat{A}, \hat{B}] = 0$ . Nevertheless, we can reverse the order of the product of two operators using,

$$\hat{A} \otimes \hat{B} = \hat{S}(\hat{B} \otimes \hat{A})\hat{S} \quad \text{with} \quad \hat{S} = \begin{pmatrix} 1 & & & \\ & 0 & 1 & \\ & 1 & 0 & \\ & & & 1 \end{pmatrix}. \quad (2.116)$$

We note, that it is important to distinguish from what space the vector came from. In our notation, the vector *before* the symbol of the tensorial product ( $\otimes$ ) is belongs to the space  $\mathcal{H}_A$ , and the one *after* the  $\otimes$  belongs to the space  $\mathcal{H}_B$ . With the definition (2.111) we can verify that the operators only act on their respective states:

$$(\mathbf{A} \otimes \mathbf{B})(|\alpha\rangle \otimes |\beta\rangle) = \mathbf{A}|\alpha\rangle \otimes \mathbf{B}|\beta\rangle. \quad (2.117)$$

**Example 7 (Tensorial product):** We can check the relationship (2.117) by

the definitions (2.110) and (2.113) of the external product,

$$\begin{aligned}
& \left[ \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \otimes \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \right] \left[ \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \otimes \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \right] \\
&= \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{11}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{11}B_{22} \\ A_{21}B_{11} & A_{11}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{11}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{pmatrix} \begin{pmatrix} \alpha_{11}\beta_{11} \\ \alpha_{11}\beta_{21} \\ \alpha_{21}\beta_{11} \\ \alpha_{21}\beta_{21} \end{pmatrix} \\
&= \begin{pmatrix} A_{11}B_{11}\alpha_{11}\beta_{11} + A_{11}B_{12}\alpha_{11}\beta_{21} + A_{12}B_{11}\alpha_{21}\beta_{11} + A_{11}B_{12}\alpha_{21}\beta_{21} \\ A_{11}B_{21}\alpha_{11}\beta_{11} + A_{11}B_{22}\alpha_{11}\beta_{21} + A_{12}B_{21}\alpha_{21}\beta_{11} + A_{11}B_{22}\alpha_{21}\beta_{21} \\ A_{21}B_{11}\alpha_{11}\beta_{11} + A_{11}B_{12}\alpha_{11}\beta_{21} + A_{22}B_{11}\alpha_{21}\beta_{11} + A_{22}B_{12}\alpha_{21}\beta_{21} \\ A_{21}B_{21}\alpha_{11}\beta_{11} + A_{11}B_{22}\alpha_{11}\beta_{21} + A_{22}B_{21}\alpha_{21}\beta_{11} + A_{22}B_{22}\alpha_{21}\beta_{21} \end{pmatrix} \\
&= \begin{pmatrix} (A_{11}\alpha_1 + A_{12}\alpha_2)(B_{11}\beta_1 + B_{12}\beta_2) \\ (A_{11}\alpha_1 + A_{12}\alpha_2)(B_{21}\beta_1 + B_{22}\beta_2) \\ (A_{21}\alpha_1 + A_{22}\alpha_2)(B_{11}\beta_1 + B_{12}\beta_2) \\ (A_{21}\alpha_1 + A_{22}\alpha_2)(B_{21}\beta_1 + B_{22}\beta_2) \end{pmatrix} \\
&= \begin{pmatrix} A_{11}\alpha_1 + A_{12}\alpha_2 \\ A_{21}\alpha_1 + A_{22}\alpha_2 \end{pmatrix} \otimes \begin{pmatrix} B_{11}\beta_1 + B_{12}\beta_2 \\ B_{21}\beta_1 + B_{22}\beta_2 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \otimes \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}.
\end{aligned} \tag{2.118}$$

**Example 8 (Mathematical definition of the tensor product):** If  $\alpha$  belongs to the Hilbert space  $\mathcal{H}_\alpha$  and  $\beta$  belongs to  $\mathcal{H}_\beta$ , then the equivalence class of  $(\alpha, \beta)$  is denoted by  $\alpha \otimes \beta$  and called the tensor product of  $\alpha$  with  $\beta$ . This use of the  $\otimes$ -symbol refers specifically to the outer product operation. An element of  $\mathcal{H}_\alpha \otimes \mathcal{H}_\beta$  that can be written in the form  $\alpha \otimes \beta$  is called a pure tensor. In general, an element of the tensor product space is not a pure tensor, but rather a finite linear combination of pure tensors. For example, if  $\alpha_1$  and  $\alpha_2$  are linearly independent, and  $\beta_1$  and  $\beta_2$  are also linearly independent, then  $\alpha_1 \otimes \beta_1 + \alpha_2 \otimes \beta_2$  cannot be written as a pure tensor. The number of pure tensors required to express an element of a tensor product is called the tensor rank. The rank should not be confused with the tensor order, which is the number of spaces one has taken the product of (in this case two), and which corresponds to the number of indices. For linear operators or matrices, thought of as  $(1, 1)$  tensors (elements of the space  $\mathcal{H}_\alpha \otimes \mathcal{H}_\alpha^*$ ), the tensor rank agrees with matrix rank.

Given bases  $\{\alpha_i\}$  and  $\{\beta_j\}$  for  $\mathcal{H}_\alpha$  and  $\mathcal{H}_\beta$  respectively, the tensors  $\{\alpha_i \otimes \beta_j\}$  form a basis for  $\mathcal{H}_\alpha \otimes \mathcal{H}_\beta$ . Therefore, if  $\mathcal{H}_\alpha$  and  $\mathcal{H}_\beta$  are finite-dimensional, the dimension of the tensor product is the product of dimensions of the original spaces; for instance  $\mathbb{R}^m \otimes \mathbb{R}^n$  is isomorphic to  $\mathbb{R}^{nm}$ .

The tensor product also operates on linear maps (called operators in quantum mechanics) between vector spaces. Specifically, given two linear maps  $\hat{A} : \mathcal{H}_\alpha \rightarrow \mathcal{H}'_\alpha$  and  $\hat{B} : \mathcal{H}_\beta \rightarrow \mathcal{H}'_\beta$  between vector spaces, the tensor product of the two linear maps  $\hat{A}$  and  $\hat{B}$  is a linear map,

$$\hat{A} \otimes \hat{B} : \mathcal{H}_\alpha \otimes \mathcal{H}_\beta \rightarrow \mathcal{H}'_\alpha \otimes \mathcal{H}'_\beta,$$

defined by,

$$(\hat{A} \otimes \hat{B})(\alpha \otimes \beta) = \hat{A}(\alpha) \otimes \hat{B}(\beta).$$

In this way, the tensor product becomes a bifunctor from the category of vector spaces to itself, covariant in both arguments. If  $\hat{A}$  and  $\hat{B}$  are both injective,

surjective or (in the case that  $\mathcal{H}_\alpha$ ,  $\mathcal{H}'_\alpha$ ,  $\mathcal{H}_\beta$ , and  $\mathcal{H}'_\beta$  are normed vector spaces or topological vector spaces) continuous, then  $\hat{A} \otimes \hat{B}$  is injective, surjective or continuous, respectively.

By choosing bases of all vector spaces involved, the linear maps  $\hat{A}$  and  $\hat{B}$  can be represented by matrices. Then, depending on how the tensor  $\alpha \otimes \beta$  is vectorized, the matrix describing the tensor product  $\hat{A} \otimes \hat{B}$  is the Kronecker product of the two matrices. For example, if  $\mathcal{H}_\alpha$ ,  $\mathcal{H}'_\alpha$ ,  $\mathcal{H}_\beta$ , and  $\mathcal{H}'_\beta$  above are all two-dimensional and bases have been fixed for all of them, and  $\hat{A}$  and  $\hat{B}$  are given by the matrices,

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

respectively, then the tensor product of these two matrices is,

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \otimes \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = \begin{pmatrix} A_{11} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} & A_{12} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \\ A_{21} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} & A_{22} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \end{pmatrix}.$$

The resultant rank is at most 4, and thus the resultant dimension is 4. Note that rank here denotes the tensor rank i.e. the number of requisite indices (while the matrix rank counts the number of degrees of freedom in the resulting array). Note  $\text{Tr } \hat{A} \otimes \hat{B} = \text{Tr } \hat{A} \times \text{Tr } \hat{B}$ .

A dyadic product is the special case of the tensor product between two vectors of the same dimension.

### 2.3.8.3 Direct external sum

Using the nomenclature (2.111) we define the external direct sum by,

$$\hat{A} \oplus \hat{B} \equiv \sum_{(ik)(jl)} |ik\rangle (A_{ij} + B_{kl}) \langle jl|, \quad (2.119)$$

that is,

$$\hat{A} \oplus \hat{B} = \begin{pmatrix} A_{11} + B_{11} & A_{11} + B_{12} & A_{12} + B_{11} & A_{12} + B_{12} \\ A_{11} + B_{21} & A_{11} + B_{22} & A_{12} + B_{21} & A_{12} + B_{22} \\ A_{21} + B_{11} & A_{21} + B_{12} & A_{22} + B_{11} & A_{22} + B_{12} \\ A_{21} + B_{21} & A_{21} + B_{22} & A_{22} + B_{21} & A_{22} + B_{22} \end{pmatrix}. \quad (2.120)$$

It can be decomposed as,

$$\hat{A} \oplus \hat{B} = \hat{A} \oplus \mathbb{O} + \mathbb{O} \oplus \hat{B} = \hat{A} \otimes \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \otimes \hat{A}. \quad (2.121)$$

Again, using the definition (2.116) of the unitary operator  $\hat{S}$ , we can reverse the order of the operator by,

$$\hat{A} \oplus \hat{B} = \hat{S}(\hat{B} \oplus \hat{A})\hat{S}. \quad (2.122)$$

**Example 9 (Direct external sum of two diagonal Hamiltonians):** As an example we consider a two-level atom excited by radiation and trapped in an external harmonic potential. We assume that the degrees of freedom do not interact. As the Hamiltonian of the HO is diagonal, the total Hamiltonian is organized into a diagonal matrix of quadratic subspaces,

$$\hat{H} = \hbar\omega(n + \frac{1}{2}) \oplus \begin{pmatrix} 0 & \hbar\Omega \\ \hbar\Omega & \hbar\Delta \end{pmatrix} = \begin{pmatrix} \frac{\hbar\omega}{2} & \frac{\hbar\omega}{2} + \hbar\Omega & 0 & 0 & \vdots \\ \frac{\hbar\omega}{2} + \hbar\Omega & \frac{\hbar\omega}{2} + \hbar\Delta & 0 & 0 & \vdots \\ 0 & 0 & \frac{3\hbar\omega}{2} & \frac{3\hbar\omega}{2} + \hbar\Omega & \vdots \\ 0 & 0 & \frac{3\hbar\omega}{2} + \hbar\Omega & \frac{3\hbar\omega}{2} + \hbar\Delta & \vdots \\ \dots & \dots & \dots & \dots & \ddots \end{pmatrix}.$$

It acts on the product state  $|n\rangle|i\rangle$ , where the first ket denotes the vibrational level and the second ket the electronic excitation of the atom.

Other examples are studied in [2.3.9.13](#) and [2.3.9.14](#).

### 2.3.8.4 Trace

The *trace* of an operator over a subspace reduces its domain to the remaining dimensions (the  $\cdot$ -symbol is a place holder for the dimension over which we do NOT want to trace):

$$\begin{aligned} \text{Tr}_B \hat{A} \otimes \hat{B} &= \sum_{(ik)(jl)(\cdot m)} \langle \cdot m | ik \rangle A_{ij} B_{kl} \langle jl | \cdot m \rangle = \sum_{(ik)(jl)(\cdot m)} |i\rangle A_{ij} B_{kl} \langle j| \delta_{km} \delta_{lm} \\ &= \sum_{(i)(j)(m)} |i\rangle A_{ij} B_{mm} \langle j| = \hat{A} \sum_m B_{mm} = \hat{A} \text{Tr}_B \hat{B}. \end{aligned} \tag{2.123}$$

For example,  $\text{Tr}_\rho \hat{A} \otimes \hat{\rho} = \hat{A}$ . See the Excs. [2.3.9.15](#) and [2.3.9.16](#).

It can be shown,

$$\text{Tr} \hat{A} \hat{B} = \text{Tr} \hat{B} \hat{A}. \tag{2.124}$$

## 2.3.9 Exercises

### 2.3.9.1 Ex: Orthogonality

Show that two eigenvectors of a Hermitian operator associated with two different eigenvalues are orthogonal.

### 2.3.9.2 Ex: Orthonormalization

Orthonormalize the base  $\langle a_1 | = (1 \ -1 \ 0)$ ,  $\langle a_2 | = (0 \ 1 \ 0)$ ,  $\langle a_3 | = (0 \ 1 \ 1)$ .

**2.3.9.3 Ex: Orthonormal base**

Construct an orthonormal basis for the following operator describing a partially degenerate three-level system,

$$\hat{A} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}.$$

**2.3.9.4 Ex: Eigenvalue equation**

Calculate the unitary matrix  $U$  transforming the Hamiltonian  $\hat{H} = \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$  into a diagonal matrix  $E = U^\dagger \hat{H} U$ .

**2.3.9.5 Ex: Spin rotation operators**

Prove the following relations for the spin rotation operator:  $e^{-i\pi\sigma_x/4}\sigma_z e^{i\pi\sigma_x/4} = -\sigma_y$  and  $e^{-i\pi\sigma_x/4}\sigma_y e^{i\pi\sigma_x/4} = \sigma_z$ .

**2.3.9.6 Ex: Eigenvalues and eigenvectors**

Find the eigenvalues and -vectors of the operator  $\hat{A} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$  and construct the unitary matrix which transforms this operator into a diagonal matrix.

**2.3.9.7 Ex: Commuting operators**

- Show that if two operators  $\hat{A}$  and  $\hat{B}$  commute and if  $|\psi\rangle$  is an eigenvector of  $\hat{A}$ ,  $\hat{B}|\psi\rangle$  also is an eigenvector of  $\hat{A}$  with the same eigenvalue.
- Show that if two operators  $\hat{A}$  and  $\hat{B}$  commute and if  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are two eigenvectors of  $\hat{A}$  with different eigenvalues, the matrix element  $\langle\psi_1|\hat{B}|\psi_2\rangle$  is equal to zero.
- Show that if two operators  $\hat{A}$  and  $\hat{B}$  commute, we can construct an orthonormal basis of eigenvectors common to  $\hat{A}$  and  $\hat{B}$ .

**2.3.9.8 Ex: Eigenvalues**

- Find the eigenvalues and eigenvectors of the operator  $\hat{A} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & \mu & 0 \\ 1 & 0 & 1 \end{pmatrix}$  for  $0 < \mu < 2$ .
- Write down the unitary matrix  $U$  satisfying the eigenvalue equation:  $\hat{A}U = UE_A$ , where  $E_A$  is the matrix that has all eigenvalues of  $\hat{A}$  in its diagonal.
- Now consider the case  $\mu = 0$ . Find a complete set of commuting operators (CSCO). That is, calculate the components of a second operator  $\hat{B}$ , which commutes with  $\hat{A}$ , as a function of its eigenvalues  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$ , and verify  $[\hat{A}, \hat{B}] = 0$ . Find the most general form of operator  $\hat{B}$ .

**2.3.9.9 Ex: Schwartz inequality**

Demonstrate the Schwartz inequality  $|\langle u|v\rangle|^2 \leq \langle u|u\rangle\langle v|v\rangle$ .

**2.3.9.10 Ex: Heisenberg's uncertainty principle**

Develop the formal derivation of Heisenberg's uncertainty principle.

**2.3.9.11 Ex: Fourier transform**

Show that  $\langle \mathbf{r}|\hat{\mathbf{P}}|\psi\rangle = \frac{\hbar}{i}\nabla\langle \mathbf{r}|\psi\rangle$  reproduces the Schrödinger equation in position representation.

**2.3.9.12 Ex: Projection of the motion of a particle**

Project the Hamiltonian of the motion of a free particle onto the plane  $x$ - $y$  at the position  $z = z_0$  using the projection operator  $\hat{P} = |z_0\rangle\langle z_0|$  and the trace defined in (2.123) generalized to continuous variables.

**2.3.9.13 Ex: Complete system of commuting operators**

Construct the Hilbert space of two independent two-level systems a and b. Consider observables  $\hat{X}_a$  and  $\hat{Y}_b$  acting on their respective systems. What will be their shapes  $\hat{X}_{ab}$ , respectively  $\hat{Y}_{ab}$ , in the total Hilbert space? Construct the expanded state  $|\psi_{ab}\rangle$  from the basis of the individual systems. Verify  $[\hat{X}_{ab}, \hat{Y}_{ab}] = 0$ . Verify that the expanded observables obey the same eigenvalue equations as the original ones.

**2.3.9.14 Ex: Liouville equation**

Show that  $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \hat{A} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \hat{B} = \hat{A} \oplus \hat{B}$ .

**2.3.9.15 Ex: Liouville equation**

Show at the example of a two-level system that the von Neumann equation,  $\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}]$ , can be written,  $\dot{\vec{\rho}} = -\frac{i}{\hbar}(\hat{H} \otimes \mathbb{I} - \mathbb{I} \otimes \hat{H})\vec{\rho}$ , using the definition of the external

product and  $\vec{\rho} \equiv \begin{pmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{21} \\ \rho_{22} \end{pmatrix}$ . **Help:** For this exercise the physical interpretation of  $\hat{\rho}$  as

the density operator does not matter. It may be regarded as a common observable.

**2.3.9.16 Ex: Unitary transformation of singlet states**

Consider two spins  $a$  and  $b$  that do not interact. Applying to each spin the same transformation to another base, show that the singlet state has in each base the following form:  $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_a|\downarrow\rangle_b - |\downarrow\rangle_a|\uparrow\rangle_b)$ .

## 2.4 Time evolutions

Quantum systems may evolve in time, as predicted by the time-dependent Schrödinger equation (2.51). In this section we show different equivalent but complementary descriptions of the temporal evolution of quantum systems depending on whether the time dependence is attributed to the state function or to observables.

### 2.4.1 Unitary transformations

The best we can do to characterize a system is, obviously, to measure all its observables. However, neither the state functions nor the observables are fixed unambiguously, since defining a unitary operator,  $U^\dagger = U^{-1}$ , we can do,

$$\langle \psi | \hat{A} | \psi \rangle = \langle \psi | U^\dagger U \hat{A} U^\dagger U | \psi \rangle = \langle U \psi | U \hat{A} U^\dagger | U \psi \rangle . \quad (2.125)$$

That is, exchanging  $|\psi\rangle$  by  $U|\psi\rangle$  and at the same time  $\hat{A}$  by  $U\hat{A}U^\dagger$ , we obtain quantities describing the same physical reality, since the eigenvalues are unchanged. This allows us to choose the best mathematical representation for a specific problem. As an example, we will apply the temporal unitary transformation to solve the dynamics of a coupled two-level system in Exc. 2.4.7.1.

### 2.4.2 Schrödinger picture

Important examples of how the same system can be represented in different ways (related by unitary transformations) are the Heisenberg, Schrödinger, and interaction pictures.

The *Schrödinger picture*, denoted by the subscript  $S$ , is defined by the choice of a Hamiltonian,

$$\hat{H}_S = \hat{H}(t, \hat{p}_S, \hat{r}_S) \quad \text{with} \quad \frac{d}{dt} \hat{p}_S = \frac{d}{dt} \hat{r}_S = 0 . \quad (2.126)$$

That is, the observables of the system  $\hat{A}_S(t, \hat{p}_S, \hat{r}_S)$  can only depend *explicitly* on time, but not via the operators  $\hat{p}_S$  and  $\hat{r}_S$ , which are stationary,

$$\frac{d}{dt} \hat{A}_S = \frac{\partial \hat{A}_S}{\partial t} + \dot{\hat{p}}_S^0 \frac{\partial \hat{A}_S}{\partial p_S} + \dot{\hat{r}}_S^0 \frac{\partial \hat{A}_S}{\partial r_S} . \quad (2.127)$$

This is,

$$\boxed{\frac{d}{dt} \hat{A}_S(t) = \frac{\partial}{\partial t} \hat{A}_S(t)} . \quad (2.128)$$

In this case, the formal solution of the Schrödinger equation,

$$\boxed{i\hbar \frac{d}{dt} |\psi_S(t)\rangle = \hat{H}_S |\psi_S(t)\rangle} , \quad (2.129)$$

can be written,

$$|\psi_S(t)\rangle = e^{-(i/\hbar)\hat{H}_S t} |\psi_S(0)\rangle \equiv U(t) |\psi_S(0)\rangle . \quad (2.130)$$

Apparently, the temporal dynamics is completely within the wave functions.



**Example 10 (The time evolution operator):** Generalizing to an arbitrary initial time  $t_0$  we write the temporal translation operator,

$$U(t, t_0)|\psi(t_0)\rangle = |\psi(t)\rangle . \quad (2.131)$$

By the expression (2.130) we find immediately, with  $t_0 < t_1 < t_2$ ,

$$U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0) \quad \text{and} \quad U(t_0, t) = U^\dagger(t, t_0) = U^{-1}(t, t_0) = U(t, t_0)^{-1} .$$

The conjugate operator of time evolution acts on the vector 'bra',

$$\langle\psi(t)| = \langle\psi(t_0)|U^\dagger(t, t_0) .$$

### 2.4.3 Heisenberg picture

As unitary transformations do not change the physics, the system described by,

$$|\psi_S(t)\rangle \longrightarrow U(t)^\dagger|\psi_S(t)\rangle \equiv |\psi_H\rangle \quad \text{and} \quad \hat{A}_S(t) \longrightarrow U(t)^\dagger\hat{A}_S(t)U(t) \equiv \hat{A}_H(t) \quad (2.132)$$

with the transformation defined by equation (2.130), is equivalent. The subscript  $H$  means the *Heisenberg picture*. In particular, we obviously have,

$$\hat{H}_S = \hat{H}_H \equiv \hat{H} . \quad (2.133)$$

Thus, the matrix element of the operator  $\hat{A}_S$  in Schrödinger's picture with the time-dependent base  $\{|\psi_S\rangle\}$  is equal to the matrix element of the operator  $\hat{A}_H = U^\dagger\hat{A}_S U$  in Heisenberg's picture with the time-independent base  $\{|\psi_H\rangle\}$ . In this picture the wavefunctions are independent of time,

$$\boxed{\frac{d}{dt}|\psi_H\rangle = \frac{d}{dt}|\psi_S(0)\rangle = 0} , \quad (2.134)$$

but the operators depend *im- and explicitly* on time,

$$\begin{aligned} \frac{d}{dt}\hat{A}_H(t) &= \frac{d}{dt}\left(U(t)^\dagger\hat{A}_S(t)U(t)\right) = \frac{dU^\dagger}{dt}\hat{A}_S(t)U(t) + U(t)^\dagger\hat{A}_S(t)\frac{dU}{dt} + U(t)^\dagger\frac{\partial\hat{A}_S(t)}{\partial t}U(t) \\ &= \frac{i}{\hbar}\hat{H}^\dagger U(t)^\dagger\hat{A}_S U(t) + U(t)^\dagger\hat{A}_S\frac{-i}{\hbar}\hat{H}U(t) + U^\dagger(t)\frac{\partial\hat{A}_S(t)}{\partial t}U(t) . \end{aligned} \quad (2.135)$$

That is,

$$\boxed{\frac{d}{dt}\hat{A}_H(t) = \frac{i}{\hbar}[\hat{H}, \hat{A}_H(t)] + \frac{\partial\hat{A}_H(t)}{\partial t}} . \quad (2.136)$$

This so-called *Heisenberg equation*, which describes the temporal evolution of an operator acting on time-independent states in the Heisenberg picture, is equivalent to the Schrödinger equation, which expresses the temporal evolution of a quantum state in Schrödinger's picture.

According to equation (2.136), the rate of temporal variation of an operator in the Heisenberg representation is given by the commutator of that operator with the

total Hamiltonian of the system. Note that if an operator representing a dynamic variable commutes with the Hamiltonian in the Schrödinger representation, it will also commute with the Hamiltonian in the Heisenberg representation and thus with the complete set of commuting observables,

$$[\hat{H}, \hat{A}_S] = 0 \quad \iff \quad [\hat{H}, \hat{A}_H] = 0 . \quad (2.137)$$

We will show this in the Exc. 2.4.7.2.

**Example 11 (Position and momentum operators in the Heisenberg picture):** We know that in Schrödinger's picture (2.126), the operators  $\hat{p}_S$  and  $\hat{r}_S$  are stationary. Using this fact in derivation (2.135), we can show for example for the momentum operator,

$$\frac{\partial}{\partial t} \hat{p}_S = 0 \quad \implies \quad \frac{\partial}{\partial t} \hat{p}_H = 0 \quad \implies \quad \frac{d}{dt} \hat{p}_H = \frac{i}{\hbar} [\hat{H}, \hat{p}_H] .$$

In the Exc. 2.4.7.3 we will use the Heisenberg picture to derive the equations of motion for a particle confined to a potential.

## 2.4.4 Interaction picture

The *interaction picture* deals with problems where the total Hamiltonian is composed of a time-independent part and a time-dependent part,

$$\hat{H} = \hat{H}_0 + \hat{V}(t) . \quad (2.138)$$

Analogously to Eq. (2.130), we define a time evolution operator in terms of the *time-independent* part of the total Hamiltonian,

$$\boxed{|\psi_I(t)\rangle = e^{i\hat{H}_0 t/\hbar} |\psi_S(t)\rangle \quad \text{and} \quad \hat{A}_I(t) = e^{i\hat{H}_0 t/\hbar} \hat{A}_S e^{-i\hat{H}_0 t/\hbar}} . \quad (2.139)$$

Now we are interested in the temporal dependence of quantum states and operators in the interaction picture. Replacing the inverse function  $|\psi_S(t)\rangle = e^{-i\hat{H}_0 t/\hbar} |\psi_I(t)\rangle$  in the Schrödinger equation (2.129) we immediately see,

$$\boxed{\hat{V}(t) |\psi_I(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle} . \quad (2.140)$$

Apparently, in the interaction picture, only the perturbative term in Hamiltonian controls the temporal evolution. Taking the time derivative of both sides of the equation (2.139) transforming an operator from the Schrödinger to the interaction picture results in,

$$\boxed{\frac{d\hat{A}_I}{dt} = \frac{i}{\hbar} [\hat{H}_0, \hat{A}_I] + \frac{\partial \hat{A}_I}{\partial t}} . \quad (2.141)$$

Therefore, we see that the time derivative can be expressed in the form of a commutator, resembling the Heisenberg equation (2.136), except that only the unperturbed term of the Hamiltonian appears in the argument of the commutation operator.

**Example 12 (Schrieffer-Wolff transformation):** The *Schrieffer-Wolff transformation* is a unitary transformation used to perturbatively diagonalize the system Hamiltonian to first order in the interaction. As such, the Schrieffer-Wolff transformation is an operator version of second-order perturbation theory. The Schrieffer-Wolff transformation is often used to project out the high energy excitations of a given quantum many-body Hamiltonian in order to obtain an effective low energy model. The Schrieffer-Wolff transformation thus provides a controlled perturbative way to study the strong coupling regime of quantum-many body Hamiltonians.

Consider a quantum system evolving under the time-independent Hamiltonian operator  $\hat{H}$  of the form  $\hat{H} = \hat{H}_0 + \hat{V}$ , where  $H_0$  is a Hamiltonian with known eigenstates  $|m\rangle$  and corresponding eigenvalues  $E_m$ , and where  $V$  is a small perturbation. Moreover, it is assumed without loss of generality that  $\hat{V}$  is purely off-diagonal in the eigenbasis of  $\hat{H}_0$ , i.e.,

$$\langle m|\hat{V}|m\rangle = 0 \quad (2.142)$$

for all  $m$ . Indeed, this situation can always be arranged by absorbing the diagonal elements of  $\hat{V}$  into  $\hat{H}_0$ , thus modifying its eigenvalues to,

$$E'_m = E_m + \langle m|\hat{V}|m\rangle . \quad (2.143)$$

The Schrieffer-Wolff transformation is a unitary transformation which expresses the Hamiltonian in a basis (the 'dressed' basis) where it is diagonal to first order in the perturbation  $\hat{V}$ . This unitary transformation is conventionally written as:

$$\hat{H}' = e^{\iota S} \hat{H} e^{-\iota S} . \quad (2.144)$$

When  $\hat{V}$  is small, the generator  $S$  of the transformation will likewise be small. The transformation can then be expanded in  $S$  using the Baker-Campbell-Hausdorff formula,

$$\hat{H}' = \hat{H} + [\iota S, \hat{H}] + \frac{1}{2}[\iota S, [\iota S, \hat{H}]] + \dots . \quad (2.145)$$

In terms of  $\hat{H}_0$  and  $\hat{V}$ , the transformation becomes,

$$\hat{H}' = \hat{H}_0 + \hat{V} + [\iota S, \hat{H}_0] + [\iota S, \hat{V}] + \frac{1}{2}[\iota S, [\iota S, \hat{H}_0]] + \frac{1}{2}[\iota S, [\iota S, \hat{V}]] + \dots . \quad (2.146)$$

The Hamiltonian can be made diagonal to first order in  $\hat{V}$  by choosing the generator  $S$  such that,

$$[\hat{H}_0, \iota S] = \hat{V} . \quad (2.147)$$

This equation always has a definite solution under the assumption that  $\hat{V}$  is off-diagonal in the eigenbasis of  $\hat{H}_0$ . Substituting this choice in the previous transformation yields:

$$\hat{H}' = \hat{H}_0 + \frac{1}{2}[\iota S, \hat{V}] + O(\hat{V}^3) . \quad (2.148)$$

This expression is the standard form of the Schrieffer-Wolff transformation. Note that all the operators on the right-hand side are now expressed in a new basis 'dressed' by the interaction  $\hat{V}$  to first order.

In the general case, the difficult step of the transformation is to find an explicit expression for the generator  $S$ . Once this is done, it is straightforward to compute the Schrieffer-Wolff Hamiltonian by computing the commutator  $[S, \hat{V}]$ . The

Hamiltonian can then be projected on any subspace of interest to obtain an effective projected Hamiltonian for that subspace. In order for the transformation to be accurate, the eliminated subspaces must be energetically well separated from the subspace of interest, meaning that the strength of the interaction  $\hat{V}$  must be much smaller than the energy difference between the subspaces. This is the same regime of validity as in standard second-order perturbation theory.

### 2.4.5 Hamiltonian under arbitrary unitary transformation

In the preceding section we have studied particular unitary transformations between the Schrödinger, Heisenberg, and interaction pictures. Let us now have a look at *arbitrary* unitary transformations.

We have seen that the unitary transformation,

$$|\psi_U\rangle = U^\dagger|\psi\rangle \quad , \quad \hat{A}_U = U^\dagger\hat{A}U \quad , \quad (2.149)$$

leaves the physics of a system unchanged. The question is now, how the Schrödinger equation,

$$\hat{H}|\psi\rangle = i\hbar\frac{d}{dt}|\psi\rangle \quad (2.150)$$

transforms into the new system, that is, what will the Hamiltonian  $\hat{H}'$  look like in the transformed equation,

$$\hat{H}'|\psi_U\rangle \stackrel{?}{=} i\hbar\frac{d}{dt}|\psi_U\rangle \quad . \quad (2.151)$$

We calculate,

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi_U\rangle &= i\hbar U^\dagger\frac{d}{dt}|\psi\rangle + i\hbar\dot{U}^\dagger|\psi\rangle = (U^\dagger\hat{H} + i\hbar\dot{U}^\dagger)|\psi\rangle \\ &= (U^\dagger\hat{H} + i\hbar\dot{U}^\dagger)U|\psi_U\rangle = (U^\dagger\hat{H}U + i\hbar\dot{U}^\dagger U)|\psi_U\rangle = \hat{H}'|\psi_U\rangle \quad . \end{aligned} \quad (2.152)$$

Hence,

$$\boxed{\hat{H}' = U^\dagger\hat{H}U + i\hbar\dot{U}^\dagger U} \quad . \quad (2.153)$$

We will apply this concept in Exc. 2.4.7.4 to a particle in the field of gravity.

**Example 13 (Interaction picture):** The above derivation is general and holds for any unitary transformation. We will now apply it to transform the Hamiltonian  $\hat{H} = \hat{H}_0 + \hat{V}(t)$  into the interaction picture via the transformation  $U = e^{-(i/\hbar)\hat{H}_0 t}$ . From

$$\dot{U}^\dagger = \frac{i}{\hbar}\hat{H}_0 e^{(i/\hbar)\hat{H}_0 t} = \frac{i}{\hbar}\hat{H}_0 U^\dagger \quad (2.154)$$

we calculate,

$$\begin{aligned} \hat{H}' &= U^\dagger\hat{H}U + i\hbar\dot{U}^\dagger U = U^\dagger\left[\hat{H}_0 + \hat{V}(t)\right]U + i\hbar\frac{i}{\hbar}\hat{H}_0 U^\dagger U \\ &= U^\dagger\left[\hat{H}_0 + \hat{V}(t)\right]U - \hat{H}_0 = U^\dagger\hat{V}(t)U \quad , \end{aligned} \quad (2.155)$$

which confirms the validity of the Schrödinger equation (2.140) in the interaction picture, provided the Hamiltonian is taken to be the perturbation part  $\hat{V}(t)$ , only. In the Heisenberg picture  $\hat{V}(t) = 0$ , such that,

$$\hat{H}' = 0 \quad . \quad (2.156)$$

### 2.4.6 Ehrenfest's theorem

For linear operators satisfying  $[\hat{A}, \hat{B}] = \imath$  we can give a generalization of the commutation relation:

$$\boxed{[\hat{A}, F(\hat{A}, \hat{B})] = \imath \frac{\delta F(\hat{A}, \hat{B})}{\delta \hat{B}}}. \quad (2.157)$$

This can be verified by a Taylor expansion of  $F(\hat{A}, \hat{B})$  by  $\hat{B}$  around  $\hat{B} = 0$ , as will be shown in Exc. 2.4.7.6. An immediate consequence of  $[\hat{p}, \hat{r}] = -\imath\hbar$  is,

$$[\hat{p}, F(\hat{r})] = -\imath\hbar \frac{\delta F(\hat{r})}{\delta \hat{r}}. \quad (2.158)$$

The momentum observable is not singularly defined by the commutation relation, because each unitarily transformed operator satisfies the relation as well. We can expand a unitarily equivalent momentum as  $\tilde{p} = UpU^\dagger = e^{\imath F(r)}pe^{-\imath F(r)} = p + \imath[F(r), p] + \frac{\imath^2}{2!}[F(r), [F(r), p]] + \dots$  using the relation (2.158).

The observables in the Heisenberg picture follow the same equations of motion as the corresponding classical quantities. This *correspondence principle* is called *Ehrenfest theorem*. For example, when working with position and momentum variables  $[\hat{r}, \hat{k}] = \imath$  and  $\hat{H} = \frac{\hbar^2}{2m}\hat{k}^2 + V(\hat{r})$ , we obtain,

$$[\hat{r}, \hat{H}] = \imath\hbar \frac{\delta \hat{H}}{\delta \hat{p}} \quad \text{and} \quad [\hat{p}, \hat{H}] = -\imath\hbar \frac{\delta \hat{H}}{\delta \hat{r}}, \quad (2.159)$$

and using the Heisenberg equation (2.136),

$$\dot{\hat{r}} = \frac{\delta \hat{H}}{\delta \hat{p}} \quad \text{and} \quad \dot{\hat{p}} = -\frac{\delta \hat{H}}{\delta \hat{r}}. \quad (2.160)$$

We will demonstrate this in Exc. 2.4.7.7 for the case of a harmonic potential.

In the Schrödinger picture the equation of motion for the eigenvalues of the observables takes the form,

$$\frac{d}{dt}\langle \hat{A}_S \rangle = \langle \partial_t \psi | \hat{A}_S | \psi \rangle + \langle \psi | \partial_t \hat{A}_S | \psi \rangle + \langle \psi | \hat{A}_S | \partial_t \psi \rangle = \frac{\partial}{\partial t}\langle \hat{A}_S \rangle + \frac{\imath}{\hbar}\langle [\hat{H}, \hat{A}_S] \rangle. \quad (2.161)$$

The eigenvalues behave as Heisenberg observables in Eq. (2.135), that is, they follow the laws of Hamilton's and Newton's mechanics.

The important result now is that the equations that govern the eigenvalues of the observables are identical in the both pictures, since from the Heisenberg picture we obtain with Eq. (2.135),

$$\frac{d}{dt}\langle \hat{A}_H \rangle = \frac{\partial}{\partial t}\langle \hat{A}_H \rangle + \frac{\imath}{\hbar}\langle [\hat{H}, \hat{A}_H] \rangle.$$

### 2.4.7 Exercises

**2.4.7.1 Ex: Coupled two-level atom**

Calculate the time evolution of an atom with two levels coupled by a light field using the Hamiltonian,

$$\hat{H} = \begin{pmatrix} 0 & \frac{1}{2}\hbar\Omega \\ \frac{1}{2}\hbar\Omega & -\hbar\Delta \end{pmatrix},$$

where  $\Delta = \omega - \omega_0$  is the detuning between the frequency of the light and the frequency of the transition and  $\Omega$  the Rabi frequency. **Help:** Determine the matrix of the eigenvalues  $\hat{E}$  and the unitary transformation  $U$  given by  $U^\dagger \hat{H} U = \hat{E}$  and use the formal solution of the Schrödinger equation:  $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi_0\rangle = e^{-iU^\dagger \hat{E} U t/\hbar}|\psi_0\rangle = U^\dagger e^{-i\hat{E}t/\hbar} U |\psi_0\rangle$ <sup>13</sup>.

**2.4.7.2 Ex: Commutator in Schrödinger's and Heisenberg's picture**

Show that operators which commute with the Hamiltonian in the Schrödinger picture also do it in the Heisenberg picture. Use the rule  $[\hat{H}, \hat{A}\hat{B}] = \hat{A}[\hat{H}, \hat{B}] + [\hat{H}, \hat{A}]\hat{B}$ .

**2.4.7.3 Ex: Motion in Heisenberg's picture**

Consider the Hamiltonian  $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2 \hat{r}^2$ . Using the relation  $[\hat{p}, \hat{r}] = -i\hbar$  calculate in the Heisenberg picture the equations of motion for the observables  $\hat{p}$ ,  $\hat{r}$ , and  $\hat{p}\hat{r}$ .

**2.4.7.4 Ex: Particle in a homogenous gravitational field**

- Consider a particle free to move along the axis of gravity. Derive the time-dependent unitary operator describing the transformation into the particle's rest frame and check, whether the transformation satisfies the expression (2.153).
- Solve the Schrödinger equation and derive the Heisenberg equations for  $\hat{x}$  and  $\hat{p}$ .
- Calculate the phase shift due to gravity from the solution of the Schrödinger equation.

**2.4.7.5 Ex: Phase shift in a Ramsey-Bordé interferometer**

- Calculate the dynamical phase accumulated by an atom in the field of gravity as a function of its initial momentum.
- Derive the phase difference of a particle wavefunction passing through a *Ramsey-Bordé interferometer*<sup>14</sup>.

**2.4.7.6 Ex: Commutator of a function of operators**

Prove the relationship (2.157).

<sup>13</sup>The MATLAB code for calculating time evolution (QM\_Fundamentals\_Evolucao.m) can be found on the web page of this course.

<sup>14</sup>A Ramsey-Bordé interferometer consists of a  $\pi/2 - \pi - \pi/2$  pulse sequence (similar to photon echo in NMR) of Bragg diffraction pulses leading to a splitting and recombination of an atomic wavefunction in momentum space. Every pulse transfers one unit of photonic recoil to the atomic center-of-mass.

### 2.4.7.7 Ex: Ehrenfest's theorem

Compare the equations of Ehrenfest's theorem with those of Hamilton-Jacobi for a classical particle subject to a time-independent potential. Discuss the classical limit, that is, when the Hamilton-Jacobi equations approach those of Ehrenfest.

## 2.5 Symmetries in quantum mechanics

We already saw in Sec. 2.3.4 that, beyond observables, there is another category of operators that does not correspond to measurable physical quantities, but is very useful in the quantum formalism. These are the *unitary transformations*. In this section we will encounter some interesting examples.

### 2.5.1 Translation and rotation

#### 2.5.1.1 Temporal translation operator

The temporal evolution of a system is described by the Schrödinger equation whose formal solution can be written as follows,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle . \quad (2.162)$$

With this we can define an *evolution operator* or temporal translation,

$$\boxed{U_{tp}(\tau) \equiv e^{-i\hat{H}\tau/\hbar} \quad \text{such that} \quad U_{tp}(\tau)|\psi(t)\rangle = |\psi(t + \tau)\rangle} . \quad (2.163)$$

The temporal evolution has already been discussed extensively in Sec. 2.4.

#### 2.5.1.2 Spatial translation operator

In this section we look for a unitary *translation operator*,

$$\mathcal{T}_{tr}\mathbf{r} \equiv \mathbf{a} + \mathbf{r} . \quad (2.164)$$

Before this, we need to derive the following calculation rule for commutators, which will be done in Exc. 2.5.5.1:

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \dots . \quad (2.165)$$

Applying this formula to the two operators  $\hat{\mathbf{p}}$  and  $\hat{\mathbf{r}}$  related by the commutation rule (2.50), we obtain,

$$e^{(i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}}\hat{\mathbf{r}}e^{(-i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}} = \hat{\mathbf{r}} + [(i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}, \hat{\mathbf{r}}] + \frac{1}{2!}[(i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}, \mathbf{a}\cdot\hat{\mathbf{p}}] + \dots = \hat{\mathbf{r}} + \mathbf{a} . \quad (2.166)$$

That is, the operator

$$\boxed{U_{tr}(\mathbf{a}) \equiv e^{(-i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}}} \quad (2.167)$$

performs a spatial translation of the position operator. The operator is unitary,

$$U_{tr}(\mathbf{a})^{-1} = U_{tr}(\mathbf{a})^\dagger , \quad (2.168)$$

and forms a group since  $U_{tr}(\mathbf{a})U_{tr}(\mathbf{b}) = U_{tr}(\mathbf{a} + \mathbf{b})$ . Summarizing the impact of the translation on the operators of space,

$$\boxed{U_{tr}^\dagger(\mathbf{a})\hat{\mathbf{r}}U_{tr}(\mathbf{a}) = \hat{\mathbf{r}} + \mathbf{a} \quad , \quad U_{tr}^\dagger(\mathbf{a})\hat{\mathbf{p}}U_{tr}(\mathbf{a}) = \hat{\mathbf{p}}} \quad , \quad (2.169)$$

where the second relation is obvious.

To demonstrate how the translation acts on a state, let us calculate,

$$\hat{\mathbf{r}}e^{(-i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}}|r\rangle = e^{(-i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}}(\hat{\mathbf{r}} + \mathbf{a})|r\rangle = (\mathbf{r} + \mathbf{a})e^{(-i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}}|r\rangle . \quad (2.170)$$

Hence,

$$\boxed{U_{tr}(\mathbf{a})|r\rangle = e^{(-i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}}|r\rangle = |\mathbf{r} + \mathbf{a}\rangle} . \quad (2.171)$$

Therefore, if a particle is in an eigenstate  $|r\rangle$  of the position operator (i.e. located exactly at the position  $\mathbf{r}$ ), then after  $U_{tr}(\mathbf{a})$  acts on it, the particle is at the position  $\mathbf{r} + \mathbf{a}$ : The translation operator  $U_{tr}(\mathbf{a})$  hence moves particles and fields by the distance  $\mathbf{a}$ .

Finally, we want to describe, how the translation operator acts on an arbitrary state  $|\psi\rangle$  represented in position-space, remembering that the position-space wavefunction is obtained via  $\psi(\mathbf{r}) \equiv \langle\mathbf{r}|\psi\rangle$ , as already mentioned in Sec. 2.3.7. We get,

$$\psi'(\mathbf{r}) \equiv \mathcal{T}_{tr}\psi(\mathbf{r}) \equiv \langle\mathbf{r}|U_{tr}(\mathbf{a})|\psi\rangle = \langle U_{tr}^\dagger(\mathbf{a})\mathbf{r}|\psi\rangle = \langle\mathbf{r} - \mathbf{a}|\psi\rangle = \psi(\mathbf{r} - \mathbf{a}) . \quad (2.172)$$

This relation is easier to remember as  $\psi'(\mathbf{r} + \mathbf{a}) = \psi(\mathbf{r})$ , which can be read as: *The value of the new wavefunction at the new point equals the value of the old wavefunction at the old point.*

**Example 14 (Translation of spatial wavefunctions):** Here is an example showing that these two descriptions (2.171) and (2.172) are equivalent. The state  $|\mathbf{x}\rangle$  corresponds to the wavefunction  $\psi(\mathbf{r}) = \delta^3(\mathbf{r} - \mathbf{x})$ , while the state  $U_{tr}(\mathbf{a})|\mathbf{x}\rangle = |\mathbf{x} + \mathbf{a}\rangle$  corresponds to the wavefunction  $\psi'(\mathbf{r}) = \delta^3(\mathbf{r} - (\mathbf{x} + \mathbf{a}))$ . These indeed satisfy  $\psi'(\mathbf{r}) = \psi(\mathbf{r} - \mathbf{a})$ .

Comparing the expansion of the translation operator,

$$\langle\mathbf{r}|U_{tr}(\mathbf{a})|\psi\rangle = \langle e^{(i/\hbar)\mathbf{a}\cdot\hat{\mathbf{p}}}\mathbf{r}|\psi\rangle = \left(1 + \frac{i}{\hbar}\mathbf{a}\cdot\hat{\mathbf{p}} - \frac{1}{\hbar^2}\frac{(\mathbf{a}\cdot\hat{\mathbf{p}})^2}{2!} + \dots\right)\langle\mathbf{r}|\psi\rangle , \quad (2.173)$$

with the Taylor expansion of the wavefunction,

$$\langle\mathbf{r} + \mathbf{a}|\psi\rangle = \psi(\mathbf{r} + \mathbf{a}) = \left(1 + \mathbf{a}\cdot\nabla + \frac{(\mathbf{a}\cdot\nabla)^2}{2!} + \dots\right)\psi(\mathbf{r}) . \quad (2.174)$$

we obtain

$$\hat{\mathbf{p}}|\mathbf{r}\rangle = \frac{\hbar}{i}\nabla|\mathbf{r}\rangle . \quad (2.175)$$

Finally, we note that the momentum operator can be defined via the translation operator,

$$\hat{\mathbf{p}} = i\hbar\nabla_{\mathbf{a}}U_{tr}(\mathbf{a})|_{\mathbf{a}=\mathbf{0}} . \quad (2.176)$$



### 2.5.1.3 Rotation operator

In this section we look for the unitary transformation corresponding to the *rotation operator* [678],

$$\mathcal{T}_{rt}\mathbf{r} \equiv e^{\vec{\alpha} \times \mathbf{r}}. \quad (2.177)$$

We calculate,

$$\begin{aligned} e^{\vec{\alpha} \times \mathbf{r}} &= \sum_n \frac{(\vec{\alpha} \times)^n}{n!} \mathbf{r} = \mathbf{r} + \vec{\alpha} \times \mathbf{r} + \frac{1}{2} \vec{\alpha} \times (\vec{\alpha} \times \mathbf{r}) + \dots \\ &= \hat{\mathbf{e}}_\alpha (\hat{\mathbf{e}}_\alpha \cdot \mathbf{r}) + \hat{\mathbf{e}}_\alpha \times \mathbf{r} \sin \alpha - \hat{\mathbf{e}}_\alpha \times (\hat{\mathbf{e}}_\alpha \times \mathbf{r}) \cos \alpha, \end{aligned} \quad (2.178)$$

as we will see in Exc. 2.5.5.2. We define the unitary rotational transformation by,

$$\boxed{U_{rt}^\dagger(\vec{\alpha}) \hat{\mathbf{r}} U_{rt}(\vec{\alpha}) = e^{\vec{\alpha} \times \hat{\mathbf{r}}} \quad , \quad U_{rt}(\vec{\alpha}) |\mathbf{r}\rangle = |e^{\vec{\alpha} \times \mathbf{r}}\rangle}. \quad (2.179)$$

To derive the explicit form of the rotation operator, we consider two rotations about the same axis  $\vec{\alpha} = \lambda_1 \hat{\mathbf{e}}_\alpha + \lambda_2 \hat{\mathbf{e}}_\alpha$ , such that

$$U_{rt}(\lambda_1 \hat{\mathbf{e}}_\alpha) U_{rt}(\lambda_2 \hat{\mathbf{e}}_\alpha) = U_{rt}(\lambda_1 \hat{\mathbf{e}}_\alpha + \lambda_2 \hat{\mathbf{e}}_\alpha). \quad (2.180)$$

Calculating the derivative of this equation by  $\lambda_1$  and then setting  $\lambda_1 = 0$ , we have,

$$\begin{aligned} \Rightarrow \quad \frac{d\lambda_1 \hat{\mathbf{e}}_\alpha}{d\lambda_1} \Big|_{\lambda_1=0} \cdot \nabla_{\vec{\alpha}} U_{rt}(\vec{\alpha}) \Big|_{\vec{\alpha}=0} U_{rt}(\lambda_2 \hat{\mathbf{e}}_\alpha) &= \frac{dU_{rt}(\lambda_1 \hat{\mathbf{e}}_\alpha + \lambda_2 \hat{\mathbf{e}}_\alpha)}{d(\lambda_1 + \lambda_2)} \Big|_{\lambda_1=0} \frac{d(\lambda_1 + \lambda_2)}{d\lambda_1} \Big|_{\lambda_1=0} \\ \Rightarrow \quad \hat{\mathbf{e}}_\alpha \cdot \frac{\hat{\mathbf{L}}}{i\hbar} U_{rt}(\lambda_2 \hat{\mathbf{e}}_\alpha) &= \frac{dU_{rt}(\lambda_2 \hat{\mathbf{e}}_\alpha)}{d\lambda_2} \end{aligned} \quad (2.181)$$

where we define the angular momentum operator,

$$\hat{\mathbf{L}} \equiv i\hbar \nabla_{\vec{\alpha}} U_{rt}(\vec{\alpha}) \Big|_{\vec{\alpha}=0}. \quad (2.182)$$

The solution of the last differential equation (2.181) is, with  $\lambda_2 \hat{\mathbf{e}}_\alpha = \vec{\alpha} \Big|_{\lambda_1=0}$ ,

$$\boxed{U_{rt}(\vec{\alpha}) = e^{(-i/\hbar) \mathbf{L} \cdot \vec{\alpha}}}. \quad (2.183)$$

The explicit form of  $\mathbf{L}$  follows from its action on a state  $|\psi\rangle$  projected into position space. In analogy with the derivation of the result (2.175), comparing the expansion of the operator (2.183),

$$\langle \mathbf{r} | U_{rt}(\vec{\alpha}) | \psi \rangle = \langle e^{(i/\hbar) \vec{\alpha} \cdot \mathbf{L}} \mathbf{r} | \psi \rangle = \left( 1 + \frac{i}{\hbar} \vec{\alpha} \cdot \mathbf{L} + \dots \right) \langle \mathbf{r} | \psi \rangle, \quad (2.184)$$

with the Taylor expansion of the wavefunction,

$$\langle e^{\vec{\alpha} \times \mathbf{r}} \mathbf{r} | \psi \rangle = \psi(\mathbf{r} + \vec{\alpha} \times \mathbf{r} + \dots) = [1 + (\vec{\alpha} \times \mathbf{r}) \cdot \nabla_{\mathbf{r}} + \dots] \psi(\mathbf{r}), \quad (2.185)$$

we find,

$$\frac{i}{\hbar} \vec{\alpha} \cdot \mathbf{L} = (\vec{\alpha} \times \mathbf{r}) \cdot \nabla_{\mathbf{r}} = \vec{\alpha} \cdot (\mathbf{r} \times \nabla_{\mathbf{r}} = \frac{i}{\hbar} \vec{\alpha} \cdot (\mathbf{r} \times \hat{\mathbf{p}}), \quad (2.186)$$

that is,

$$\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}. \quad (2.187)$$

Therefore, the observable  $\hat{\mathbf{L}}$  is the *orbital angular momentum* of the particle producing the rotations.

### 2.5.2 Kick operator, Galilei and Lorentz boosts

The *Galilei transform* (or *Galilei boost*) is defined by,

$$\mathcal{T}_{\mathbf{v}}\mathbf{r} = \mathbf{r} + \mathbf{v}t \quad \text{and} \quad \mathcal{T}_{\mathbf{v}}\mathbf{p} = \mathbf{p} + m\mathbf{v} . \quad (2.188)$$

It describes the transformation of a system into a moving frame. Obviously, the Galilei transform must satisfy  $\mathcal{T}_{\mathbf{v}_1}\mathcal{T}_{\mathbf{v}_2} = \mathcal{T}_{\mathbf{v}_1+\mathbf{v}_2}$ , while this certainly does not hold for relativistic velocities. We derive the expression for the operator of this transformation from its actions on the position and momentum states. For the position we have with (2.167),

$$U_G(\mathbf{v})|\mathbf{r}\rangle \propto e^{(-i/\hbar)\hat{\mathbf{p}}\cdot\mathbf{v}t}|\mathbf{r}\rangle = |\mathbf{r} + \mathbf{v}t\rangle . \quad (2.189)$$

For the momentum we can proceed analogously,

$$U_G(\mathbf{v})|\mathbf{p}\rangle \propto e^{(i/\hbar)\hat{\mathbf{r}}\cdot\mathbf{v}m}|\mathbf{p}\rangle = |\mathbf{p} + m\mathbf{v}\rangle . \quad (2.190)$$

This is the prescription for the so-called *kick operator*, which will play a prominent role in the discussion of photonic recoil (see 3.6.2).

By defining

$$\hat{\mathbf{G}} = \hat{\mathbf{p}}t - \hat{\mathbf{r}}m = i\hbar\nabla_{\mathbf{v}}U_G(\mathbf{v})|_{\mathbf{v}=0} , \quad (2.191)$$

the unitary transformation

$$U_G(\mathbf{v}) = e^{(-i/\hbar)\mathbf{v}\cdot\hat{\mathbf{G}}} \quad (2.192)$$

meets the requirements (2.189) and (2.190)<sup>15</sup>. We just need to check,

$$e^{(i/\hbar)\mathbf{v}\cdot\hat{\mathbf{r}}m}|\mathbf{r}\rangle = e^{(i/\hbar)\mathbf{v}\cdot\hat{\mathbf{r}}m} \int_{\mathbb{R}^3} |\mathbf{p}\rangle\langle\mathbf{p}|\mathbf{r}\rangle d^3p = \frac{1}{h^{3/2}} \int_{\mathbb{R}^3} |\mathbf{p}\rangle e^{-(i/\hbar)\mathbf{r}\cdot(\mathbf{p}-\mathbf{v}m)} d^3p = |\mathbf{r}\rangle \quad (2.193)$$

and analogously,

$$e^{(-i/\hbar)\mathbf{v}\cdot\hat{\mathbf{p}}t}|\mathbf{p}\rangle = e^{(-i/\hbar)\mathbf{v}\cdot\hat{\mathbf{p}}t} \int_{\mathbb{R}^3} |\mathbf{r}\rangle\langle\mathbf{r}|\mathbf{p}\rangle d^3p = \frac{1}{h^{3/2}} \int_{\mathbb{R}^3} |\mathbf{r}\rangle e^{(i/\hbar)\mathbf{p}\cdot(\mathbf{r}-\mathbf{p}t)} d^3p = |\mathbf{p}\rangle . \quad (2.194)$$

With the commutator of  $\hat{\mathbf{p}}$  and  $\hat{\mathbf{r}}$  we derive,

$$[\mathbf{G} \cdot \mathbf{a}, \mathbf{G} \cdot \mathbf{b}] = 0 , \quad (2.195)$$

for any vectors  $\mathbf{a}$  and  $\mathbf{b}$ , and with that, using the Baker-Hausdorff formula (3.108), we verify,

$$U_G(\mathbf{v}_1)U_G(\mathbf{v}_2) = e^{(-i/\hbar)(\mathbf{v}_1+\mathbf{v}_2)\cdot\mathbf{G} - [\mathbf{v}_1\cdot\mathbf{G}, \mathbf{v}_2\cdot\mathbf{G}]/2\hbar^2} = U_G(\mathbf{v}_1 + \mathbf{v}_2) . \quad (2.196)$$

Obviously, for very high velocities, the Galilei-boost should be replaced by the *Lorentz transform* (or *Lorentz boost*) [361]. Here, we only note, that the additivity of velocities expressed by equation (2.195) does not hold for non-collinear relativistic velocities<sup>16</sup>.

<sup>15</sup>We need to keep in mind that, following Glauber's rule,  $e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}+[\hat{A},\hat{B}]/2}$  with  $\hat{A} \equiv \mathbf{v} \cdot \hat{\mathbf{p}}t$  and  $\hat{B} \equiv \mathbf{v} \cdot \hat{\mathbf{r}}m$ . However, the commutator  $[\mathbf{v} \cdot \hat{\mathbf{p}}t, \mathbf{v} \cdot \hat{\mathbf{r}}m] = -i\hbar m t \mathbf{v}^2$  is independent of  $\hat{\mathbf{p}}$  and  $\hat{\mathbf{r}}$ , such that it only contributes an unimportant phase.

<sup>16</sup>See script on *Electrodynamics* (2020).

### 2.5.3 Gauge transformations

We learn in electrodynamics <sup>17</sup>, that the motion of a particle carrying the charge  $q$  and interacting with an electrical potential  $\Phi(\mathbf{r}, t)$  and a magnetic vector potential  $\mathbf{A}(\mathbf{r}, t)$  is governed by the electric and the magnetic field,

$$\vec{\mathcal{E}}(\mathbf{r}, t) = -\nabla\Phi - \partial_t\mathbf{A} \quad \text{and} \quad \vec{\mathcal{B}}(\mathbf{r}, t) = \nabla \times \mathbf{A} . \quad (2.197)$$

Also, we know that the fields are invariant under the substitution,

$$\Phi \rightarrow \Phi' \equiv \Phi - \partial_t\chi \quad \text{and} \quad \mathbf{A} \rightarrow \mathbf{A}' \equiv \mathbf{A} + \nabla\chi , \quad (2.198)$$

where  $\chi(\mathbf{r}, t)$  is a scalar field called *gauge field*.

In quantum mechanics the *gauge transformation* defined by,

$$\boxed{U_{gg}(\chi) = e^{-iq\chi(\mathbf{r}, t)/\hbar}} \quad (2.199)$$

obviously must keep the Schrödinger equation invariant. Transforming operators and wave functions as,

$$\hat{H} \rightarrow U_{gg}\hat{H}U_{gg}^{-1} \equiv \hat{H}_U \quad \text{and} \quad |\psi\rangle \rightarrow U_{gg}|\psi\rangle \equiv |\psi_U\rangle , \quad (2.200)$$

we calculate for the energy,

$$\begin{aligned} \hat{H}_U|\psi_U\rangle &= U_{gg}i\hbar\frac{d}{dt}U_{gg}^{-1}|\psi_U\rangle = U_{gg}i\hbar U_{gg}^{-1}\frac{d}{dt}|\psi_U\rangle + U_{gg}i\hbar\left(\frac{-iq}{\hbar}U_{gg}^{-1}\frac{d\chi}{dt}\right)|\psi_U\rangle \\ &= i\hbar\left(\frac{d}{dt} - \frac{iq}{\hbar}\frac{d\chi}{dt}\right)|\psi_U\rangle , \end{aligned} \quad (2.201)$$

in accordance with the transformation rule (2.153) for time-dependent unitary transformations. For the momentum, we get analogously,

$$\begin{aligned} \hat{\mathbf{p}}_U|\psi_U\rangle &= U_{gg}(-i\hbar\nabla)U_{gg}^{-1}|\psi_U\rangle = U_{gg}(-i\hbar)U_{gg}^{-1}(\nabla|\psi_U\rangle) + U_{gg}(-i\hbar)\left(\frac{-iq}{\hbar}U_{gg}^{-1}\nabla\chi\right)|\psi_U\rangle \\ &= (-i\hbar)\left[\nabla - \frac{iq}{\hbar}(\nabla\chi)\right]|\psi_U\rangle , \end{aligned} \quad (2.202)$$

This corresponds to the substitutions <sup>18</sup>,

$$\boxed{U_{gg}i\hbar\frac{d}{dt}U_{gg}^{-1} = i\hbar\frac{d}{dt} + q\frac{d\chi}{dt} \quad \text{and} \quad U_{gg}\hat{\mathbf{p}}U_{gg}^{-1} = \hat{\mathbf{p}} - q\nabla\chi} . \quad (2.203)$$

This shows that the gauge transformation applies to the *minimal coupling* rule,

$$\hat{H} = \hat{H}_{kin} + q\Phi \xrightarrow{U_{gg}} \hat{H}_{kin} + q\Phi + q\partial_t\chi \quad \text{and} \quad m\mathbf{v} = \mathbf{p} - q\mathbf{A} \xrightarrow{U_{gg}} \mathbf{p} - q\mathbf{A} - q\nabla\chi , \quad (2.204)$$

confirming the rules (2.198). That is, the Hamiltonian of a particle carrying the charge  $q$  and interacting with an electric potential  $\Phi$  and a magnetic vector potential  $\mathbf{A}$  is,

$$\hat{H} = \frac{1}{2m}(\mathbf{p} - q\mathbf{A} - q\nabla\chi)^2 + q\Phi + q\partial_t\chi . \quad (2.205)$$

<sup>17</sup>See script on *Electrodynamics* (2020).

<sup>18</sup>In quadrivetorial notation  $i\hbar\partial_\mu \rightarrow i\hbar\partial_\mu + q\partial_\mu\chi$ .

### 2.5.4 Noether's theorem and conservation laws

The fundamental laws of physics are often expressed as symmetries. The knowledge of symmetries allows the characterization of a system and its behavior without the need to know its details. We can often deduce the differential equation of motion from the symmetries. The fundamental symmetries define the fundamental laws of physics. Following *Noether's theorem* each symmetry corresponds to a conserved quantity, that is, a quantities that remains invariant for all time. The invariance of a system under symmetry transformation represents a *conservation law*. For example, the homogeneity of space corresponds to the conservation of linear momentum.

In quantum mechanics, a *symmetry transformation* is defined by,

$$|\psi\rangle \longrightarrow U|\psi\rangle \quad \text{and} \quad \hat{Q} \longrightarrow U\hat{Q}U^\dagger . \quad (2.206)$$

Therefore, to find a conservation law, i.e., an invariable observable (also called *constant of motion*), we must verify that the observable and the transformed wavefunctions simultaneously satisfy the same fundamental equations (that is, Schrödinger's or Heisenberg's equation) as the original observable and wavefunctions. For example, if the wavefunction  $|\psi\rangle$  satisfies the Schrödinger equation, the wave function  $U|\psi\rangle$  must do this too,

$$\hat{H}U|\psi\rangle \stackrel{!}{=} i\hbar \frac{d}{dt}U|\psi\rangle = i\hbar \frac{dU}{dt}|\psi\rangle + i\hbar U \frac{d}{dt}|\psi\rangle = i\hbar \frac{dU}{dt}|\psi\rangle + U\hat{H}|\psi\rangle . \quad (2.207)$$

Consequently, we obtain the relation,

$$[\hat{H}, U] = i\hbar \dot{U} . \quad (2.208)$$

As shown in (2.161) and (2.162), an operator that commutes with the Hamiltonian does not explicitly depend on time, that is, it is *conserved*.

#### 2.5.4.1 Temporal homogeneity

*Temporal homogeneity* means invariance under translation in time by a fixed time interval  $\tau$ , that is, under the unitary temporal transformation,

$$U(\tau) \equiv |\psi(\tau)\rangle\langle\psi(0)| = e^{(i/\hbar)\hat{E}\tau} . \quad (2.209)$$

Since  $\frac{d}{dt}e^{(i/\hbar)\hat{E}\tau} = 0$ , this means  $[e^{(i/\hbar)\hat{E}\tau}, \hat{H}] = 0$ , which implies conservation of energy  $[\hat{E}, \hat{H}] = 0$ . This will be verified in the Exc. 2.5.5.3.

**Example 15 (Homogeneity of time):** We imagine the following mental experiment or *Gedankenexperiment*: We consider two attractive bodies that move away from each other until they reach the perihelia. At this point, before the bodies reapproach, we change the laws, for example, by modifying the force of attraction. As a consequence, when the bodies arrive at the initial point, the total energy is non-zero. Therefore, the conservation of energy indicates that the laws are invariant.

### 2.5.4.2 Temporal isotropy

The fundamental laws of classical physics and quantum mechanics are all symmetrical under *time reversal*. That is, they remain invariant when we change the arrow of time,  $t \rightarrow -t$ .

### 2.5.4.3 Spatial homogeneity

*Spatial homogeneity* means invariance under spatial translation, that is, under the unitary translational transformation,

$$U_{tr}(\mathbf{a}) \equiv \int |\mathbf{r} + \mathbf{a}\rangle \langle \mathbf{r}| d^3r = e^{(-i/\hbar)\hat{\mathbf{p}} \cdot \mathbf{a}} . \quad (2.210)$$

This is equivalent to momentum conservation  $[\hat{\mathbf{p}}, \hat{H}] = 0$ <sup>19</sup>.

**Example 16 (Homogeneity of space):** Ehrenfest's theorem says  $[\hat{\mathbf{p}}, H] = -i\hbar \frac{\partial H}{\partial \hat{\mathbf{p}}}$ . Therefore, the commutator is not zero when there is a potential,  $\hat{H} = \hat{\mathbf{p}}^2/2m + V(\hat{\mathbf{r}})$ . This is obvious, because the potential introduces an energy inhomogeneity to a particle interacting with the potential. However, this does not mean that the space itself is inhomogeneous, because in order to verify the translational invariance of space, we must displace the entire system, that is, the particle together with the potential. For example, if the potential is generated by another particle we must consider the Hamiltonian  $\hat{H} = \hat{\mathbf{p}}_1^2/2m_1 + \hat{\mathbf{p}}_2^2/2m_2 + V(\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2)$ .

### 2.5.4.4 Spatial isotropy

*Spatial isotropy* means invariance under rotation, that is, under rotational unitary transformation,

$$U_{rt}(\phi) \equiv e^{(-i/\hbar)\hat{\mathbf{L}}\phi} . \quad (2.211)$$

This is equivalent to the conservation of angular momentum  $[\hat{\mathbf{L}}, \hat{H}] = 0$ .

### 2.5.4.5 Parity conservation

Besides continuous symmetry transformations there exist discrete transformations. Discrete symmetries are important in elementary particle physics. The *parity conservation* means invariance to spatial reflection:  $\mathbf{r} \rightarrow -\mathbf{r}$ . A parity transformation is

<sup>19</sup>Imagine that the forces attracting two bodies to each other are not equal: Contrary to Newton's third law, body A attracts body B, more than the body B attracts the body A. In that case after a while the two bodies have different momenta. With the unitary transformation  $U_{tr}(\mathbf{a}) = e^{-i\hat{\mathbf{p}} \cdot \mathbf{a}/\hbar} \simeq 1 - i\epsilon \hat{\mathbf{p}} \cdot \mathbf{a}/\hbar + \dots$  we have,

$$U_{tr}H|\psi\rangle = U_{tr}E_\psi|\psi\rangle = E_\psi U|\psi\rangle = H|\psi(\mathbf{r} + \mathbf{a})\rangle =? = H|\psi(\mathbf{r})\rangle .$$

Since,  $[H, \hat{p}] = 0$ , Heisenberg's equation yields,

$$\frac{\partial}{\partial t} \langle \psi | \hat{p} \cdot \mathbf{a} | \psi \rangle = \frac{1}{i\hbar} \langle \psi | [\hat{p} \cdot \mathbf{a}, \hat{H}] | \psi \rangle = 0 .$$

defined by the mirroring of the wavefunction through a point in space, for example  $\mathbf{r} = 0$ ,

$$\hat{P}|\psi(\mathbf{r})\rangle \equiv |\psi(-\mathbf{r})\rangle . \quad (2.212)$$

with

$$\hat{P}^2 = \hat{P} . \quad (2.213)$$

We talk about *even* parity when  $\hat{P}|\psi(\mathbf{r})\rangle = |\psi(\mathbf{r})\rangle$  and *odd* parity when  $\hat{P}|\psi(\mathbf{r})\rangle = -|\psi(\mathbf{r})\rangle$ . See Exc. 2.5.5.4.

### 2.5.4.6 Invariance to the velocity of the inertial system

The *Galilei boost* asks for Galilei invariance regarding the transformation,

$$U_G(\mathbf{v}) \equiv \iint |\mathbf{r} + \mathbf{v}t, \mathbf{p} + m\mathbf{v}\rangle \langle \mathbf{r}, \mathbf{p} | d^3r d^3p , \quad (2.214)$$

that is, the independence of the inertial system on its velocity  $\mathbf{v}$ .

### 2.5.4.7 Charge conservation

Let us consider again the *gauge transform* (2.198). We know that the Lagrangian density in free space is given in terms of the potentials by,

$$\begin{aligned} \mathcal{L}(x^\mu) &= \frac{1}{4\mu_0} F^{\mu\nu} F_{\mu\nu} - A_\mu j^\mu = \frac{\epsilon_0}{2} \vec{\mathcal{E}}^2 - \frac{1}{2\mu_0} \vec{\mathcal{B}}^2 - A_\mu j^\mu \\ &= \frac{\epsilon_0}{2} [\nabla\Phi + \partial_t \mathbf{A}]^2 - \frac{1}{2\mu_0} [\nabla \times \mathbf{A}]^2 - \Phi\rho + \mathbf{A} \cdot \mathbf{j} , \end{aligned} \quad (2.215)$$

and the *action* is simply the fourth-dimensional integral,

$$S = \int \mathcal{L}(x^\mu) dV dt . \quad (2.216)$$

From the Lagrangian formulation, Maxwell's equations can be derived by requiring the action to be minimal,  $\delta S = 0$ , which yields the Euler-Lagrange equations. As the field equations do not change under gauge transformation, this implies that the action is also unchanged.

To find the relation with *charge conservation*, we simply have to compare the actions in different gauges. First, we express the Lagrangian transformed into the old gauge,

$$\begin{aligned} \mathcal{L}'(x^\mu) &= \frac{\epsilon_0}{2} \{ \nabla[\Phi - \partial_t \chi] + \partial_t[\mathbf{A} + \nabla\chi] \}^2 - \frac{1}{2\mu_0} \{ \nabla \times [\mathbf{A} + \nabla\chi] \}^2 \\ &\quad - [\Phi - \partial_t \chi]\rho + [\mathbf{A} + \nabla\chi] \cdot \mathbf{j} \\ &= \mathcal{L} + (\partial_t \chi)\rho + \nabla\chi \cdot \mathbf{j} . \end{aligned} \quad (2.217)$$

With this result, we can calculate the difference between the actions under gauge transformation and recall, that they can not be different:

$$0 \stackrel{!}{=} S' - S = \int [(\partial_t \chi)\rho + \nabla\chi \cdot \mathbf{j}] dV dt = - \int \chi [\partial_t \rho + \nabla \cdot \mathbf{j}] dV dt , \quad (2.218)$$

using partial integration<sup>20</sup> and choosing volumes so large, that every charge is inside. This is the *continuity equation* derived from the gauge invariance of the action. The calculation really is nothing more than an application of Noether's theorem from which we could have derived directly the continuity equation,  $\partial_\mu j^\mu = 0$ .

In summary, the conservation of charge means invariance with respect to gauge transformations,

$$U_{cl}(\chi) \equiv e^{-iq\chi(\mathbf{r},t)/\hbar}, \quad (2.219)$$

where  $\chi$  is the gauge field. We note that  $q$  and  $\chi$  are conjugated observables. Therefore, if  $[\chi, \hat{H}] = 0$ , then the charge  $q$  is a conserved quantity.

Transformations can be combined. For example, we believe that nowadays all laws are invariant with respect to CPT transformation, that is, a combination of *charge conjugation*, *parity inversion*, and  *$\theta$ -transform*.

## 2.5.5 Exercises

### 2.5.5.1 Ex: Calculus with commutator

Derive the rule (2.165) via a Taylor expansion of the operator  $\hat{G}(\tau) \equiv e^{\tau\hat{A}}\hat{B}e^{-\tau\hat{A}}$ .

### 2.5.5.2 Ex: Rotation operator

Derive the rule  $e^{\vec{\alpha} \times \mathbf{r}} = \sum_n \frac{(\vec{\alpha} \times)^n}{n!} \mathbf{r} = \hat{\mathbf{e}}_\alpha (\hat{\mathbf{e}}_\alpha \cdot \mathbf{r}) + \hat{\mathbf{e}}_\alpha \times \mathbf{r} \sin \alpha - \hat{\mathbf{e}}_\alpha \times (\hat{\mathbf{e}}_\alpha \times \mathbf{r}) \cos \alpha$ .

### 2.5.5.3 Ex: Constants of motion

Show at the example of energy conservation using the relation (2.208), that energy commutes with the Hamiltonian if  $\dot{E} = 0$ .

### 2.5.5.4 Ex: Parity

Show that the eigenfunctions of the Hamiltonian  $\hat{H} = -(\hbar/2m)(d^2/dx^2) + V(x)$  have well-defined parity, i.e., parity is a *good quantum number* in cases where the energy is an even function of position,  $V(x) = V(-x)$ .

## 2.6 Further reading

Ph.W. Courteille (2020), *Script on Optical spectroscopy: A practical course* [[http](#)]

Ph.W. Courteille (2020), *Script on Electrodynamics: Electricity, magnetism, and radiation* [[http](#)]

Ph.W. Courteille (2020), *Script on Quantum mechanics applied to atomic and molecular physics* [[http](#)]

W.R. Theis, Teubner (1985), *Grundzüge der Quantentheorie* [[ISBN](#)]

<sup>20</sup>Think about the argument, because  $\int \partial_t |\chi| p dt = 0!$

- C. Cohen-Tannoudji, B. Diu, F. Laloe, Wiley Interscience, *Quantum mechanics, vol. 1,2* [\[ISBN\]](#)
- L.I. Schiff, McGraw-Hill Book Company (1968), *Quantum mechanics* [\[ISBN\]](#)
- J.J. Sakurai, J.J. Napolitano, 2<sup>nd</sup> ed. Springer (2011), *Modern Quantum Mechanics* [\[ISBN\]](#)
- H.A. Bethe, R. Jackiw, 3<sup>rd</sup> ed. Taylor & Francis (1997), *Intermediate Quantum Mechanics* [\[ISBN\]](#)
- D.J. Griffiths, *Introduction to Quantum Mechanics* [\[ISBN\]](#)
- Photonics101, *How the Gauge Invariance of the Action implies Charge Conservation* [\[http\]](#)





# Chapter 3

## Linear motion / Separable potentials

In this chapter we will analyze the translational and vibrational motion of a quantum particle. We will give special consideration to the rectangular potential and the harmonic oscillator.

### 3.1 Translational motion

In one dimension the Hamiltonian of a free particle is,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} . \quad (3.1)$$

Therefore, the general solution of the Schrödinger stationary equation,

$$\hat{H}\psi(x) = E\psi(x) , \quad (3.2)$$

is,

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{with} \quad k = \sqrt{\frac{2mE}{\hbar^2}} . \quad (3.3)$$

Note that the  $e^{ikx}$  functions are not quadratically integrable, since  $\int_{-\infty}^{\infty} |e^{ikx}|^2 dx = \int_{-\infty}^{\infty} dx \rightarrow \infty$ . On the other side, they do not represent actual physical systems. In practice, we need to consider wave packets or specify a finite volume for the particle. Note also that the spectrum of eigenvalues is continuous. Do the Exc. [3.1.4.1](#).

#### 3.1.1 Quadratic integrability

To allow for an interpretation as probability density we need to ask for quadratic integrability,

$$\int |\psi|^2 d^3r = 1 . \quad (3.4)$$

This means that the wavefunction can not be infinite inside a finite volume. But it can be infinite within an infinitely small volume. Also, since the Schrödinger equation contains the second derivative by position, the wavefunction must be continuous and have a continuous derivative.

### 3.1.2 Separation of dimensions

Frequently, a 3D potential can be written in the way,

$$V(x, y, z) = V_x(x) + V_y(y) + V_z(z) . \quad (3.5)$$

This is the case, for example, for a rectangular well with  $V_x(x) = V_y(y) = V_z(z) = V_0/3$  inside the well and  $V(x, y, z) = 0$  outside. It also holds for a harmonic potential,

$$V(\mathbf{r}) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) . \quad (3.6)$$

In these cases, the following ansatz for the wavefunction is generally useful,

$$\psi(\mathbf{r}) = \psi_x(x)\psi_y(y)\psi_z(z) , \quad (3.7)$$

since inserting the ansatz into the Schrödinger equation,

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) + V_x(x) + V_y(y) + V_z(z) \right] \psi_x(x)\psi_y(y)\psi_z(z) = E\psi_x(x)\psi_y(y)\psi_z(z) , \quad (3.8)$$

the equation separates into three independent one-dimensional equations,

$$-\frac{\hbar^2}{2m} \frac{\psi_x''(x)}{\psi_x(x)} + V_x(x) = \text{const.} \equiv E_x , \quad (3.9)$$

and the same for  $y$  and  $z$ . Since,  $E = E_x + E_y + E_z$  may have the same value for different combinations of  $E_x$ ,  $E_y$  and  $E_z$ , multidimensional systems are often degenerate.

### 3.1.3 Homogeneous force fields, gravity

The behavior of a wavefunction in a homogeneous force field has been studied in Excs. 2.4.7.4 and 2.4.7.5.

### 3.1.4 Exercises

#### 3.1.4.1 Ex: Trapped particle

Consider the problem of a particle of mass  $m$  forced to move in a single direction and completely confined to a box, with walls placed at the positions  $x = 0$  and  $x = a$ .

- The particle be in the ground state, what is its energy and its wavefunction?
- Suppose the particle has the following wavefunction:

$$\psi_I(x) = \frac{1}{\sqrt{7a}} \left[ 2 \cos\left(\frac{\pi}{2a}(6x - a)\right) - 3i \sin\left(\frac{2\pi}{a}x\right) + \cos\left(\frac{\pi}{2a}(2x - a)\right) \right] ,$$

what is the probability that a measurement of the energy yields the result  $E = \frac{2\pi^2\hbar^2}{ma^2}$ ?

c. Considering again the ground state of item (a), what is the probability distribution for the momentum of the particle in this state?

d. Still starting from the ground state, suppose we remove (instantaneously) the walls,

leaving the particle free ( $\hat{H} = \hat{p}^2/2m$ ). What is the energy of this free particle?

**Formulae:**

$$\int_0^L e^{iBx} \sin\left(\frac{n\pi x}{L}\right) dx = \frac{n\pi L[1 - (-1)^n e^{iBL}]}{n^2\pi^2 - B^2L^2} \quad \text{for } n = 1, 2, 3, \dots$$

$$\int_{-\infty}^{\infty} \frac{x^2}{(1-x^2)^2} \cos^2 \frac{\pi x}{2} dx = \frac{\pi^2}{4}$$

## 3.2 Rectangular potentials

The continuity equation (2.16) teaches us that the probability flux of a moving particle cannot make abrupt changes. That is, even if the particle encounters an obstacle represented by a smooth or abrupt variation of the potential depth, the wavefunction and its derivative must remain continuous, unless the potential step is infinitely high.

### 3.2.1 Box potential

Let us now place the particle into a rectangular potential well, such that the Hamiltonian is,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad \text{with} \quad V(x) = \begin{cases} 0 & \text{for } x \in [0, L] \\ \infty & \text{for } x \notin [0, L] \end{cases}. \quad (3.10)$$

As the potential barriers are high, the walls are hard, that is, the particle, even being a quantum particle, can not penetrate. The wavefunction and the possible energy values are,

$$\boxed{\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad \text{and} \quad E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}}. \quad (3.11)$$

The Exc. 3.2.5.1 asks to demonstrate the result (3.11) illustrated in Fig. 3.1.

Obviously the spectrum of eigenvalues is now discrete. They can be enumerated by an integer  $n$  called *quantum number*. Note that the energy levels are not equidistant.

**Example 17 (Localization energy):** There is a minimal energy  $E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$  which is called *zero point energy* or *localization energy*. This energy can be understood as a consequence of Heisenberg's *uncertainty principle*. We can make the following gross estimation of the zero point energy. Obviously, the particle is localized with an uncertainty lower than  $\Delta x < L$ . Hence,  $\Delta p > \hbar/\Delta x > \hbar/L$ . The average kinetic energy is,

$$\frac{\langle p^2 \rangle}{2m} = \frac{\langle p \rangle^2 + \Delta p^2}{2m} = \frac{\Delta p^2}{2m} > \frac{\hbar^2}{2mL^2}.$$

The fact that the numerical value is different from the value calculated by the formula (3.11) comes from the particular geometry of the box potential.

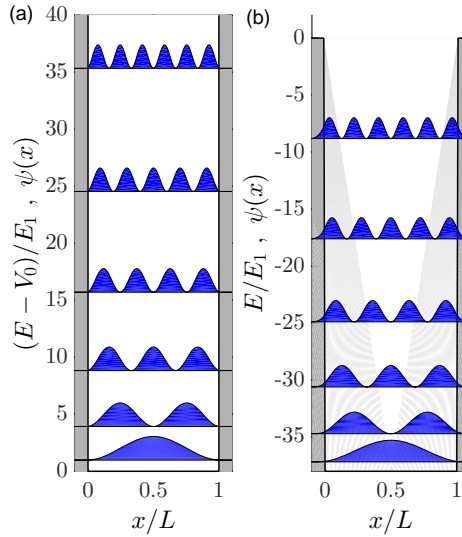


Figure 3.1: (code) (a) Wavefunctions and energies in the box potential. (b) The rectangular potential well with the reference energy set to the height of the well.

### 3.2.2 Multidimensional box potential

In a multidimensional well there can be degeneracy if the well exhibits symmetries. In the case of a 2D quadratic well  $L_x = L_y$ , the eigenenergies are doubly degenerate, since  $E_{n_x, n_y} = E_{n_y, n_x}$ . In the case of a 3D cubic well  $L_x = L_y = L_z$ , the eigenenergies are 6-fold degenerate, because  $E_{n_x, n_y, n_z} = E_{n_y, n_z, n_x} = E_{n_z, n_x, n_y} = E_{n_z, n_y, n_x} = E_{n_y, n_x, n_z} = E_{n_x, n_z, n_y}$ . The states and energies of the 2D well are calculated in Exc. 3.2.5.2.

### 3.2.3 Potentials with several sections of constant depths

To find the global wavefunction in potentials with several sections of constant depths, we solve Schrödinger's equations separately for each section,

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_a \right) \psi_a(x) = E \psi_a(x) . \quad (3.12)$$

The general solution for a section  $a$  with potential energy  $V_a$  is,

$$\boxed{\psi_a(x) = A_a e^{ik_a x} + B_a e^{-ik_a x}} , \quad (3.13)$$

where  $k_a = \frac{1}{\hbar} \sqrt{2m(E - V_a)}$ . If  $E > V_a$ , the wave is propagating.  $k_a$  is the Broglie wavevector of the wave. If  $E < V_a$ , the wave is evanescent. That is, the wave decays within a distance  $\kappa_a = -ik_a$ .

If the particle is confined, that is, if  $E < V(x \rightarrow \pm\infty)$ , the possible energy levels are quantized and the spectrum is discrete.

For every transition between two sections  $a = 1$  and  $a = 2$  we require the boundary conditions,

$$\psi_1(x) = \psi_2(x) \quad \text{and} \quad \psi'_1(x) = \psi'_2(x) . \quad (3.14)$$

Together with the normalization,  $1 = \int_{-\infty}^{\infty} |\psi|^2 dx$ , these conditions are sufficient to determine the wavefunction unambiguously.

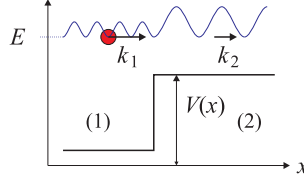


Figure 3.2: Scheme of a potential with several sections of constant depths.

### 3.2.4 Potential well

Consider a particle with energy  $E$  and a potential well of finite depth such that  $V(x) = V_0 < 0$  for  $-L/2 > x > L/2$  and  $V(x) = 0$  otherwise, as illustrated in Fig. 3.3(a). The particle be confined,  $E < 0$ .

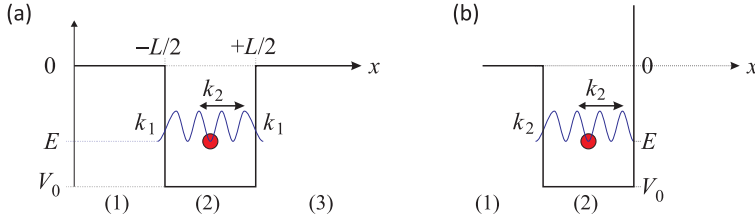


Figure 3.3: (a) Scheme of a two-sided and (b) one-sided potential well.

The wavevectors are

$$k_1 = k_3 = \frac{1}{\hbar} \sqrt{2mE} = \frac{1}{\hbar} \sqrt{2m|E|} = \imath \kappa_1 \quad \text{and} \quad k_2 = \frac{1}{\hbar} \sqrt{2m(E - V_0)} . \quad (3.15)$$

with  $\kappa_1 \in \mathbb{R}^+$ . The boundary conditions yield,

$$\begin{aligned} A_1 e^{-\imath k_1 L/2} + B_1 e^{\imath k_1 L/2} &= A_2 e^{-\imath k_2 L/2} + B_2 e^{\imath k_2 L/2} \\ -\imath k_1 A_1 e^{-\imath k_1 L/2} + \imath k_1 B_1 e^{\imath k_1 L/2} &= -\imath k_2 A_2 e^{-\imath k_2 L/2} + \imath k_2 B_2 e^{\imath k_2 L/2} \\ A_2 e^{\imath k_2 L/2} + B_2 e^{-\imath k_2 L/2} &= A_3 e^{\imath k_1 L/2} + B_3 e^{-\imath k_1 L/2} \\ \imath k_2 A_2 e^{\imath k_2 L/2} - \imath k_2 B_2 e^{-\imath k_2 L/2} &= \imath k_1 A_3 e^{\imath k_1 L/2} - \imath k_1 B_3 e^{-\imath k_1 L/2} . \end{aligned} \quad (3.16)$$

For confined particles,  $E < 0$ , the problem is totally symmetric. In addition, the wavefunction must disappear for  $x \rightarrow \pm\infty$ . Therefore, we can simplify,

$$A_1 = 0 = B_3 \quad \text{and} \quad A_3 = B_1 . \quad (3.17)$$

The first two equations (3.16) now give,

$$B_1 e^{\iota k_1 L/2} = A_2 e^{-\iota k_2 L/2} + B_2 e^{\iota k_2 L/2} = \frac{k_2}{k_1} \left( -A_2 e^{-\iota k_2 L/2} + B_2 e^{\iota k_2 L/2} \right). \quad (3.18)$$

We now consider the quotient  $B_2/A_2$ . Using the right part of equation (3.18),

$$\frac{B_2}{A_2} = \frac{e^{-\iota k_2 L/2} (k_2 + k_1)}{e^{\iota k_2 L/2} (k_2 - k_1)} = \frac{e^{-\iota k_2 L} (k_2 + \iota \kappa_1)^2}{k_2^2 + \kappa_1^2}. \quad (3.19)$$

Since the amplitudes are real, the imaginary part of the quotient (3.19) should disappear, which is the case when,

$$\begin{aligned} 0 &= \text{Im} e^{-\iota k_2 L} (k_2 + \iota \kappa_1)^2 = 2\kappa_1 k_2 \cos k_2 L + (\kappa_1^2 - k_2^2) \sin k_2 L \quad (3.20) \\ \implies \tan k_2 L &= \frac{2\kappa_1 k_2}{-\kappa_1^2 + k_2^2}. \end{aligned}$$

In order to construct graphically the values of the momenta  $k_2$  of the particle associated with the allowed energy levels, we introduce a constant  $\beta \equiv \hbar / (L\sqrt{2m|V_0|})$ . Hence,

$$\tan k_2 L = \tan \frac{1}{\beta} \sqrt{1 - |E/V_0|} = \frac{2\sqrt{|E/V_0|} \sqrt{1 - |E/V_0|}}{1 - 2|E/V_0|} = \frac{2\kappa_1 k_2}{-\kappa_1^2 + k_2^2}. \quad (3.21)$$

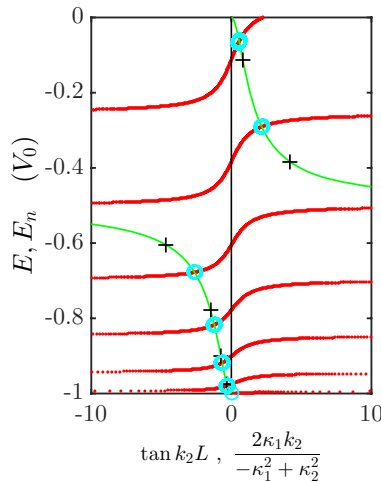


Figure 3.4: (code) Graphical solution for a finite bilateral potential well. The red dotted curves represent the tangents (left side of the equation (3.21)), the solid green curves the hyperbolas (right side of the equation), the circles in cyan are the eigenenergies. When  $0 < E - V_0 \ll E$ , they converge to the eigenenergies of the infinitely deep well (black crosses and vertical black line).

At the bottom of deep potentials, that is, when  $0 < E - V_0 \ll E$ , or equivalently,  $E \simeq V_0$ , we have  $k_2 \ll \kappa_1$  and hence,  $\tan k_2 L \rightarrow 0 \implies k_2 L = n\pi$ . The energies are

then,

$$E - V_0 = \frac{\hbar^2}{k_2^2} 2m = \frac{\hbar^2 \pi^2}{2mL^2} n^2. \quad (3.22)$$

Apply the notions obtained in this section to solve Excs. 3.2.5.3 and 3.2.5.4.

### 3.2.5 Exercises

#### 3.2.5.1 Ex: Particle in a box

Obtain the wavefunctions and associated energy levels of a particle confined in a box, where  $V(x) = 0$  for  $0 \leq x \leq l$  and  $V(x) = \infty$  outside.

#### 3.2.5.2 Ex: Particle in a two-dimensional box

Obtain the wavefunctions and associated energy levels of a particle trapped in a two-dimensional box inside which the particle is confined to a rectangular surface with dimensions  $L_1$  in  $x$ -direction and  $L_2$  in  $y$ -direction,  $V(x, y) = 0$  for  $0 \leq x \leq L_1$  and  $0 \leq y \leq L_2$  and  $V(x, y) = \infty$  else.

#### 3.2.5.3 Ex: Particle in a well

Obtain the energies of the bound states of a particle in the potential well in which  $V(x) = \infty$  for  $x < 0$ ,  $V(x) = -V_0$  for  $0 \leq x \leq L/2$  and  $V(x) = 0$  to  $x > L/2$ . Compare the obtained values with those of the symmetrical well discussed in Sec. 3.2.4 and the well with infinitely high walls discussed in Sec. 3.2.1.

#### 3.2.5.4 Ex: Least bound states and localization energy

Calculate, based on the discussion in Sec. 3.2.4, the minimum required potential depth  $V_0$  of a three-dimensional finite rectangular well potential of size  $L$  to have a bound state capable of trapping an  $^{87}\text{Rb}$  atom. Assuming a trap volume of  $L = 10$  nm, how deep should the trap be?

## 3.3 Potential barrier

The linear momentum of a particle described by  $\psi(x, t) = Ae^{ikx}$  is,

$$\langle \psi | \hat{p} | \psi \rangle = \langle \psi | \frac{\hbar}{i} \frac{d}{dx} | \psi \rangle = \hbar k. \quad (3.23)$$

Therefore, this particle propagates towards  $+\infty$ . On the contrary, the particle  $Be^{-ikx}$  propagates towards  $-\infty$ . Thus, the two solutions (3.13) of the Schrödinger equation (3.12) correspond to propagating particle waves. From here on we will use the letter  $A$  ( $B$ ) to denote the amplitudes of waves propagating in direction  $\infty$  ( $-\infty$ ).

In locations where the potential changes abruptly, the particle can be partially reflected.



### 3.3.1 $\mathcal{T}$ -scattering matrix

As we have already shown in the previous section, we can write the transformation of the amplitudes due to a potential step at position  $L$  as,

$$\begin{aligned} A_2 e^{\imath k_2 L} + B_2 e^{-\imath k_2 L} &= A_1 e^{\imath k_1 L} + B_1 e^{-\imath k_1 L} \\ \imath k_2 A_2 e^{\imath k_2 L} - \imath k_2 B_2 e^{-\imath k_2 L} &= \imath k_1 A_1 e^{\imath k_1 L} - \imath k_1 B_1 e^{-\imath k_1 L} . \end{aligned} \quad (3.24)$$

We can summarize these two equations in a matrix formalism,

$$\boxed{\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}} = \mathcal{T} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \quad (3.25)$$

with the *scattering matrix*  $\mathcal{T}$  for a particle with energy  $E$  (see Fig. 3.2),

$$\begin{aligned} \mathcal{T} &= \frac{1}{2} \begin{pmatrix} \left(1 + \frac{k_1}{k_2}\right) e^{\imath(k_1 - k_2)L} & \left(1 - \frac{k_1}{k_2}\right) e^{\imath(-k_1 - k_2)L} \\ \left(1 - \frac{k_1}{k_2}\right) e^{\imath(k_1 + k_2)L} & \left(1 + \frac{k_1}{k_2}\right) e^{\imath(-k_1 + k_2)L} \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} e^{-\imath k_2 L} & 0 \\ 0 & e^{\imath k_2 L} \end{pmatrix} \begin{pmatrix} 1 + \frac{k_1}{k_2} & 1 - \frac{k_1}{k_2} \\ 1 - \frac{k_1}{k_2} & 1 + \frac{k_1}{k_2} \end{pmatrix} \begin{pmatrix} e^{\imath k_1 L} & 0 \\ 0 & e^{-\imath k_1 L} \end{pmatrix} . \end{aligned} \quad (3.26)$$

If there are more zones with different depths, we may concatenate the scattering matrices. Denoting by  $\mathcal{T}_{m \rightarrow n}$  the scattering matrix describing a transition at position  $L_{m,n}$  of a potential of the depth  $V_m$  to another potential  $V_n$ , we write,

$$\mathcal{T} = \mathcal{T}_{2 \rightarrow 3} \mathcal{T}_{1 \rightarrow 2} . \quad (3.27)$$

### 3.3.2 $\mathcal{S}$ -scattering matrix

Another common definition is the *scattering matrix*  $\mathcal{S}$ ,

$$\boxed{\begin{pmatrix} A_2 \\ B_1 \end{pmatrix}} = \mathcal{S} \begin{pmatrix} B_2 \\ A_1 \end{pmatrix}. \quad (3.28)$$

To see how the scattering matrices are interconnected, we start with

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \mathcal{T} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} \mathcal{T}_{11} A_1 + \mathcal{T}_{12} B_1 \\ \mathcal{T}_{21} A_1 + \mathcal{T}_{22} B_1 \end{pmatrix}, \quad (3.29)$$

Multiplying the first line with  $\mathcal{T}_{22}$  and the second with  $-\mathcal{T}_{12}$  and adding them,

$$\mathcal{T}_{22} A_2 - \mathcal{T}_{12} B_2 = (\mathcal{T}_{11} \mathcal{T}_{22} - \mathcal{T}_{12} \mathcal{T}_{21}) A_1 . \quad (3.30)$$

This equation resolved by  $A_2$  along with the second equation (3.29) resolved by  $B_1$  give,

$$\begin{pmatrix} A_2 \\ B_1 \end{pmatrix} = \mathcal{S} \begin{pmatrix} B_2 \\ A_1 \end{pmatrix} = \begin{pmatrix} \mathcal{T}_{12}/\mathcal{T}_{22} & \mathcal{T}_{11} - \mathcal{T}_{12}\mathcal{T}_{21}/\mathcal{T}_{22} \\ 1/\mathcal{T}_{22} & -\mathcal{T}_{21}/\mathcal{T}_{22} \end{pmatrix} \begin{pmatrix} B_2 \\ A_1 \end{pmatrix}. \quad (3.31)$$

The matrix  $\mathcal{S}$  describes the causality of scattering process more adequately: The amplitude  $A_2$  in region (2) results from the superposition of a wave  $B_2$  being reflected by the barrier and a wave  $A_1$  being transmitted by the barrier. The amplitude  $B_1$  in region (1) results from the superposition of a wave  $A_1$  being reflected by the barrier and a wave  $B_2$  being transmitted by the barrier. Therefore, the matrix  $\mathcal{S}$  is more appropriate for the description of the quantum reflection, as we will discuss in the next section. However, it has the disadvantage that it can not be concatenated in the same way as the  $\mathcal{T}$  matrices.

Unlike the  $\mathcal{T}$  matrix the  $\mathcal{S}$  matrix is *unitary*, since

$$\det \mathcal{S} = \mathcal{S}_{11}\mathcal{S}_{22} - \mathcal{S}_{12}\mathcal{S}_{21} = -\frac{\mathcal{T}_{11}}{\mathcal{T}_{22}} = -e^{2ik_1L}. \quad (3.32)$$

Also, it is possible to show,

$$\mathcal{S}^\dagger \mathcal{S} = \begin{pmatrix} \mathcal{S}_{11}^* & \mathcal{S}_{21}^* \\ \mathcal{S}_{12}^* & \mathcal{S}_{22}^* \end{pmatrix} \begin{pmatrix} \mathcal{S}_{11} & \mathcal{S}_{12} \\ \mathcal{S}_{21} & \mathcal{S}_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (3.33)$$

### 3.3.3 Quantum reflection at a potential step

The *quantum reflection* is a non-classical property of the motion of a particle. An example is the *reflection* of a quantum particle by an *attractive* potential. To study this effect, we consider a plane wave  $e^{ik_1x}$  propagating in region (1) ( $E_1 > V_1$ ) encountering a potential step up or down at position  $x = 0$  leading to another region (2). Using the  $S$  matrix formalism introduced in the previous section,

$$\mathcal{S} = \frac{1}{k_1 + k_2} \begin{pmatrix} k_2 - k_1 & 2k_1 \\ 2k_2 & k_1 - k_2 \end{pmatrix}, \quad (3.34)$$

we find that one part of the wave is reflected into the region (1), another is transmitted into the region (2),

$$\begin{aligned} \begin{pmatrix} A_2 \\ B_1 \end{pmatrix} &= \mathcal{S} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \mathcal{T}_{11} - \mathcal{T}_{12}\mathcal{T}_{21}/\mathcal{T}_{22} \\ -\mathcal{T}_{21}/\mathcal{T}_{22} \end{pmatrix} = \begin{pmatrix} \frac{(1+k_1/k_2)^2 - (1-k_1/k_2)^2}{2(1+k_1/k_2)} \\ -\frac{1-k_1/k_2}{1+k_1/k_2} \end{pmatrix} \\ &= \frac{1}{k_1 + k_2} \begin{pmatrix} 2k_1 \\ k_1 - k_2 \end{pmatrix}. \end{aligned} \quad (3.35)$$

We use  $B_2 = 0$ , since no wave comes from the side of region (2), and  $A_1 = 1$ , because it simplifies the formulas and does not affect the generality of the results. The interesting results are:

- Even when  $E_2 < V_2$ , the particle enters the classically prohibited region:  $\psi_2(x) \propto e^{-\kappa_2 x}$  with  $\kappa_2 = \frac{1}{\hbar} \sqrt{2m(V_2 - E_2)}$ , i.e. the transmission is non-zero,  $|A_2| > 0$ .
- Even with  $E_2 > V_2$ , the particle has a probability of being reflected at the step,  $|B_1| > 0$ .

**Example 18 (Contrast of a partially reflected wave):** Defining  $K_\pm \equiv \frac{1}{2} (\max |\psi_1|^2 \pm \min |\psi_1|^2)$ , the *contrast* of the wavefunction in region (1) is given

by  $K_-/K_+$ . Writing the function as  $\psi_1 = e^{ik_1x} + B_1e^{-ik_1x}$  it is easy to show, that

$$|B_1| = \frac{\sqrt{K_+ + K_-} - \sqrt{K_+ - K_-}}{\sqrt{K_+ + K_-} + \sqrt{K_+ - K_-}} \simeq \frac{K_-}{2K_+}. \quad (3.36)$$

This formula can be understood as an analogue of *Fresnel formula* for matter waves <sup>1</sup>.

In Exc. 3.3.7.1 we calculate the behavior of a Broglie wave passing through a potential step and entering a classically forbidden region. In Exc. 3.3.7.2 we investigate a model describing the collision between attracting or repelling particles via a partial reflection at a potential step.

### 3.3.4 Continuity of probability flow

The continuity equation (2.16) requires that the *probability flux* be preserved in stationary situations,

$$0 = \frac{dj}{dx} = \frac{d}{dx} \frac{\hbar}{2mi} \left[ \psi^* \left( \frac{d}{dx} \psi \right) - \left( \frac{d}{dx} \psi^* \right) \psi \right]. \quad (3.37)$$

Applying this to a potential step separating the regions  $n = 1, 2$ , we find,

$$\begin{aligned} j_n &= \frac{\hbar}{2mi} \left[ \psi^* \frac{d}{dx} \psi - \psi \frac{d}{dx} \psi^* \right] \\ &= \frac{\hbar}{2mi} [(A_n^* e^{-ik_n x} + B_n^* e^{ik_n x})(ik_n A_n e^{ik_n x} - ik_n B_n e^{-ik_n x}) \\ &\quad - (A_n e^{ik_n x} + B_n e^{-ik_n x})(-ik_n A_n^* e^{-ik_n x} + ik_n B_n^* e^{ik_n x})] \\ &= \frac{\hbar k_n}{m} (|A_n|^2 - |B_n|^2). \end{aligned} \quad (3.38)$$

Hence,  $j_1 = j_2$  implies  $k_1|A_1|^2 - k_1|B_1|^2 = k_2|A_2|^2 - k_2|B_2|^2$ . Assuming that the particle comes from side 1 and  $B_2 = 0$ , we have,

$$1 = |B_1|^2 + \frac{k_2}{k_1} |A_2|^2 = R + T, \quad (3.39)$$

defining the *transmission*  $T$  and the *reflection*  $R$  as,

$$T \equiv \frac{k_2}{k_1} |S_{12}|^2 = \frac{k_2}{k_1} |A_2|^2 \quad \text{and} \quad R \equiv |S_{22}|^2 = |B_1|^2. \quad (3.40)$$

### 3.3.5 Tunneling and quantum reflection at a potential well

Particles thrown with a kinetic energy  $E$  against potential barriers can cross them even if  $V_0 > E$  or be reflected even when  $V_0 < E$ , as illustrated in Fig. 3.5(a). This can be verified by considering a particle propagating from  $x = -\infty$  towards  $x = +\infty$  through a potential well located at  $x \in [0, a]$ . We determine the concatenation  $\mathcal{T} = \mathcal{T}_{2 \rightarrow 3} \mathcal{T}_{1 \rightarrow 2}$ . Then we find the  $\mathcal{S}$  matrix that corresponds to the  $\mathcal{T}$  matrix and solve the

<sup>1</sup>In this sense light reflection at an optical interface (with typical losses of 4% for glass) can be interpreted as quantum reflection of light

problem in the same way as in the previous section. For example, we can calculate the transmission and reflection probabilities. The formula is derived in Exc. 3.3.7.3,

$$R = 1 - T = \left( 1 + \frac{16E/V_0(1 - E/V_0)}{(e^{\kappa L} - e^{-\kappa L})^2} \right)^{-1}, \quad (3.41)$$

and sketched in Fig. 3.5(b).

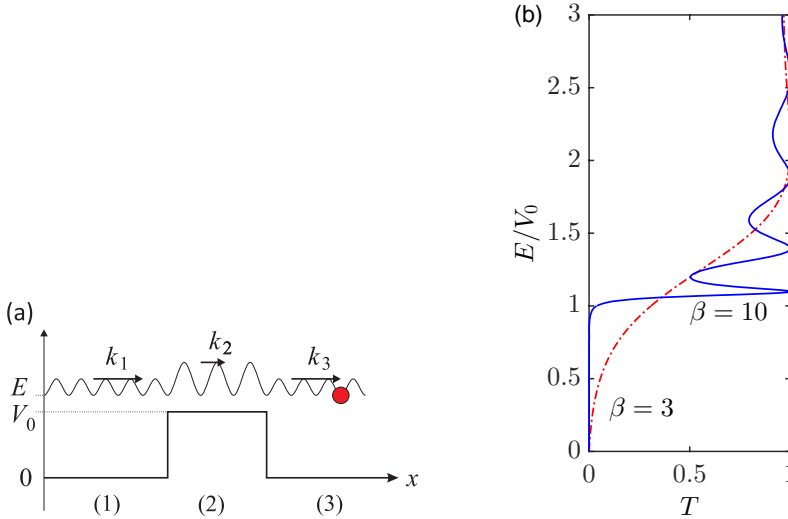


Figure 3.5: (code) (a) Tunnel effect and quantum transmission and reflection at a potential barrier. (b) Coefficients of transmission and reflection (horizontal) through the shown potential barrier as a function of the energy normalized to the height of the barrier  $E/V_0$ . The dashed red curve corresponds to a low barrier,  $\beta \equiv \frac{1}{\hbar}L\sqrt{2mV_0} = 3$ , the blue solid curve corresponds to a deep barrier  $\beta = 10$ .

### 3.3.6 The delta-potential

In quantum mechanics the  $\delta$ -potential can be used to simulate situations, where a particle is free to move in two regions of space with a barrier in between. For example, an electron can move almost freely in a conducting material, but when two conducting surfaces are put close together, the interface between them acts as a barrier for the electron that can be approximated by a  $\delta$ -potential. The  $\delta$ -potential is a limiting case of the finite potential well when we decrease its width while maintained the product of its width and its depth constant. Here, for simplicity, we only consider a one-dimensional potential well, but the analysis can be expanded to more dimensions.

The time-independent Schrödinger equation for the wavefunction  $\psi(x)$  of a particle in one dimension is,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \alpha\delta(x)\psi(x) = E\psi(x), \quad (3.42)$$

The potential is called a  $\delta$ -potential well if  $\alpha$  is negative and a  $\delta$ -potential barrier if  $\alpha$  is positive.

The potential splits the space in two parts ( $x < 0$  and  $x > 0$ ). In each of these parts the potential energy is zero, and the Schrödinger equation reduces to,

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi. \quad (3.43)$$

The solutions of this differential equation are linear combinations of  $e^{ikx}$  and  $e^{-ikx}$ , where the wavenumber  $k$  is related to the energy by  $k = \frac{\sqrt{2mE}}{\hbar}$ . In general, due to the presence of the  $\delta$ -potential in the origin, the coefficients of the solution need not be the same in both half-spaces:

$$\psi(x) = \begin{cases} \psi_1(x) = A_1 e^{ikx} + B_1 e^{-ikx} & \text{for } x < 0 \\ \psi_2(x) = A_2 e^{ikx} + B_2 e^{-ikx} & \text{for } x > 0 \end{cases}, \quad (3.44)$$

where, in the case of positive energies (real  $k$ ),  $e^{ikx}$  represents a wave traveling to the right, and  $e^{-ikx}$  one traveling to the left. One obtains a relation between the coefficients by imposing that the wavefunction be continuous at the origin,

$$\psi(0) = \psi_1(0) = \psi_2(0) = A_1 + B_1 = A_2 + B_2. \quad (3.45)$$

A second relation can be found by studying the derivative of the wavefunction. Normally, we could also impose differentiability at the origin, but this is not possible because of the  $\delta$ -potential. However, if we integrate the Schrödinger equation around  $x = 0$  over an interval  $[-\epsilon, +\epsilon]$ :

$$-\frac{\hbar^2}{2m} \int_{-\epsilon}^{+\epsilon} \psi''(x) dx + \int_{-\epsilon}^{+\epsilon} V(x)\psi(x) dx = E \int_{-\epsilon}^{+\epsilon} \psi(x) dx. \quad (3.46)$$

In the limit  $\epsilon \rightarrow 0$  the right-hand side of this equation vanishes,

$$-\frac{\hbar^2}{2m} [\psi_2'(0) - \psi_1'(0)] + \alpha\psi(0) = 0. \quad (3.47)$$

Substituting the definition of  $\psi$  into this expression, we obtain,

$$-\frac{\hbar^2}{2m} ik(A_1 - B_1 - A_2 + B_2) + \alpha(A_1 + B_1) = 0. \quad (3.48)$$

The boundary conditions thus give the following restrictions on the coefficients,

$$\boxed{\begin{aligned} A_1 + B_1 - A_2 - B_2 &= 0 \\ A_1 - B_1 - A_2 + B_2 &= \frac{2m\alpha}{ik\hbar^2}(A_1 + B_1) \end{aligned}}. \quad (3.49)$$

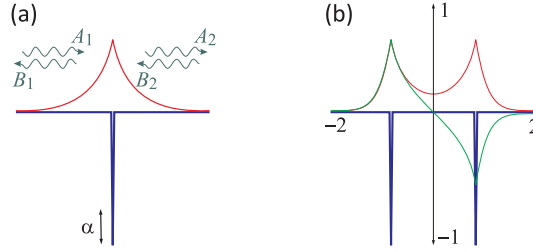


Figure 3.6: (a) The  $\delta$ -potential (green) and the bound state wavefunction (blue). (b) Double  $\delta$ -potential (green).

### 3.3.6.1 Bound states

The bound state wavefunction solution to the  $\delta$ -function potential is continuous everywhere, but its derivative is not defined at  $x = 0$ .

In any one-dimensional attractive potential there will be a bound state. To find its energy, note that for negative energies,  $E < 0$ , the wavenumber  $k = \iota\sqrt{2m|E|}/\hbar = \iota\kappa$  is imaginary and the wavefunctions are exponentially increasing or decreasing functions of  $x$  (see above). Requiring that the wavefunctions do not diverge at infinity eliminates half of the terms:  $A_2 = B_1 = 0$ . The wavefunction is then an evanescent wave,

$$\psi(x) = \begin{cases} \psi_1(x) = A_1 e^{\kappa x} & \text{for } x < 0 \\ \psi_2(x) = B_2 e^{-\kappa x} & \text{for } x > 0 \end{cases}. \quad (3.50)$$

From the boundary conditions and normalization conditions, it follows that,

$$A_1 = B_2 = \sqrt{\kappa} \quad \text{and} \quad \kappa = -\frac{m\alpha}{\hbar^2}, \quad (3.51)$$

from which follows that  $\alpha$  must be negative, that is the bound state only exists for the well, and not for the barrier. The Fourier transform of this wavefunction is a Lorentzian function. The energy of the bound state is then,

$$E_b = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}. \quad (3.52)$$

The  $\delta$ -potential well and its wavefunction are exhibited in Fig. 3.6(a).

### 3.3.6.2 Scattering

For positive energies, the wavefunctions are oscillating functions of  $x$ . That is, the particle is free to move in either half-space:  $x < 0$  or  $x > 0$ , but it may be scattered at the  $\delta$ -potential. The quantum case can be studied in the following situation: a particle incident on the barrier from the left side ( $A_1$ ) may be reflected ( $B_1$ ) or transmitted ( $A_2$ ). To find the amplitudes for reflection and transmission for incidence from the left, we set in the equations (3.49)  $A_1 = 1$  (incoming particle),  $B_1 = r$  (reflection),  $B_2 = 0$  (no incoming particle from the right), and  $A_2 = t$  (transmission), and solve

for  $r$  and  $t$ ,

$$t = \frac{1}{1 - \frac{m\alpha}{i\hbar^2 k}} \quad , \quad r = \frac{1}{\frac{i\hbar^2 k}{m\alpha} - 1} . \quad (3.53)$$

Due to the mirror symmetry of the model, the amplitudes for incidence from the right are the same as those from the left. The result is that there is a non-zero probability,

$$R = |r|^2 = \frac{1}{1 + \frac{\hbar^4 k^2}{m^2 \alpha^2}} = \frac{1}{1 + \frac{2\hbar^2 E}{m\alpha^2}} . \quad (3.54)$$

for the particle to be reflected. This does not depend on the sign of  $\alpha$ , that is, a barrier has the same probability of reflecting the particle as a well. This is a significant difference from classical mechanics, where the reflection probability would be 1 for the barrier (the particle simply bounces back), and 0 for the well (the particle passes through the well undisturbed). The probability for transmission is,

$$T = |t|^2 = 1 - R = \frac{1}{1 + \frac{m^2 \alpha^2}{\hbar^4 k^2}} = \frac{1}{1 + \frac{m\alpha^2}{2\hbar^2 E}} . \quad (3.55)$$

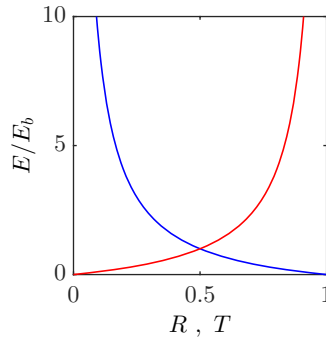


Figure 3.7: (code) Transmission (red) and reflection (blue) probability of a  $\delta$ -potential well. The energy  $E > 0$  is in units of  $E_b = m\alpha^2/2\hbar^2$ .

An application example regards the interfaces between two conducting materials. In the bulk of the materials, the motion of the electrons is quasi-free and can be described by the kinetic term in the above Hamiltonian with an effective mass  $m$ . Often, the surfaces of such materials are covered with oxide layers or are not ideal for other reasons. This thin, non-conducting layer may then be modeled by a local  $\delta$ -function potential. Electrons may then tunnel from one material to the other giving rise to a current.

**Example 19 (Double delta potential):** The  $\delta$ -function model is actually a one-dimensional version of the hydrogen atom. The model becomes particularly useful when applied to the hydrogen molecule ion, as shown in the following.

The double-well  $\delta$ -function models a diatomic hydrogen molecule by the corresponding Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}(x) + V(x)\psi(x) = E\psi(x),$$

where the potential is now:

$$V(x) = -q\lambda \left[ \delta\left(x + \frac{R}{2}\right) + \delta\left(x - \frac{R}{2}\right) \right]$$

where  $0 < R < \infty$  is the 'internuclear' distance with  $\delta$ -function (negative) peaks located at  $x = \pm R/2$  (shown in brown in the diagram). Keeping in mind the relationship of this model with its three-dimensional molecular counterpart, we use atomic units and set  $\hbar = m = 1$ . Here  $0 < \lambda < 1$  is a formally adjustable parameter. From the single well case, we can infer the 'ansatz' for the solution to be:

$$\psi(x) = Ae^{-d|x+\frac{R}{2}|} + Be^{-d|x-\frac{R}{2}|}.$$

Matching of the wavefunction at the  $\delta$ -function peaks yields the determinant:

$$\begin{vmatrix} q-d & qe^{-dR} \\ q\lambda e^{-dR} & q\lambda-d \end{vmatrix} = 0 \quad \text{where} \quad E = -\frac{d^2}{2}.$$

Thus,  $d$  is found to be governed by the pseudo-quadratic equation:

$$d_{\pm}(\lambda) = \frac{1}{2}q(\lambda+1) \pm \frac{1}{2} \left\{ q^2(1+\lambda)^2 - 4\lambda q^2[1 - e^{-2d_{\pm}(\lambda)R}] \right\}^{1/2},$$

which has two solutions  $d = d_{\pm}$ . For the case of equal charges (symmetric homonuclear case),  $\lambda = 1$  and the pseudo-quadratic reduces to:

$$d_{\pm} = q[1 \pm e^{-d_{\pm}R}].$$

The '+' case corresponds to a wave function symmetric about the midpoint (shown in red in the diagram) where  $A = B$  and is called gerade. Correspondingly, the '-' case is the wavefunction that is anti-symmetric about the midpoint where  $A = -B$  is called ungerade (shown in green in the diagram). They represent an approximation of the two lowest discrete energy states of the three-dimensional  $\text{H}_2^+$  and are useful in its analysis. Analytical solutions for the energy eigenvalues for the case of symmetric charges are given by:

$$d_{\pm} = q + W(\pm qRe^{-qR})/R,$$

where  $W$  is the standard Lambert function. Note that the lowest energy corresponds to the symmetric solution  $d_+$ . In the case of unequal charges, and for that matter the three-dimensional molecular problem, the solutions are given by a generalization of the Lambert function (see section on generalization of Lambert function and references herein).

One of the most interesting cases is when  $qR \leq 1$ , which results in  $d_- = 0$ . Thus, one has a non-trivial bound state solution with  $E = 0$ . For these specific parameters, there are many interesting properties that occur, one of which is the unusual effect that the transmission coefficient is unity at zero energy.



### 3.3.7 Exercises

#### 3.3.7.1 Ex: Tunneling

A rubidium-87 atom moves in free space (region 0) with velocity  $v = 1 \text{ cm/s}$  (see diagram). Suddenly it encounters a gap with depth  $V_1 = -k_B \cdot 1\mu\text{K}$ .

- What is the particle's Broglie wavelength in region 1?
- Now the atom encounters a barrier of height  $V_2 = -V_1$ . What is the probability that the particle will enter region 2?
- What is the probability of finding the particle inside region 2 up to a depth of  $x_2 = 10 \text{ nm}$ ?

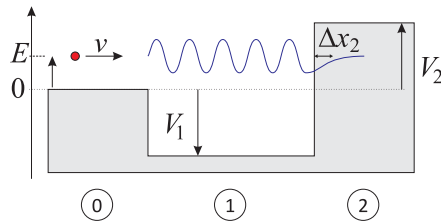


Figure 3.8: Particle in a potential landscape.

#### 3.3.7.2 Ex: Collisions

A *collision* between attractive or repulsive particles can be described by the Schrödinger equation as a one-dimensional scattering,

$$-\frac{\hbar^2}{2m}\psi''(x) + \alpha\delta(x)\psi(x) = E\psi(x).$$

The energy spectrum may be a discrete spectrum of bound states and a continuum of free states.

- Calculate the transmission coefficient for the case of a particle with energy  $E$  thrown against the potential energy barrier  $V(x) = \alpha\delta(x)$ . Does the result change for the case when  $V(x) = -\alpha\delta(x)$ , with  $\alpha > 0$ ?
- For this last potential, find the energy of the bound state and its corresponding wavefunction.

#### 3.3.7.3 Ex: Energy barrier

Consider a particle with energy  $E$  thrown (in the direction  $\hat{e}_x$ ) against a potential energy barrier of finite height and width, such that  $V(x) = 0$  for  $x < 0$  or  $x > L$  and  $V(x) = V_0$  for  $0 \leq x \leq L$ .

- Obtain the reflection and transmission coefficients  $R$  and  $T$  for the case  $E > V_0$ . Discuss the result.
- Do the same for the case  $E < V_0$ .

### 3.3.7.4 Ex: Wavepacket reflected at a potential barrier

Simulate the reflection of a Gaussian wavepacket at a potential barrier for various kinetic energies using the Julia programming language.

## 3.4 Numerical approaches for arbitrary potentials

In practice, many potentials are not box-shaped or harmonic, which renders an analytic treatment difficult or impossible. To some extent approximation methods can be used, as discussed in Sec. 6.5, but many problems can only be solved numerically. In Sec. 3.4.1 we will first show at the example of arbitrary one-dimensional potentials, how the Schrödinger equation can be solved numerically and how this allows one to determine the eigenenergies of bound states. In Sec. 3.4.2 we will introduce the very efficient Fourier grid method for calculating bound state energies and wavefunctions.

### 3.4.1 Calculation of free and bound states wavefunctions

Numerical routines or packages are available for solving ordinary differential equations (ODE). Generally it is advantageous to convert the one-dimensional second-order Schrödinger equation into two first-order differential equations via,

$$\varphi'(x) = \frac{2m}{\hbar^2} [E - V(x)]\psi(x) \quad \text{and} \quad \psi'(x) = \varphi(x) . \quad (3.56)$$

For free states,  $E > V(x)$ , we just solve equation (3.56) specifying the kinetic energy of the particle. The magenta curve in Fig 3.9(a) is an example of a collisional wavefunction in a Morse-type interatomic potential.

For bound states, we must additionally satisfy the eigenvalue problem, since only specific discrete eigenenergies  $E$  are permitted. A possible procedure consists in guessing an eigenvalue  $E$ , calculating the associated wavefunction  $\psi(x)$  using an ODE solver, check whether it diverges for  $x \rightarrow \pm\infty$ , and vary  $E$  until  $\psi(x)$  no longer diverges. Then we repeat the procedure for bound state energies, until we got them all. The red curve in Fig 3.9(a) shows the wavefunction of a vibrational state in a Morse-type potential obtained by solving the Schrödinger equation and adjusting the energy until the function stops diverging in the classically forbidden range. In this example the iteration process was stopped when the wavefunction diverged at around  $R \approx 19a_B$ . In Exc. 3.4.4.1 we will practice this technique at the example of Hermite's differential equation, and in Exc. 3.4.4.2 we will study the case of a potential whose depth linearly increases with the distance from origin.

### 3.4.2 The Fourier grid method for bound states

The objective of the *Fourier grid method* is to analytically solve the 1D Schrödinger equation with an arbitrary potential  $V(r)$  on a grid of  $2N + 1$  equally spaced spatial points  $r_i$ , where  $i = 0, \pm 1, \dots, \pm N$ . That is, we assume the potential  $V(r_i)$  to be given at these points. Scaling by the spatial coordinate  $r$  by  $r/L = x/2\pi$ , we get for the dimensionless coordinate  $x$  the Schrödinger equation,

$$\left[ -\frac{\hbar^2}{2mL^2} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x) , \quad (3.57)$$

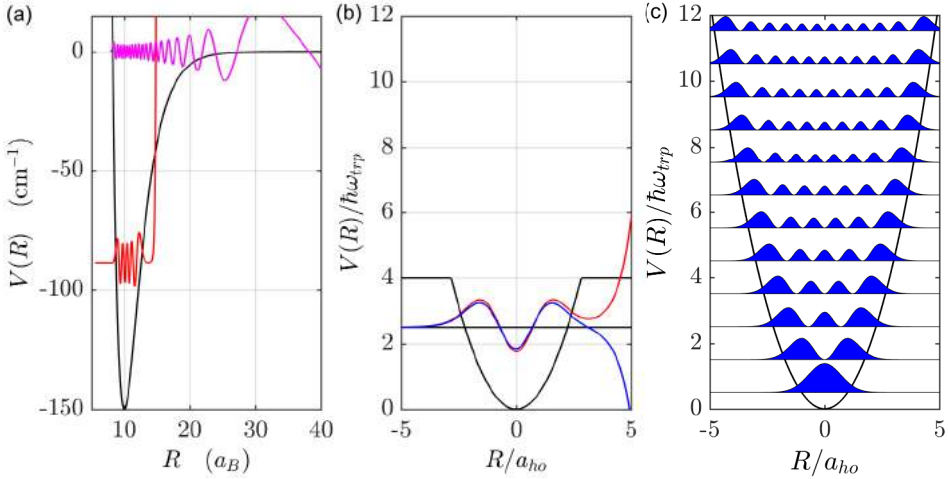


Figure 3.9: (code) (a) Free particle (magenta) and bound state wavefunction (red) calculated using a MATLAB ODE solver. (b) Bound state wavefunction of the harmonic oscillator calculated using a MATLAB ODE solver. For the red curve the eigenvalue has been slightly overestimated and for the blue curve underestimated. (c) Calculation of the harmonic oscillator energies and wave functions using the Fourier grid method.

with the grid given by,

$$x_i \equiv \frac{2\pi i}{2N+1} . \quad (3.58)$$

The main difficulty for numerically solving such eigenvalue equations is obviously the derivative. Numerical differentiation schemes can be cast into the following general form [479],

$$f'(x_i) = \sum_{j=-N}^N D_{ij} f(x_j) , \quad (3.59)$$

that is, they can be expressed as a multiplication of the discretized wavefunction represented as a vector  $f(x_j)$  and a matrix  $D_{ij}$ . These schemes are usually based on interpolation polynomials and are the more accurate, the higher the order of these polynomials is chosen to be.

Instead of using interpolation polynomials, one may now consider over-all approximation of a function  $f(x)$  by a Fourier series of  $N$ -th order, i.e. to assume,

$$f(x) = \sum_{k=-\infty}^{\infty} c_k e^{ikx} \simeq \sum_{k=-N}^N c_k e^{ikx} . \quad (3.60)$$

The highest harmonics of the Fourier expansion  $N$  is set by the distance between two grid points. The expansion coefficients are,

$$c_k = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-ikx} dx \longrightarrow \frac{1}{2\pi} \sum_{j=-N}^N f(x_j) e^{-ikx_j} \Delta x = \frac{1}{2N+1} \sum_{j=-N}^N f(x_j) e^{-ikx_j} . \quad (3.61)$$

Now, substituting  $x$  by the discrete variable  $x_i$ , we take the derivative  $f'(x_i)$  of the function (3.60), insert the expansion coefficients (3.61), and compare the resulting expression to the linear combination (3.59) of the functional values  $f(x_j)$ ,

$$\begin{aligned} f'(x_i) &= \sum_{k=-N}^N ikc_k e^{ikx_i} = \frac{i}{2N+1} \sum_{k=-N}^N k \sum_{j=-N}^N f(x_j) e^{ik(x_i-x_j)} \\ &= \frac{2}{2N+1} \sum_{k=1}^N k \sum_{j=-N}^N f(x_j) \sin k(x_j - x_i) \equiv \sum_{j=-N}^N D_{ij} f(x_j). \end{aligned} \quad (3.62)$$

From this we see, that the matrix elements  $D_{j'j}$  are given by,

$$D_{ij} = \frac{2}{2N+1} \sum_{k=1}^N k \sin k(x_j - x_i) = \frac{2}{2N+1} \sum_{k=1}^N k \sin \frac{2\pi k(i-j)}{2N+1}. \quad (3.63)$$

The sum can be evaluated analytically, as shown in Exc. 3.4.4.3 [656],

$$D_{ii} = 0 \quad \text{and} \quad D_{i \neq j} = \frac{(-1)^{i-j}}{2 \sin \frac{x_i - x_j}{2}} = \frac{(-1)^{i-j}}{2 \sin \frac{\pi(i-j)}{2N+1}}. \quad (3.64)$$

We may proceed similarly for the second derivative,

$$\begin{aligned} f''(x_i) &= - \sum_{k=-N}^N k^2 c_k e^{ikx_i} = \frac{-1}{2N+1} \sum_{k=-N}^N k^2 \sum_{j=-N}^N f(x_j) e^{ik(x_i-x_j)} \\ &= \frac{-2}{2N+1} \sum_{k=1}^N k^2 \sum_{j=-N}^N f(x_j) \cos k(x_j - x_i) \equiv \sum_{j=-N}^N (D^2)_{ij} f(x_j), \end{aligned} \quad (3.65)$$

yielding,

$$(D^2)_{ij} = \frac{-2}{2N+1} \sum_{k=1}^N k^2 \cos k(x_j - x_i) = \frac{-2}{2N+1} \sum_{k=1}^N k^2 \cos \frac{2\pi k(i-j)}{2N+1}. \quad (3.66)$$

Again, the sum can be evaluated analytically, as shown in Exc. 3.4.4.3 [656],

$$(D^2)_{ii} = -\frac{N^2+2}{12} \quad \text{and} \quad (D^2)_{i \neq j} = -\frac{(-1)^{i-j}}{2 \sin^2 \frac{\pi(i-j)}{2N+1}}. \quad (3.67)$$

With this scheme of differentiation, the set of difference equations representing the problem (3.67) is readily found to be [456, 215, 656],

$$\hat{H}\psi = E\psi \quad \text{with} \quad \hat{H}_{ij} = -\frac{h^2}{2mL^2} (D^2)_{ij} + V(x_j)\delta_{ij}. \quad (3.68)$$

This eigenvalue problem can easily be solved on a computer, see Fig 3.9(b).

### 3.4.3 Steepest descent of the ground state

The softwares 'Maple' or 'Mathematics' are useful for analytical calculations, that is, multiplying matrices or determining eigenvalues. For numerical calculations the software 'Matlab' is more adapted. For example, the time evolution of a Schrödinger equation,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle, \quad (3.69)$$

can be calculated in a single command line using the Matlab 'expm' function.

When the system varies temporally,  $\hat{H}(t)$ , we may divide time into small units  $dt$  and propagate the wavefunction as,

$$|\psi(t+dt)\rangle = e^{-i\hat{H}(t)dt/\hbar}|\psi(t)\rangle \simeq |\psi(t)\rangle \left(1 - i\frac{\hat{H}}{\hbar}dt\right), \quad (3.70)$$

continuously reinserting the solution into the equation. This *Newton method* does not converge quickly ( $dt$  should be chosen small enough, when  $\hat{H}(t)$  varies rapidly), but there are other more sophisticated methods like the *Runge-Kutta method*.

A variation of this method is called *steepest descent method*. This method is similar to the Newton Eq. (3.70), but replaces the time  $dt$  with an imaginary time. Thus, the coherent temporal evolution of the Schrödinger equation is replaced by a dissipative evolution. The loss of energy automatically takes the system to the ground state. However, in order to preserve the normalization of the wavefunction, it must be renormalized at each iteration step,

$$|\psi(t+dt)\rangle \rightarrow \frac{|\psi(t+dt)\rangle}{\sqrt{\langle\psi(t+dt)|\psi(t+dt)\rangle}}. \quad (3.71)$$

The method also applies to more complicated equations than the Schrödinger equation, for example, the *Gross-Pitaevskii equation*. We will deepen this technique in Sec. 26.3.3.

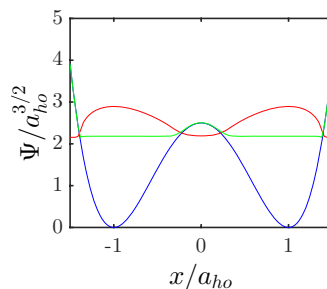


Figure 3.10: (code) Condensate wavefunction (red) in a double-well potential (blue) numerically calculated using the steepest descent method. Also shown is the chemical potential (green).

Another numerical method often used in quantum mechanics is the method called the quantum *Monte Carlo simulation* of the wavefunction [496]. This method simulates trajectories of quantum systems treating intrinsic quantum noise as random processes disrupting the uniformity of the trajectory. The advantage of this method is that it also applies to dissipative systems.

### 3.4.4 Exercises

#### 3.4.4.1 Ex: Numerical resolution of the Hermite differential equation

Solve the Hermite differential equation (3.90) numerically for  $n = 8$ , e.g. using the 'ode45' ordinary differential equation solver of Matlab, or similar. Plot the wavefunction of the 8-th vibrational level of a harmonic oscillator.

#### 3.4.4.2 Ex: Numerical resolution of the Schrödinger equation

Paramagnetic atoms, such as rubidium, can be confined in quadrupolar magnetic traps, which are characterized by a linear increase of the magnetic field in any direction of space. Let us consider one dimension of such a potential, given by  $V(x) = \mu_B \partial_x B |x| - V_0$  wherever  $V(x)$  is negative and  $V(x) = 0$  else. Here  $\mu_B$  is the Bohr magneton. Be  $\partial_x B = 200$  G/cm the magnetic field gradient and  $V_0 = h$  15 kHz the potential depth.

a. Calculate the energy and wavefunction of the lowest bound state of this potential by numerical integration of the stationary Schrödinger equation using Matlab or another software.

b. Obtain all bound state energies and wavefunctions using the Fourier grid method.

#### 3.4.4.3 Ex: The Fourier grid method

Derive (a) the formula (3.64) and (b) the formula (3.67) for  $N \gg 1$  using the formula (1.352) from [277].

#### 3.4.4.4 Ex: Derivation of the Fourier grid method from the FFT

The Fast Fourier Transform (FFT) is defined by,

$$H_n = \sum_{k=0}^{N-1} e^{-2\pi i n k / N} h_k$$

$$= \sum_{k=0}^{N-1} e^{-2\pi i n k / (N/2)} h_{2k} + e^{-2\pi i n k / N} \sum_{k=0}^{N/2-1} e^{-2\pi i n k / (N/2)} h_{2k+1} = \text{even} + \text{odd} .$$

the inverse transform is,

$$h_k = \frac{1}{N} \sum_{n=0}^{N-1} e^{2\pi i n k / N} H_n .$$

The sinus transform of a real vector  $s_k$  is,

$$S_n = \frac{2}{N} \sum_{k=1}^{N-1} s_k \sin \pi n k / N .$$

Calculate the inverse transform of the matrix  $T_{rs} = k_r^2 \delta_{rs}$ .

### 3.4.4.5 Ex: Infinite rectangular double-well potential

- a. Consider the rectangular double-well potential sketched in Fig. 3.11 and calculate the energy levels according to the procedure taught in Sec. 3.3.5.
- b. For the same type of potential as in (a) prepare a numerical calculation of the wavefunctions, e.g. using the Fourier grid method introduced in Sec. 11.2.5, for  $^{87}\text{Rb}$  using the following dimensions of the potential:  $V_0 = h \times 15 \text{ MHz}$ ,  $L = 40 \text{ nm}$ , and  $b = 3 \text{ nm}$ .

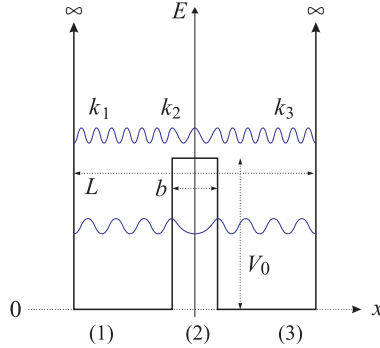


Figure 3.11: Scheme of the rectangular double-well potential.

## 3.5 Harmonic oscillator

Many systems oscillate. Common examples are vibrations of atoms bound in a molecule or in a crystalline lattice, of particles trapped in applied electric or magnetic fields, or light in an electromagnetic mode. Most periodic movements are approximately harmonic for small amplitude vibrations and can be treated in a way that we will detail now.

We start with the unidimensional *harmonic oscillator* (OH),

$$\left[ \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) - E \right] \psi(x) = 0 \quad \text{where} \quad V(x) = \frac{m}{2} \omega^2 x^2. \quad (3.72)$$

### 3.5.1 Factorization of the Hamiltonian and Fock states

Respecting the fact that the operators  $\hat{p}$  and  $\hat{x}$  do not commute,  $\frac{i}{\hbar} [\hat{p}, \hat{x}] = 1$ , we can rewrite the Hamiltonian of the harmonic oscillator in the following way,

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m}{2} \omega^2 \hat{x}^2 = \hbar\omega \left[ \left( \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - i\sqrt{\frac{1}{2m\hbar\omega}} \hat{p} \right) \left( \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + i\sqrt{\frac{1}{2m\hbar\omega}} \hat{p} \right) + \frac{1}{2} \right] \\ &= \hbar\omega \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right), \end{aligned} \quad (3.73)$$

with the abbreviation  $\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + i\sqrt{\frac{1}{2m\hbar\omega}} \hat{p}$  and its Hermitian transposition  $\hat{a}^\dagger$ . Now let's try to find out the properties of the operators  $\hat{a}^\dagger$  and  $\hat{a}$ . First of all, the

commutator is,

$$\begin{aligned} [\hat{a}, \hat{a}^\dagger] &= \left[ \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + i\sqrt{\frac{1}{2m\hbar\omega}} \hat{p}, \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - i\sqrt{\frac{1}{2m\hbar\omega}} \hat{p} \right] = \frac{i}{2\hbar} [\hat{x} + \hat{p}, \hat{x} - \hat{p}] \\ &= \frac{i}{\hbar} [\hat{p}, \hat{x}] = 1. \end{aligned} \quad (3.74)$$

Knowing  $\hat{H}|\psi\rangle = E|\psi\rangle$  is it clear that  $\hat{a}^\dagger\hat{a}$  is an observable with the eigenvalue  $n \equiv \frac{E}{\hbar\omega} - \frac{1}{2}$ ,

$$\hat{a}^\dagger\hat{a}|\psi\rangle = \left(\frac{E}{\hbar\omega} - \frac{1}{2}\right) |\psi\rangle \equiv n|\psi\rangle \implies |\psi\rangle = |n\rangle. \quad (3.75)$$

Now, we show that the states  $\hat{a}|\psi\rangle$  are eigenstates of the operator defined as  $\hat{n} \equiv \hat{a}^\dagger\hat{a}$ , since,

$$\begin{aligned} \hat{a}^\dagger\hat{a}\hat{a}|\psi\rangle &= (\hat{a}\hat{a}^\dagger - [\hat{a}, \hat{a}^\dagger])\hat{a}|\psi\rangle = (\hat{a}\hat{a}^\dagger\hat{a} - \hat{a})|\psi\rangle = \hat{a}(\hat{a}^\dagger\hat{a} - 1)|\psi\rangle = (n-1)\hat{a}|\psi\rangle \\ &\implies \hat{a}|\psi\rangle \propto |n-1\rangle \equiv C|n-1\rangle \\ &\implies n = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = C^2\langle n-1|n-1\rangle \\ &\implies C = \sqrt{n}. \end{aligned} \quad (3.76)$$

We note that the quantum number of the new  $|n-1\rangle$  is decreased by 1. Similarly, we show for the state  $\hat{a}^\dagger|\psi\rangle$ ,

$$\begin{aligned} \hat{a}^\dagger\hat{a}\hat{a}^\dagger|\psi\rangle &= \hat{a}^\dagger([\hat{a}, \hat{a}^\dagger] + \hat{a}^\dagger\hat{a})|\psi\rangle = \hat{a}^\dagger(1 + \hat{a}^\dagger\hat{a})|\psi\rangle = (n+1)\hat{a}^\dagger|\psi\rangle \\ &\implies \hat{a}^\dagger|\psi\rangle \propto |n+1\rangle \equiv C|n+1\rangle \\ &\implies n+1 = \langle n|\hat{a}^\dagger\hat{a} + [\hat{a}, \hat{a}^\dagger]|n\rangle = C^2\langle n+1|n+1\rangle \\ &\implies C = \sqrt{n+1}. \end{aligned} \quad (3.77)$$

Therefore, this new state is also an eigenvector  $|n+1\rangle$ , with a quantum number increased by one unit.  $\hat{a}^\dagger$  and  $\hat{a}$  are creation and annihilation operators of an energy packet,

$$\boxed{\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad \text{and} \quad \hat{a}|n\rangle = \sqrt{n}|n-1\rangle}. \quad (3.78)$$

The matrix representation of the field operators is,

$$\hat{a}^\dagger = \sum_n \sqrt{n+1}|n+1\rangle\langle n| \quad \text{and} \quad \hat{a} = \sum_n \sqrt{n}|n-1\rangle\langle n|. \quad (3.79)$$

Now it is clear, that  $\hat{n}$  can be understood as a number operator <sup>2</sup>. The energy spectrum of the harmonic oscillator is equidistant,

$$\boxed{E_n = \hbar\omega \left(n + \frac{1}{2}\right)}. \quad (3.80)$$

The state with  $n$  quanta can be created from the vacuum,

$$|n\rangle = \frac{\hat{a}^\dagger}{\sqrt{n}}|n-1\rangle = \frac{\hat{a}^{\dagger n}}{\sqrt{n!}}|0\rangle. \quad (3.81)$$

The state  $|n\rangle$  is called *number state* or *Fock state*.

<sup>2</sup>Also, we can define phase operators by  $\widehat{\exp}(i\phi) = \sum_n |n+1\rangle\langle n|$ .



### 3.5.1.1 Uncertainty in Fock states

We consider an OH of mass  $m$  and angular frequency  $\omega$  prepared in the stationary state  $|n\rangle$  which is an eigenstate of the Hamiltonian  $\hat{H}$  with eigenvalue  $(n + \frac{1}{2})\hbar\omega$ . Defining the characteristic size of the OH,  $a_{ho} = \sqrt{\hbar/m\omega}$ , the annihilation and creation operators can be written,

$$\hat{a} = \frac{1}{\sqrt{2}} \left( \frac{\hat{x}}{a_{ho}} + i \frac{a_{ho}}{\hbar} \hat{p} \right) \quad \text{and} \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}} \left( \frac{\hat{x}}{a_{ho}} - i \frac{a_{ho}}{\hbar} \hat{p} \right). \quad (3.82)$$

Therefore, the position and momentum operators are,

$$\sqrt{2} \frac{1}{a_{ho}} \hat{x} = \hat{a} + \hat{a}^\dagger \quad \text{and} \quad \sqrt{2} i \frac{a_{ho}}{\hbar} \hat{p} = \hat{a} - \hat{a}^\dagger. \quad (3.83)$$

The mean squared deviations of the position  $\hat{x}$  and the momentum  $\hat{p}$  are,

$$\begin{aligned} \Delta x^2 &= \langle n | \hat{x}^2 | n \rangle = \frac{a_{ho}^2}{2} \langle n | \hat{a}\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger | n \rangle = \frac{a_{ho}^2}{2} \langle n | 2\hat{n} + 1 | n \rangle \\ &= \frac{a_{ho}^2}{2} (2n + 1) \\ \Delta p^2 &= \langle n | \hat{p}^2 | n \rangle = \frac{-\hbar^2}{2a_{ho}^2} \langle n | \hat{a}\hat{a} - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger | n \rangle = \frac{-\hbar^2}{2a_{ho}^2} \langle n | -2\hat{n} - 1 | n \rangle \\ &= \frac{\hbar^2}{2a_{ho}^2} (2n + 1). \end{aligned} \quad (3.84)$$

From the results of the previous item we obtain the uncertainty relation  $\Delta x \Delta p$  for the OH in the state  $|n\rangle$ ,

$$\Delta p \Delta x = \frac{\hbar}{2} (2n + 1). \quad (3.85)$$

**Example 20 (Localization energy):** The non-vanishing energy of the fundamental state of the harmonic oscillator,  $E_0 = \hbar\omega/2$ , is an immediate consequence of the Heisenberg principle  $\Delta x \Delta p \geq \hbar$ , because in analogy with Example 17 we calculate,

$$\frac{\langle p^2 \rangle}{2m} = \frac{\Delta p^2}{2m} > \frac{\hbar^2}{2m\Delta x^2} > \frac{\hbar^2}{2ma_{ho}^2} = \frac{\hbar\omega}{2}.$$

In the case of an electromagnetic field this energy is called *vacuum fluctuation*.

### 3.5.2 Harmonic oscillator in spatial representation

To simplify the Schrödinger equation in spatial representation,

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m}{2} \omega^2 x^2 \right] \psi(x) = \hbar\omega \left( n + \frac{1}{2} \right) \psi(x), \quad (3.86)$$

we use the scale  $\tilde{x} \equiv x/a_{ho}$ , where  $a_{ho} = \sqrt{\hbar/m\omega}$  is the spatial extent of the ground state. Therefore,

$$\begin{aligned} \frac{2}{\hbar\omega} \left[ -\frac{\hbar^2}{2m} \frac{d^2}{d(a_{ho}\tilde{x})^2} + \frac{m}{2} \omega^2 (a_{ho}\tilde{x})^2 \right] \tilde{\psi}(\tilde{x}) &= \frac{2}{\hbar\omega} \left[ -\frac{\hbar\omega}{2} \frac{d^2}{d\tilde{x}^2} + \frac{\hbar\omega}{2} \tilde{x}^2 \right] \tilde{\psi}(\tilde{x}) \\ &= \left[ -\frac{d^2}{d\tilde{x}^2} + \tilde{x}^2 \right] \tilde{\psi}(\tilde{x}) = (2n + 1) \tilde{\psi}(\tilde{x}). \end{aligned}$$

Now we start looking for asymptotic solutions. For  $\tilde{x} \rightarrow \pm\infty$ , that is, when the particle enters the classically forbidden region, we can neglect the total energy of the particle,

$$\left[ -\frac{d^2}{d\tilde{x}^2} + \tilde{x}^2 \right] \tilde{\psi}_\infty(\tilde{x}) \simeq 0. \quad (3.87)$$

The solution of this equation is  $\tilde{\psi}_\infty(\tilde{x}) = Ce^{-\tilde{x}^2/2}$ , since

$$\begin{aligned} \left[ -\frac{d^2}{d\tilde{x}^2} + \tilde{x}^2 \right] e^{-\tilde{x}^2/2} &= -\frac{d}{d\tilde{x}}(-\tilde{x})e^{-\tilde{x}^2/2} + \tilde{x}^2 e^{-\tilde{x}^2/2} \\ &= -\tilde{x}^2 e^{-\tilde{x}^2/2} + e^{-\tilde{x}^2/2} + \tilde{x}^2 e^{-\tilde{x}^2/2} = e^{-\tilde{x}^2/2} \simeq 0. \end{aligned} \quad (3.88)$$

This motivates the ansatz  $\tilde{\psi}(\tilde{x}) \equiv e^{-\tilde{x}^2/2} H(\tilde{x})$  for the complete differential equation (3.86),

$$\begin{aligned} \left[ -\frac{d^2}{d\tilde{x}^2} + \tilde{x}^2 \right] e^{-\tilde{x}^2/2} H(\tilde{x}) &= -e^{-\tilde{x}^2/2} \frac{d^2 H(\tilde{x})}{d\tilde{x}^2} - 2 \frac{de^{-\tilde{x}^2/2}}{d\tilde{x}} \frac{dH(\tilde{x})}{d\tilde{x}} - \frac{d^2 e^{-\tilde{x}^2/2}}{d\tilde{x}^2} H(\tilde{x}) + \tilde{x}^2 e^{-\tilde{x}^2/2} H(\tilde{x}) \\ &= -e^{-\tilde{x}^2/2} \frac{d^2 H(\tilde{x})}{d\tilde{x}^2} - 2(-\tilde{x})e^{-\tilde{x}^2/2} \frac{dH(\tilde{x})}{d\tilde{x}} + \left[ -\tilde{x}^2 e^{-\tilde{x}^2/2} + e^{-\tilde{x}^2/2} \right] H(\tilde{x}) + \tilde{x}^2 e^{-\tilde{x}^2/2} H(\tilde{x}) \\ &\equiv (2n+1)e^{-\tilde{x}^2/2} H(\tilde{x}). \end{aligned} \quad (3.89)$$

Thus, the functions  $H(\tilde{x})$  must satisfy the differential equation,

$$H''(\tilde{x}) = 2\tilde{x}H'(\tilde{x}) - 2nH(\tilde{x}). \quad (3.90)$$

We can verify that the Hermite polynomials defined by,

$$H_n(\tilde{x}) = (-1)^n e^{\tilde{x}^2} \frac{d^n}{d\tilde{x}^n} e^{-\tilde{x}^2}, \quad (3.91)$$

transform the differential equation into a recursion formula,

$$H_{n+1}(\tilde{x}) = 2\tilde{x}H_n(\tilde{x}) - 2nH_{n-1}(\tilde{x}), \quad (3.92)$$

which allows us to easily calculate the polynomials,

$$H_0(\tilde{x}) = 1, \quad H_1(\tilde{x}) = 2\tilde{x}, \quad H_2(\tilde{x}) = 4\tilde{x}^2 - 2, \quad \dots \quad (3.93)$$

In summary, the eigenfunction of a harmonic oscillator in the state of excitation  $n$  is,

$$\langle x|n\rangle = \psi_n(x) = C_n e^{-x^2/2a_{ho}^2} H_n(x/a_{ho}), \quad (3.94)$$

where the constant  $C_n$  is determined by the normalization condition (7.18),  $\langle \psi_m | \psi_n \rangle = \delta_{m,n}$ ,

$$C_n = \frac{1}{\sqrt{a_{ho}} \sqrt{\pi 2^n n!}}. \quad (3.95)$$

The Hermite functions,  $H_n$ , are found in mathematical tables, see Sec. 7.3. The spatial and momentum wavefunctions for the vibrational ground state are,

$$\langle x|0\rangle = \frac{1}{\pi^{1/4} \sqrt{a_{ho}}} e^{-x^2/2a_{ho}^2} \quad \text{and} \quad \langle p|0\rangle = \frac{1}{\pi^{1/4}} \sqrt{\frac{a_{ho}}{\hbar}} e^{-a_{ho}^2 p^2/2\hbar^2}. \quad (3.96)$$

Here we will only show the graphical representation of  $|\psi|^2$  in Fig. 3.12. The Exc. 3.5.6.1 asks to evaluate HO in a classically forbidden region and in Exc. 3.5.6.2 we will calculate the spectrum of a semi-harmonic HO.

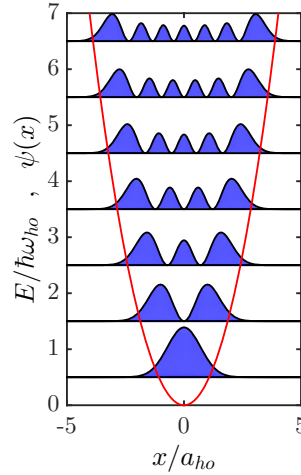


Figure 3.12: (code) Wavefunctions and energies for a harmonic potential.

### 3.5.3 Properties of the harmonic oscillator

We note that there are regions where  $\psi(\tilde{x}) \neq 0$  even though  $V(x) > E$ . This effect is purely quantum. Classically, we can not find a particle in regions where its energy is below the potential.

We also note that for high quantum numbers,  $n \rightarrow \infty$ , we expect to recover the classical predictions, i.e.,

$$\lim_{n \rightarrow \infty} |\psi(x)|^2 = P_E(x) , \quad (3.97)$$

where  $P_E$  is the probability density of finding the oscillating particle at position  $x$ . The probability of finding the particle in a range  $dx$  close to the location  $x$  is easily calculated,

$$\begin{aligned} E &= \frac{m}{2} v^2 + \frac{m}{2} \omega^2 x^2 \\ \Rightarrow P_E(x) dx &= \frac{t(x+dx) - t(x)}{T} = \frac{dx}{vT} = \frac{dx}{T} \frac{1}{\sqrt{2E/m - \omega^2 x^2}} . \end{aligned} \quad (3.98)$$

We see that for high energy values the wavefunction approaches the classical expectation.

We already mentioned that there exist solutions only for certain energies  $E_n = \hbar\omega(2n + 1)$ . Consequently, the energy levels are equidistant,  $E_{n+1} - E_n = \hbar\omega$ , as if there were a box into which we add, one after the other, particles with the energy  $\hbar\omega$  until we have accumulated  $n$  portions of energy. These particles are called *phonons* in the case of vibrations of massive particles, and *photons* in the case of a radiation field.

The fact that the energy distribution is the same as the one proposed by Planck for the black-body radiation suggests the use of the harmonic oscillator to describe the second quantization.

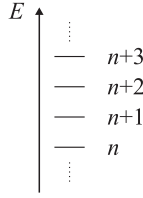


Figure 3.13: Ladder of levels.

### 3.5.4 Time evolution of the unperturbed harmonic oscillator

Here we study the temporal evolution of a population distribution in a harmonic oscillator. The formal solution of the Schrödinger equation is,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle . \quad (3.99)$$

As the Hamiltonian is diagonal in the basis  $|n\rangle$ ,

$$\hat{H} = \hbar\omega \left(\hat{n} + \frac{1}{2}\right) . \quad (3.100)$$

we can write,

$$e^{-i\hat{H}t/\hbar} = \sum_n |n\rangle e^{-i\omega t(n+1/2)} \langle n| . \quad (3.101)$$

If the initial state is  $|\psi(0)\rangle = \sum_m c_m |m\rangle$ , the final state and the eigenvalue of any observable will be,

$$|\psi(t)\rangle = \sum_n |n\rangle e^{-i\omega t(n+1/2)} \langle n|\psi(0)\rangle = \sum_n e^{-i\omega t(n+1/2)} c_n |n\rangle \quad (3.102)$$

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \sum_m \langle m| e^{i\omega t(m+1/2)} c_m^* \hat{A} \sum_n e^{-i\omega t(n+1/2)} c_n |n\rangle = \sum_{m,n} c_m^* c_n e^{i\omega t(m-n)} \langle m|\hat{A}|n\rangle .$$

If the oscillator is initially in an eigenstate,  $|\psi(0)\rangle = |k\rangle$ , we obtain,

$$|\psi(t)\rangle = e^{-i\omega t(k+1/2)} |k\rangle \quad \text{and} \quad \langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle k|\hat{A}|k\rangle , \quad (3.103)$$

that is, the *state remains stationary*. Motion needs non-diagonal elements of  $\hat{A}$ .

Another observation is that the populations do not change, even in the case of an initial superposition, since,

$$P_k(t) = |\langle k|\psi(t)\rangle|^2 = |e^{-i\omega t(k+1/2)} c_k|^2 = |c_k|^2 . \quad (3.104)$$

We conclude that

- movement of an observable  $\hat{A}$  is possible, but only due to *variations of the phase factors*;
- to carry out transitions between the vibrational states is necessary to *perturb the oscillator*, e.g. by applying fields of electromagnetic radiation.

**Example 21 (Motion of a harmonic oscillator):** We now consider some specific examples. If the studied observable is the Hamiltonian and the initial state an arbitrary superposition, then

$$\langle \psi(t) | \hat{H} | \psi(t) \rangle = \hbar\omega \sum_{m,n} c_m^* c_n e^{i\omega t(m-n)} \langle m | \hat{n} + \frac{1}{2} | n \rangle = \hbar\omega \sum_n |c_n|^2 \left(n + \frac{1}{2}\right) .$$

That is, the total energy of the oscillator is the sum of the energies of the states weighted with the populations of those states. In the case of the position operator,

$$\begin{aligned} \langle \psi(t) | \hat{x} | \psi(t) \rangle &= \frac{a_{ho}}{\sqrt{2}} \sum_{m,n} c_m^* c_n e^{i\omega t(m-n)} \langle m | \hat{a} + \hat{a}^\dagger | n \rangle \\ &= \frac{a_{ho}}{\sqrt{2}} \sum_n \left( c_{n-1}^* c_n e^{-i\omega t} \sqrt{n} + c_{n+1}^* c_n e^{i\omega t} \sqrt{n+1} \right) \\ &\xrightarrow{m,n \rightarrow \infty} a_{ho} \sqrt{2} \sum_n \sqrt{n} |c_n|^2 \cos \omega t . \end{aligned}$$

That is, *the particle can only oscillate, if there are populations in consecutive states*. If this is not the case,  $\langle \psi(t) | \hat{x} | \psi(t) \rangle = 0$ . The oscillation frequency is always  $\omega$ , independent of the energy of the particle. We will study this in Excs. 3.5.6.3, leaving the discussion of the temporal evolution of perturbed oscillators to later sections.

### 3.5.5 Multidimensional harmonic oscillator

The 3D harmonic potential is given by

$$V_{ho}(\mathbf{r}) = \frac{m}{2} \omega_x^2 x^2 + \frac{m}{2} \omega_y^2 y^2 + \frac{m}{2} \omega_z^2 z^2 . \quad (3.105)$$

Making the ansatz

$$\psi(\mathbf{r}) = \psi_x(x) \psi_y(y) \psi_z(z) , \quad (3.106)$$

we can separate the spatial directions and obtain a one-dimensional equation for each coordinate, such that the coordinates can be considered separately. Each function  $\psi_k(x_k)$  is of the form (3.94) and the energies are,

$$E_k = \hbar\omega_k \left(n_k + \frac{1}{2}\right) , \quad (3.107)$$

where  $k = x, y, z$ .

### 3.5.6 Exercises

#### 3.5.6.1 Ex: Ground state of a harmonic oscillator

Equating the ground state energy of quantum HO to that of its classical analog, obtain the maximum elongation  $x_m$ . Now, knowing that the ground state wavefunction is proportional to the Gaussian  $\psi_0 \propto e^{-x^2/2x_m^2}$ , obtain the expression for the probability of finding the HO outside the classical limits and estimate its value.

**3.5.6.2 Ex: Particle in a semi-harmonic well**

Find the energy levels of a particle in a potential energy well of the form  $V(x) = \infty$  for  $x < 0$  and  $V(x) = \frac{m\omega^2 x^2}{2}$  for  $x > 0$ . What is the parity of the allowed states?

**3.5.6.3 Ex: Vibration of a harmonic oscillator**

Consider a HO of mass  $m$  and angular frequency  $\omega$ . At time  $t = 0$  the oscillator's state is  $|\psi(0)\rangle = \sum_n c_n |n\rangle$ , where  $|n\rangle$  are the stationary states of the HO with energy  $(n + 1/2)\hbar\omega$ .

a. What is the probability  $P$  for measuring, at an arbitrary time  $t > 0$ , an energy of the HO higher than  $2\hbar\omega$ ? For the case when  $P = 0$ , what are the non-zero coefficients  $c_n$ ?

b. From now on, we assume that only  $c_0$  and  $c_1$  are nonzero. Write down the normalization condition for  $|\psi(0)\rangle$  and the mean value  $\langle \hat{H} \rangle$  of energy in terms of  $c_0$  and  $c_1$ . With the additional requirement  $\langle \hat{H} \rangle = \hbar\omega$ , calculate  $|c_0|^2$  and  $|c_1|^2$ .

c. Given that the normalized state vector  $|\psi(0)\rangle$  is defined to less than an overall phase factor, we determine this factor by choosing the real and positive coefficients  $c_0$  and  $c_1 = |c_1|e^{i\theta}$ . Assuming  $\langle \hat{H} \rangle = \hbar\omega$  and  $\langle \hat{x} \rangle = \frac{1}{2}\sqrt{\hbar/m\omega}$ , calculate  $\theta$ .

d. With  $|\psi(0)\rangle$  determined (according to the previous item), write down  $|\psi(t)\rangle$  for  $t > 0$  and calculate the value  $\theta$  at this time  $t$ . Deduce the average value  $\langle \hat{x} \rangle(t)$  of the position at time  $t$ .

**3.6 Superposition states of a harmonic oscillator**

As any other quantum system, a harmonic oscillator does not need to be in a particular vibrational eigenstate. In fact, it is much more common to encounter them in superpositions of many states. In a system in thermal equilibrium, the energetic distribution of occupied states reflects the temperature of the system.

**3.6.1 Coherent states**

The most common superposition for a harmonic oscillation is a Poissonian probability distribution of occupied vibrational (Fock) states. This state, called coherent or Glauber state, has particular features that we will discuss in the following sections.

**3.6.1.1 Glauber's formula**

A useful formula that we will use later is the *Glauber formula* (or *Baker-Hausdorff formula*),

$$\boxed{e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}+[\hat{A},\hat{B}]/2}}, \quad (3.108)$$

which holds for  $[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$ , i.e. when  $\hat{A}$  and  $\hat{B}$  commute with their commutator.

**Example 22 (The Baker-Hausdorff formula):** In order to prove the Baker-Hausdorff formula, we consider the operator,

$$\hat{G}(\tau) \equiv e^{\tau(\hat{A}+\hat{B})}e^{-\tau\hat{B}}e^{-\tau\hat{A}}.$$

The derivative is,

$$\begin{aligned}\hat{G}'(\tau) &= (\hat{A} + \hat{B})e^{\tau(\hat{A}+\hat{B})}e^{-\tau\hat{B}}e^{-\tau\hat{A}} - e^{\tau(\hat{A}+\hat{B})}\hat{B}e^{-\tau\hat{B}}e^{-\tau\hat{A}} - e^{\tau(\hat{A}+\hat{B})}e^{-\tau\hat{B}}\hat{A}e^{-\tau\hat{A}} \\ &= e^{\tau(\hat{A}+\hat{B})} \left[ \hat{A}e^{-\tau\hat{B}} - e^{-\tau\hat{B}}\hat{A} \right] e^{-\tau\hat{A}} = e^{\tau(\hat{A}+\hat{B})} \left[ \hat{A} - e^{-\tau\hat{B}}\hat{A}e^{\tau\hat{B}} \right] e^{-\tau\hat{B}}e^{-\tau\hat{A}} \\ &= e^{\tau(\hat{A}+\hat{B})} \left[ \hat{A} - \left( \hat{A} + [-\tau\hat{B}, \hat{A}] + \frac{1}{2!}[-\tau\hat{B}, [-\tau\hat{B}, \hat{A}]] + \dots \right) \right] e^{-\tau\hat{B}}e^{-\tau\hat{A}},\end{aligned}$$

using the formula (2.165). If now  $[\hat{A}, [\hat{A}, \hat{B}]] = 0 = [\hat{B}, [\hat{A}, \hat{B}]]$ , then,

$$\hat{G}'(\tau) = e^{\tau(\hat{A}+\hat{B})}\tau[\hat{B}, \hat{A}]e^{-\tau\hat{B}}e^{-\tau\hat{A}} = -\tau[\hat{A}, \hat{B}]e^{\tau(\hat{A}+\hat{B})}e^{-\tau\hat{B}}e^{-\tau\hat{A}} = -\tau[\hat{A}, \hat{B}]\hat{G}(\tau).$$

The solution of this differential equation is,

$$\hat{G}(\tau) \equiv e^{-(\tau^2/2)[\hat{A}, \hat{B}]} \hat{G}(0).$$

With  $\hat{G}(0) = 1$  we obtain at the point  $\tau = 1$ ,

$$e^{\hat{A}+\hat{B}}e^{-\hat{B}}e^{-\hat{A}} = e^{-(1/2)[\hat{A}, \hat{B}]}.$$

### 3.6.1.2 Displacement operator

We now consider the so-called *displacement operator*<sup>3</sup>,

$$\hat{D}(\alpha) \equiv e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}, \quad (3.109)$$

and try to discover its features.

$\hat{D}(\alpha)$  is a unitary operator, since using Glauber's formula (3.108) we get,

$$\begin{aligned}\hat{D}^\dagger(\alpha)\hat{D}(\alpha) &= e^{\alpha^*\hat{a} - \alpha\hat{a}^\dagger}e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = e^{\alpha^*\hat{a} - \alpha\hat{a}^\dagger + \alpha\hat{a}^\dagger - \alpha^*\hat{a} + [\alpha^*\hat{a} - \alpha\hat{a}^\dagger, \alpha\hat{a}^\dagger - \alpha^*\hat{a}]/2} \\ &= e^{[\alpha^*\hat{a} - \alpha\hat{a}^\dagger, \alpha\hat{a}^\dagger - \alpha^*\hat{a}]/2} = e^{[\alpha^*\hat{a}, \alpha\hat{a}^\dagger]/2 + [-\alpha\hat{a}^\dagger, \alpha\hat{a}^\dagger]/2 + [\alpha^*\hat{a}, -\alpha^*\hat{a}]/2 + [-\alpha\hat{a}^\dagger, -\alpha^*\hat{a}]/2} \\ &= e^{|\alpha|^2[\hat{a}, \hat{a}^\dagger]/2 + |\alpha|^2[\hat{a}^\dagger, \hat{a}]/2} = e^0 = \hat{1}.\end{aligned} \quad (3.110)$$

We can rewrite the displacement operator like this:

$$\begin{aligned}\hat{D}(\alpha) &= e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}e^{-[\alpha\hat{a}^\dagger, -\alpha^*\hat{a}]/2} = e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}e^{|\alpha|^2[\hat{a}^\dagger, \hat{a}]/2} \\ &= e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}e^{-|\alpha|^2/2}.\end{aligned} \quad (3.111)$$

The state resulting from the action of the operator  $\hat{D}(\alpha)$  onto the ground state of the HO is,

$$\begin{aligned}|\alpha\rangle \equiv \hat{D}(\alpha)|0\rangle &= e^{-|\alpha|^2/2}e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}|0\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha\hat{a}^\dagger)^n}{n!} |0\rangle \\ &= e^{-|\alpha|^2/2} \left( 1 + \alpha\hat{a}^\dagger + \frac{(\alpha\hat{a}^\dagger)^2}{2!} + \dots \right) |0\rangle = e^{-|\alpha|^2/2} \left( |0\rangle + \frac{\alpha}{1!}\sqrt{1}|1\rangle + \frac{\alpha^2}{2!}\sqrt{2!}|2\rangle + \dots \right),\end{aligned} \quad (3.112)$$

<sup>3</sup>The operator acts on the phase space spanned by the operators  $\hat{a}$  and  $\hat{a}^\dagger$ , that is,  $\hat{x} \propto \text{Re } \hat{a}$  and  $\hat{p} \propto \text{Im } \hat{a}$ .

that is, the state  $|\alpha\rangle$  is a superposition distributed according to the *Poisson distribution*,

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (3.113)$$

Applying the step-down operator  $\hat{a}$  onto the state  $|\alpha\rangle$ , we find,

$$\begin{aligned} \hat{a}|\alpha\rangle &= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \hat{a}|n\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n} |n-1\rangle \\ &= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{(n-1)!}} |n-1\rangle, \end{aligned} \quad (3.114)$$

that is,

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle. \quad (3.115)$$

We can also write,

$$\langle\alpha|\hat{a}^\dagger = (\hat{a}|\alpha\rangle)^\dagger = (\alpha|\alpha\rangle)^\dagger = \langle\alpha|\alpha^*.$$

The state  $|\alpha\rangle$  is called *coherent state* or *Glauber state*<sup>4</sup>. We note that, in spite of its appearance, the equation (3.115) is not an eigenvalue equation, since  $\hat{a}$  is not observable.

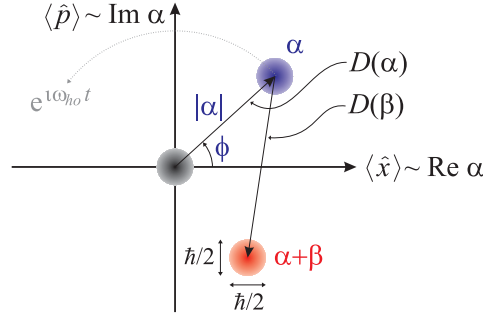


Figure 3.14: Illustration of the action of displacement operators  $D(\alpha)$  and  $D(\beta)$  on Glauber states in the phase space spanned by  $\alpha = \text{Re } \alpha + i \text{Im } \alpha = |\alpha|e^{i\phi}$ . The uncertainty of Glauber states  $\Delta x$  and  $\Delta p$  is represented by a finite distribution of the amplitude  $\alpha$  in the phase space.

Using the formula (2.165), we verify immediately,

$$\hat{D}^\dagger(\alpha)\hat{a}\hat{D}(\alpha) = \hat{a} + \alpha \quad , \quad \hat{D}^\dagger(\alpha)\hat{a}^\dagger\hat{D}(\alpha) = \hat{a}^\dagger + \alpha^* \quad . \quad (3.116)$$

Furthermore, the product of two displacement operators is, apart from a phase factor, another displacement operator satisfying,

$$\hat{D}(\alpha)\hat{D}(\beta) = e^{(\alpha\beta^* - \alpha^*\beta)/2} \hat{D}(\alpha + \beta) \quad , \quad (3.117)$$

<sup>4</sup>We can also define a *Bargmann state* as the eigenstate corresponding to the step-up operator using the notation  $\hat{a}^\dagger|\alpha\rangle = \alpha|\alpha\rangle$ .



as will be verified in Exc. 3.6.6.1. When acting on an eigenket, the phase factor  $e^{(\alpha\beta^* - \alpha^*\beta)/2}$  appears in each term of the resulting state, which makes it physically irrelevant.

### 3.6.1.3 Uncertainty in Glauber states

Consider a HO prepared in a state  $|\alpha\rangle$ . The eigenvalues of the observables  $\hat{x} \equiv \frac{a_{ho}}{\sqrt{2}}(\hat{a}^\dagger + \hat{a})$  and  $\hat{p} \equiv \frac{i\hbar}{a_{ho}\sqrt{2}}(\hat{a}^\dagger - \hat{a})$  are,

$$\begin{aligned} \frac{\sqrt{2}}{a_{ho}}\langle\alpha|\hat{x}|\alpha\rangle &= \langle\alpha|\hat{a} + \hat{a}^\dagger|\alpha\rangle = \alpha + \alpha^* \\ \frac{ia_{ho}\sqrt{2}}{\hbar}\langle\alpha|\hat{p}|\alpha\rangle &= \langle\alpha|\hat{a} - \hat{a}^\dagger|\alpha\rangle = \alpha - \alpha^*. \end{aligned} \quad (3.118)$$

With this the eigenvalues of the quadratures become,

$$\begin{aligned} \frac{2}{a_{ho}^2}\langle\alpha|\hat{x}^2|\alpha\rangle &= \langle\alpha|(\hat{a} + \hat{a}^\dagger)^2|\alpha\rangle = \langle\alpha|\hat{a}\hat{a} + 1 + 2\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger|\alpha\rangle \\ &= \alpha^2 + 1 + 2|\alpha|^2 + \alpha^{*2} = 1 + (\alpha + \alpha^*)^2 = 1 + \frac{2}{a_{ho}^2}\langle\alpha|\hat{x}|\alpha\rangle^2 \\ -\frac{a_{ho}^2}{\hbar^2}\langle\alpha|\hat{p}^2|\alpha\rangle &= \langle\alpha|(\hat{a} - \hat{a}^\dagger)^2|\alpha\rangle = \langle\alpha|\hat{a}\hat{a} - 1 - 2\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger|\alpha\rangle \\ &= \alpha^2 - 1 - 2|\alpha|^2 + \alpha^{*2} = -1 + (\alpha - \alpha^*)^2 = -1 - \frac{2a_{ho}^2}{\hbar^2}\langle\alpha|\hat{p}|\alpha\rangle^2. \end{aligned} \quad (3.119)$$

The uncertainties defined in (2.67) become,

$$\begin{aligned} \Delta x^2 &= \langle\alpha|\hat{x}^2|\alpha\rangle - \langle\alpha|\hat{x}|\alpha\rangle^2 = \frac{a_{ho}^2}{2} \\ \Delta p^2 &= \langle\alpha|\hat{p}^2|\alpha\rangle - \langle\alpha|\hat{p}|\alpha\rangle^2 = \frac{\hbar^2}{2a_{ho}^2}. \end{aligned} \quad (3.120)$$

And finally, we find the Heisenberg relation,

$$\Delta p \Delta x = \frac{\hbar}{2}. \quad (3.121)$$

Comparing with the uncertainty relation (3.85) derived for Fock states, we conclude that the uncertainty is always *smallest* for Glauber states. In this sense, the Glauber states are the ones which are closest to classical states characterized by the absence of uncertainty.

### 3.6.1.4 Orthogonality of Glauber states

Glauber are not orthogonal, since,

$$|\langle\alpha|\beta\rangle|^2 = e^{-|\alpha-\beta|^2}. \quad (3.122)$$

We leave the demonstration for Exc. 3.6.6.2, but we note here already that for  $|\alpha - \beta| \gg 0$  the states are approximately orthogonal. The reason for this is, that the respective population distributions through the Fock states,  $|\langle n|\alpha\rangle|^2$  and  $|\langle n|\beta\rangle|^2$ , do not overlap and hence do not interfere. The state  $|\alpha\rangle + |-\alpha\rangle$  is sometimes called *Schrödinger cat state*. In Exc. 3.6.6.4 we will show why such states are very difficult to detect.

### 3.6.2 Kicking a harmonic oscillator

Let us now study the dynamics of a harmonic oscillator subject to a *kick*. By kicking we understand a translation in momentum space defined by the Galilei boost operator (2.190),

$$U_G(\mathbf{k}) \equiv e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}, \quad (3.123)$$

where  $\mathbf{p} = \hbar\mathbf{k}$  is the gain in momentum due to the kick. A common situation where such a kick occurs is the photonic recoil that an atom receives upon absorption of a photon. Using the relationship (2.165) derived in Exc. 2.5.5.1 it is easy to verify the following expressions of the left-hand panel,

$$\left. \begin{array}{l} e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}|r\rangle = |r\rangle \\ e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}|\mathbf{p}\rangle = |\mathbf{p} + \hbar\mathbf{k}\rangle \\ e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}\hat{\mathbf{r}}e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} = \hat{\mathbf{r}} \\ e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}\hat{\mathbf{p}}e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} = \hat{\mathbf{p}} + \hbar\mathbf{k} \\ e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}\frac{\hat{\mathbf{p}}^2}{2m}e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} = \frac{(\hat{\mathbf{p}} + \hbar\mathbf{k})^2}{2m} \end{array} \right\}, \quad \left. \begin{array}{l} e^{-i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar}|r + \mathbf{b}\rangle = |r + \mathbf{b}\rangle \\ e^{-i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar}|\mathbf{p}\rangle = |\mathbf{p}\rangle \\ e^{i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar}\hat{\mathbf{r}}e^{-i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar} = \hat{\mathbf{r}} + \mathbf{b} \\ e^{i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar}\hat{\mathbf{p}}e^{-i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar} = \hat{\mathbf{p}} \\ e^{i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar}V(\hat{\mathbf{r}})e^{-i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar} = V(\hat{\mathbf{r}} + \mathbf{b}) \end{array} \right\} \quad (3.124)$$

The rule imply  $[e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}, \hat{\mathbf{p}}] \neq 0 \neq [e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}, \hat{H}]$ . That is, we describe the kick by simply adding the corresponding momentum  $\hbar\mathbf{k}$  to the system and adjusting the kinetic energy accordingly. Of course the assumption of an infinitely fast transition is an idealization and the ultimate reason for the non-conservation of momentum and energy by the system. In real situations, such as in the case of photonic recoil, the dynamics should be described by a collision process which conserves momentum and energy.

The right-hand panel of Eq. (3.124) summarizes rules for calculating with the spatial displacement operator introduced in Sec. 2.5.1,

$$U_{tr}(\mathbf{b}) \equiv e^{-i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar}. \quad (3.125)$$

By analogy we find  $[e^{-i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar}, \hat{\mathbf{r}}] \neq 0 \neq [e^{-i\mathbf{b}\cdot\hat{\mathbf{p}}/\hbar}, \hat{H}]$ .

#### 3.6.2.1 Transitions between vibrational states via momentum kick

Let us now restrict to one dimension and study, how the transformation operators  $U_G = e^{ik\hat{x}}$  and  $U_{tr} = e^{-ib\hat{p}/\hbar}$  couple the vibrational states of a harmonic oscillator. With the formalism developed in the last sections and with the abbreviation,

$$\alpha \equiv ika_{ho}/\sqrt{2}, \quad (3.126)$$

we find,

$$e^{ik\hat{x}} = e^{\frac{ika_{ho}}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger)} = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = D(\alpha), \quad (3.127)$$

which is nothing else than the displacement operator (3.112) generating coherent states,  $|\alpha\rangle = D(\alpha)|0\rangle$ . That is, the momentum kick attempts to put the oscillator

into a coherent state with the mean occupation number  $n = |\alpha|^2 = \frac{1}{2}k^2 a_{ho}^2$ . Note that the same effect is obtained setting,

$$\alpha \equiv -b/(a_{ho}\sqrt{2}) \quad (3.128)$$

and applying the translation operator

$$\boxed{e^{-ib\hat{p}/\hbar} = e^{\frac{-b}{a_{ho}\sqrt{2}}(\hat{a}-\hat{a}^\dagger)} = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = D(\alpha)} . \quad (3.129)$$

Now,

$$\begin{aligned} \langle n|e^{ik\hat{x}}|0\rangle &= \langle n|\alpha\rangle = \langle n|e^{-|\alpha|^2/2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}}|m\rangle \\ &= e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}} = e^{-|ka_{ho}|^2/4} \frac{(ika_{ho})^n}{\sqrt{2^n n!}} . \end{aligned} \quad (3.130)$$

This formula tells us that for small  $\alpha$ , transitions may only occur to the vibrational states  $|0\rangle$  and  $|1\rangle$ , since,

$$\langle n|e^{ik\hat{x}}|0\rangle \xrightarrow{ka_{ho} \rightarrow 0} \frac{\alpha^n}{\sqrt{n!}} \simeq \delta_{n,0} + \alpha\delta_{n,1} . \quad (3.131)$$

On the other hand for very large  $\alpha$ , the exponential in (3.130) pulls the transition rate to a particular vibrational state  $|n\rangle$  to zero, but this is simply due to the fact that the population is redistributed over many states, since,

$$\sum_n |\langle n|e^{ik\hat{x}}|0\rangle|^2 = e^{-(ka_{ho})^2/2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} = e^{-(ka_{ho})^2/2} e^{|\alpha|^2} = 1 . \quad (3.132)$$

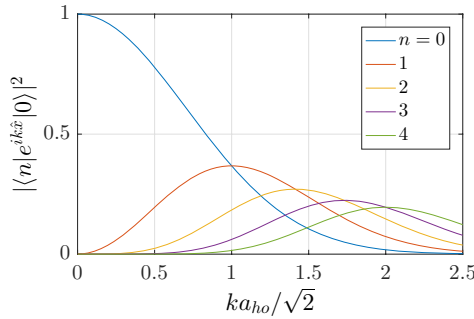


Figure 3.15: (code) Transition matrix element  $|\langle n|e^{ik\hat{x}}|0\rangle|^2$  as a function of  $ka_{ho}$ . The curves are Poisson distributions of photon numbers in coherent states.

For small momentum kicks we may approximate the transition matrix elements by,

$$\begin{aligned} \langle m|e^{ik\hat{x}}|n\rangle &\simeq \langle m|1 + ik\frac{a_{ho}}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger)|n\rangle \\ &= \delta_{m,n} + \frac{ika_{ho}}{\sqrt{2}}(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}) , \end{aligned} \quad (3.133)$$

such that,

$$\sum_{m \neq n} |\langle m | e^{ik\hat{x}} | n \rangle|^2 \simeq k^2 a_{ho}^2 (n + \frac{1}{2}). \quad (3.134)$$

Formula (3.134) tell us that the probability for a transition between vibrational states depends on the parameter  $ka_{ho}$ , which we will discuss in the next section. For small  $ka_{ho}$  it gets increasingly more difficult for the system to leave the original vibrational state  $|n\rangle$  and to form a coherent state. After a momentum kick, the population is coherently distributed over several vibrational states in a way to fulfill momentum and energy conservation. Let us consider, for simplicity, an initial state  $|0\rangle$ . If the kick is weak or the trap strong (i.e. if  $|\alpha| < 1$ ), the atom will stay in  $|0\rangle$  with a high probability amplitude and go to  $|1\rangle$  only with a small probability amplitude. We will derive in Exc. 3.6.6.5 the general expression for the transition matrix element for arbitrary values of  $\alpha$ ,

$$\langle m | e^{ik\hat{x}} | n \rangle = e^{|\alpha|^2/2} \sum_{k=0}^n \sqrt{\binom{n}{k} \binom{m}{k}} \langle n-k | \alpha \rangle \langle m-k | \alpha \rangle. \quad (3.135)$$

The formula satisfies,

$$\sum_m |\langle m | e^{ik\hat{x}} | n \rangle|^2 = \sum_m \langle n | e^{ikx} | m \rangle \langle m | e^{-ikx} | n \rangle = \langle n | e^{ikx} e^{-ikx} | n \rangle = 1. \quad (3.136)$$

Kicking a harmonic oscillator initially in state  $|0\rangle$  we obtain for the expectation value of position and momentum,

$$\begin{aligned} \langle \alpha | \hat{p} | \alpha \rangle &= \langle 0 | D(\alpha)^\dagger \hat{p} D(\alpha) | 0 \rangle = \langle 0 | e^{ik\hat{x}} \hat{p} e^{-ik\hat{x}} | 0 \rangle = \langle 0 | \hat{p} | 0 \rangle + \hbar k \\ \langle \alpha | \hat{x} | \alpha \rangle &= \langle 0 | \hat{x} | 0 \rangle \end{aligned}$$

### 3.6.2.2 Lamb-Dicke regime

We already introduced  $|\alpha|$  as the amplitude of the coherent vibrational state created by kicking a harmonic oscillator. Defined as,

$$\eta \equiv |\alpha| = \frac{1}{\sqrt{2}} ka_{ho} \quad \text{with} \quad a_{ho} \equiv \sqrt{\frac{\hbar}{m\omega_{ho}}}. \quad (3.137)$$

the so-called *Lamb-Dicke parameter* measures the *degree of confinement* of a particle in a harmonic trap with respect to the momentum shift. We say that we are in the *Lamb-Dicke regime*, when the particle is localized to a volume smaller than wavelength,  $2\pi x_0 \ll \lambda$ , corresponding to the momentum kick.

We can also rewrite the Lamb-Dicke parameter in terms of the trap's secular frequency,  $\omega_{ho}$ , and the recoil-shift,

$$\eta = \sqrt{\frac{\omega_{rec}}{\omega_{ho}}} \quad \text{with} \quad \omega_{rec} \equiv \frac{\hbar k^2}{2m}, \quad (3.138)$$

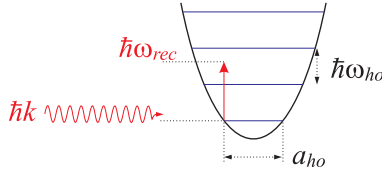


Figure 3.16: Illustration of the Lamb-Dicke parameter.

where we understand the recoil-energy  $\hbar\omega_{rec}$  as the kinetic energy gained through the recoil acceleration. In this form the Lamb-Dicke parameter tells us that, in the Lamb-Dicke regime, the energy of the momentum kick is not sufficient to efficiently excite vibrational states,

$$(2n + 1)\hbar^2 k/m \ll \omega_{ho} . \quad (3.139)$$

That is, cold particles in low vibrational states  $n$  can not accommodate the recoil shift within the vibrational spectrum of the trap. Consequently, the recoil cannot be transferred to the particle itself, but must be absorbed by the entire trap. This is the case of the *strong binding regime* in ion traps, which is analogous to the *Möbbauser effect* discussed in Sec. 18.3.3.

Finally, the Lamb-Dicke parameter can be rewritten in terms of the *inverse Doppler modulation index*,

$$\boxed{\eta = \frac{kv_{max}}{2\omega_{ho}}} \quad \text{with} \quad \frac{m}{2}v_{max}^2 = \hbar\omega_{ho} . \quad (3.140)$$

Accelerated by the momentum kick, the atom will execute harmonic oscillations with frequency  $\omega_{ho}$  and with the maximum velocity-excursions  $v_{max}$ . Hence, any quantity depending on the atomic velocity, e.g. the Doppler-shift, will be modulated. We will discuss this in Sec. 18.3.3, as well.

**Example 23 (Absorption of recoil by a molecular dimer):** To be able to discuss the validity of energy and momentum conservation in a kicked system, let us consider a molecule made of two atoms with masses  $m_1$  and  $m_2$ . Then we kick atom 1 via the momentum shift operator  $e^{ik\hat{x}_1}$  (e.g. during a photon absorption process with the associated recoil) and analyze the motional dynamics of the whole system. (We restrict ourselves to one dimension.)

The first step is to write down the Hamiltonian,

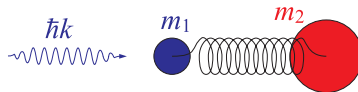


Figure 3.17: Illustration of the kicking.

$$\hat{H} = -\frac{\hbar^2}{2m_1} \frac{d^2}{dx_1^2} - \frac{\hbar^2}{2m_2} \frac{d^2}{dx_2^2} + \frac{\mu}{2}\omega_{ho}^2(x_1 - x_2)^2 ,$$

We transform in the center-of-mass system via,

$$M \equiv m_1 + m_2 \quad \text{and} \quad \frac{1}{\mu} \equiv \frac{1}{m_1} + \frac{1}{m_2}$$

$$R = \frac{m_1 x_1 + m_2 x_2}{M} \quad \text{and} \quad r = x_1 - x_2 .$$

Applying the separation ansatz  $\psi(x_1, x_2) = \Theta(R)\phi(r)$  to the Schrödinger equation,

$$\left[ -\frac{\hbar^2}{2m_1} \frac{d^2}{dx_1^2} - \frac{\hbar^2}{2m_2} \frac{d^2}{dx_2^2} + \frac{\mu}{2} \omega_{ho}^2 (\hat{x}_1 - \hat{x}_2)^2 \right] \psi(x_1, x_2) = E_{tot} \psi(x_1, x_2) ,$$

we calculate,

$$\frac{d}{dx_{1,2}} = \frac{dR}{dx_{1,2}} \frac{d}{dR} + \frac{dr}{dx_{1,2}} \frac{d}{dr} = \frac{m_{1,2}}{M} \frac{d}{dR} \pm \frac{d}{dr}$$

$$\frac{d^2}{dx_{1,2}^2} = \frac{m_{1,2}^2}{M^2} \frac{d^2}{dR^2} \pm 2 \frac{m_{1,2}}{M} \frac{d}{dR} \frac{d}{dr} + \frac{d^2}{dr^2}$$

$$-\frac{\hbar^2}{2m_1} \frac{d^2}{dx_1^2} - \frac{\hbar^2}{2m_2} \frac{d^2}{dx_2^2} = -\frac{\hbar^2}{2M} \frac{d^2}{dR^2} - \frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} .$$

Hence, we get,

$$-\frac{\hbar^2}{2M} \frac{d^2}{dR^2} \Theta(R) = (E_{tot} - E) \Theta(R) \quad , \quad \left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\mu}{2} \omega_{ho}^2 \hat{r}^2 \right] \phi(r) = E \phi(r) .$$

Now, we analyze the kick operator  $e^{ik\hat{x}_1}$  with  $\hat{x}_1 = \hat{R} - \frac{m_2}{M} \hat{r}$ . We find that, because of  $[\hat{R}, \hat{r}] = 0$ ,

$$e^{ik\hat{x}_1} = e^{ik\hat{R}} e^{-ik\frac{m_2}{M} \hat{r}} .$$

This means that the kick operator simultaneously acts on both: the center-of-mass receives a recoil accelerating it by an amount  $p_{cm} = \hbar k$ , and the vibrational relative motion receives a kick of an amount  $p_{rl} = \hbar k m_2 / M$  following the dynamics described in Sec. 3.6.2.

Obviously, the total system conserves momentum, which is imparted to the center-of-mass motion. Whether the kick also excites the relative motion depends on mass ratio. In the limit  $m_1 \ll m_2$  we find  $p_{rl} = \hbar k$ , while in the limit  $m_1 \gg m_2$  we get  $p_{rl} \rightarrow 0$ . In terms of the Lamb-Dicke parameter, we find,

$$\eta = \frac{p_{rl} a_{ho}}{\hbar \sqrt{2}} = \frac{km_2}{M \sqrt{2}} \sqrt{\frac{\hbar}{\mu \omega_{ho}}} = \frac{km_2}{m_1 + m_2} \sqrt{\frac{\hbar}{2\omega_{ho}}} \left( \frac{1}{m_1} + \frac{1}{m_2} \right) .$$

Hence, in the limit  $m_1 \ll m_2$  we expect a much larger Lamb-Dicke parameter than for  $m_1 \gg m_2$ .

### 3.6.3 Shaking a harmonic oscillator

As we mentioned below the formulae (3.124), the transformation in momentum space is not a realistic concept for a *kick*. In practice, a kick will always be the results of a collision, which is understood here as a scattering of a free (massive or massless) particle at our harmonically trapped particle. And the scattering process will take a

finite amount of time, e.g. the duration of a radiative  $\pi$ -pulse required to excite an atomic transition.

As a first example let us consider a harmonic oscillator subject to periodic forcing,

$$\hat{H}(t) = \hat{H}^{(0)} + \hat{H}^{(1)} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m}{2} \omega_{ho}^2 \hat{x}^2 + \frac{\hbar\Omega}{2} (\hat{a}e^{i\nu t} + \hat{a}^\dagger e^{-i\nu t}), \quad (3.141)$$

and study its time evolution,

$$|\psi(t)\rangle = e^{-(i/\hbar)\hat{H}t} \sum_n a_n |n\rangle \xrightarrow{a_n = \delta_{n,0}} e^{-(i/\hbar)\hat{H}t} |0\rangle, \quad (3.142)$$

when the oscillator is initially in the state  $|0\rangle$ . We rewrite the time evolution propagator as,

$$e^{-(i/\hbar)\hat{H}t} = e^{-i\omega_{ho}t(\hat{n}+1/2) - (i\Omega t/2)(\hat{a}e^{i\nu t} + \hat{a}^\dagger e^{-i\nu t})}. \quad (3.143)$$

To simplify the propagator, we first have a closer look at the terms  $\hat{a}e^{i\omega_{ho}t}$  and  $\hat{a}^\dagger e^{-i\omega_{ho}t}$ , which we evaluate through their action on the complete system of unperturbed eigenfunctions,

$$\begin{aligned} e^{-(i/\hbar)\hat{H}^{(0)}t} \hat{a} e^{(i/\hbar)\hat{H}^{(0)}t} |n\rangle &= e^{-(i/\hbar)\hat{H}^{(0)}t} \hat{a} e^{(i/\hbar)E_n^{(0)}t} |n\rangle \\ &= e^{-(i/\hbar)E_{n-1}^{(0)}t} e^{(i/\hbar)E_n^{(0)}t} \hat{a} |n\rangle = e^{i\omega_{ho}t} \hat{a} |n\rangle. \end{aligned} \quad (3.144)$$

Hence, defining the detuning  $\Delta \equiv \nu - \omega_{ho}$ ,

$$\begin{aligned} \hat{a}e^{i\nu t} &= e^{i\omega_{ho}t} \hat{a}e^{i\Delta t} = e^{-i\omega_{ho}t(\hat{n}+1/2)} \hat{a}e^{i\Delta t} e^{i\omega_{ho}t(\hat{n}+1/2)} \\ \hat{a}^\dagger e^{-i\nu t} &= e^{-i\omega_{ho}t} \hat{a}^\dagger e^{-i\Delta t} = e^{-i\omega_{ho}t(\hat{n}+1/2)} \hat{a}^\dagger e^{-i\Delta t} e^{i\omega_{ho}t(\hat{n}+1/2)} \\ \hat{n} &= e^{-i\omega_{ho}t(\hat{n}+1/2)} \hat{n} e^{i\omega_{ho}t(\hat{n}+1/2)} \end{aligned} \quad (3.145)$$

Substituting these expression into the propagator (3.143) we get,

$$e^{-(i/\hbar)\hat{H}t} = e^{-i\omega_{ho}t(\hat{n}+1/2) - (i\Omega t/2)\hat{a}e^{i\Delta t} - (i\Omega t/2)\hat{a}^\dagger e^{-i\Delta t}} e^{i\omega_{ho}t(\hat{n}+1/2)}. \quad (3.146)$$

Now, making use of the relationship,

$$e^{e^{-\hat{A}} \hat{B} e^{\hat{A}}} = \sum_n \frac{(e^{-\hat{A}} \hat{B} e^{\hat{A}})^n}{n!} = \sum_n \frac{e^{-\hat{A}} \hat{B}^n e^{\hat{A}}}{n!} = e^{-\hat{A}} e^{\hat{B}} e^{\hat{A}}, \quad (3.147)$$

which is easy to show by expansion of  $e^{\hat{B}}$ , we find <sup>5</sup>,

$$e^{-(i/\hbar)\hat{H}t} = e^{-i\omega_{ho}t(\hat{n}+1/2)} e^{-i\omega_{ho}t(\hat{n}+1/2) - (i\Omega t/2)(\hat{a}e^{i\Delta t} + \hat{a}^\dagger e^{-i\Delta t})} e^{i\omega_{ho}t(\hat{n}+1/2)}. \quad (3.148)$$

In particular, for  $\Delta = 0$ ,

$$\langle n | e^{-(i/\hbar)\hat{H}t} | 0 \rangle = e^{-ni\omega_{ho}t} \langle n | e^{-i\omega_{ho}t(\hat{n}+1/2) - (i\Omega t/2)(\hat{a} + \hat{a}^\dagger)} | 0 \rangle. \quad (3.149)$$

The dynamics is illustrated in Fig. 3.18. In Exc. 3.6.6.6 we will study how to generalize the problem to non-resonant excitation,  $\Delta \neq 0$ .

<sup>5</sup>Note, that this formula can not be simplified using the Baker-Hausdorff formula, because  $[\hat{n}, [\hat{n}, \hat{a}]] \neq 0$ .

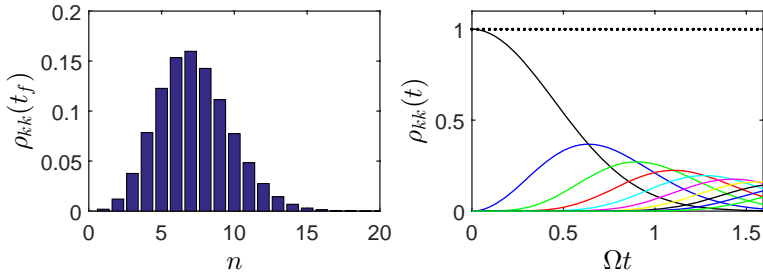


Figure 3.18: (code) (a) Populations of the vibrational states after a given interaction time. (b) Time evolution of the lowest populations.

### 3.6.4 Forcing a harmonic oscillator

The transfer of momentum is the result of a (generally) constant force applied for a certain amount of time,

$$\hbar k = \int_{-\infty}^{\infty} mg \Theta_{[0, \Delta t]}(t) dt, \quad (3.150)$$

where  $g$  denotes the acceleration. That is, we expect that a harmonic oscillator,

$$\hat{H}(t) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m}{2} \omega_{ho}^2 \hat{x}^2 - mg \hat{x} \Theta_{[0, \Delta t]}(t), \quad (3.151)$$

forced for a period of time  $\Delta t$  should have suffered a kick.

#### 3.6.4.1 Displaced harmonic oscillator

To begin with, we will derive the dynamics of a harmonic oscillator suddenly exposed to a homogeneous constant force  $F(t) = mg \Theta_{[0, \infty]}(t)$ . It is easy to see, that the above perturbed Hamiltonian can be cast into the form,

$$\hat{H}(t) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m}{2} \omega_{ho}^2 \left( \hat{x} - \frac{g}{\omega_{ho}^2} \right)^2 - \frac{mg^2}{2\omega_{ho}^2}, \quad (3.152)$$

where the last constant term plays no role in the dynamics. Knowing the eigenvalues and -states of the unperturbed Hamiltonian, the obvious solution of the perturbed eigenvalue problem is,

$$\hat{H}|\psi_n^{(1)}\rangle = E_n^{(1)}|\psi_n^{(1)}\rangle \quad (3.153)$$

$$\text{with } E_n^{(1)} = E_n - \frac{mg^2}{2\omega_{ho}^2}$$

$$\text{and } \langle x|\psi_n^{(1)}\rangle = \psi_n^{(1)}(x) = \psi_n\left(x - \frac{g}{\omega_{ho}^2}\right) = \langle x - \frac{g}{\omega_{ho}^2}|n\rangle.$$

Using the properties (2.167) and (2.169) we may write,

$$\langle x - \frac{g}{\omega_{ho}^2}|n\rangle = \langle x|U_{tr}^\dagger\left(-\frac{g}{\omega_{ho}^2}\right)|n\rangle = \langle x|e^{-(i/\hbar)(g/\omega_{ho}^2)\hat{p}}|n\rangle, \quad (3.154)$$



and using the representation (3.83) of the momentum operator by the field operators and introducing the abbreviation  $\beta \equiv \frac{g}{\omega_{ho}^2 a_{ho} \sqrt{2}}$  we can rewrite,

$$\langle x - \frac{g}{\omega_{ho}^2} | n \rangle = e^{-\beta(\hat{a} - \hat{a}^\dagger)} \langle x | n \rangle . \quad (3.155)$$

Note, that the transition from (3.151) to (3.153) can also be obtained by a redefinition of the field operators according to,

$$\hat{b} \equiv \hat{a} - \frac{mga_{ho}}{\hbar\omega_{ho}\sqrt{2}} , \quad (3.156)$$

since,

$$\hat{H} = \hbar\omega_{ho}(\hat{a}^\dagger\hat{a} + \frac{1}{2}) - \frac{mga_{ho}}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger) = \hbar\omega_{ho}(\hat{b}^\dagger\hat{b} + \frac{1}{2}) - \frac{mg^2}{2\omega_{ho}^2} \quad (3.157)$$

and  $\hat{a} - \hat{a}^\dagger = \hat{b} - \hat{b}^\dagger$ .

The temporal evolution is given by the time-dependent Schrödinger equation. Since the jump is finite, the solution must be well behaved at time  $t = 0$ ,

$$\begin{aligned} \langle x | \psi_n^{(1)}(t) \rangle &= \langle x | e^{-(i/\hbar)\hat{H}t} | \psi_n^{(1)}(0) \rangle \\ &= \langle x | e^{-(i/\hbar)\hat{H}t} e^{-\beta(\hat{a} - \hat{a}^\dagger)} | n \rangle \\ &= \langle x | e^{-(i/\hbar)\hat{H}t} e^{-\beta(\hat{a} - \hat{a}^\dagger)} e^{(i/\hbar)\hat{H}t} e^{-(i/\hbar)\hat{H}t} | n \rangle . \end{aligned} \quad (3.158)$$

To simplify the first three exponential functions, we use the relationships (3.147) and (3.144)<sup>6</sup>,

$$e^{-(i/\hbar)\hat{H}t} e^{-\beta(\hat{a} - \hat{a}^\dagger)} e^{(i/\hbar)\hat{H}t} = e^{-\beta e^{-(i/\hbar)\hat{H}t} (\hat{a} - \hat{a}^\dagger) e^{(i/\hbar)\hat{H}t}} = e^{-\beta(e^{i\omega_{ho}t}\hat{a} - e^{-i\omega_{ho}t}\hat{a}^\dagger)} , \quad (3.159)$$

and write the temporal solution,

$$\begin{aligned} \psi_n^{(1)}(x, t) &= e^{-\beta(\hat{a}e^{i\omega_{ho}t} - \hat{a}^\dagger e^{-i\omega_{ho}t})} e^{-(i/\hbar)\hat{H}t} \psi_n(x) \\ &= e^{-\beta(\hat{a} - \hat{a}^\dagger) \cos \omega_{ho}t - i\beta(\hat{a} + \hat{a}^\dagger) \sin \omega_{ho}t} e^{-(i/\hbar)E_n^{(0)}t} \psi_n(x) . \end{aligned} \quad (3.160)$$

Using Glauber's formula (3.108) we find,

$$\begin{aligned} \psi_n^{(1)}(x, t) &= e^{-i\beta(\hat{a} + \hat{a}^\dagger) \sin \omega_{ho}t} e^{-\beta(\hat{a} - \hat{a}^\dagger) \cos \omega_{ho}t} e^{i\beta^2 \sin \omega_{ho}t \cos \omega_{ho}t} e^{-(i/\hbar)E_n^{(0)}t} \psi_n(x) \\ &= e^{-i(mg/\hbar\omega_{ho})\hat{x} \sin \omega_{ho}t} e^{-(i/\hbar)(g/\omega_{ho}^2)\hat{p} \cos \omega_{ho}t} e^{i\beta^2 \sin \omega_{ho}t \cos \omega_{ho}t} e^{-(i/\hbar)E_n^{(0)}t} \psi_n(x) \\ &= e^{-i\beta(\hat{a} + \hat{a}^\dagger) \sin \omega_{ho}t} e^{i\beta^2 \sin \omega_{ho}t \cos \omega_{ho}t} e^{-(i/\hbar)E_n^{(0)}t} \psi_n(x - b \cos \omega_{ho}t) . \end{aligned} \quad (3.161)$$

Finally,

$$\boxed{|\psi_n^{(1)}(x, t)|^2 = |\psi_n(x - \bar{x}(t))|^2 \quad \text{where} \quad \bar{x}(t) \equiv \frac{g}{\omega_{ho}^2} \cos \omega_{ho}t} . \quad (3.162)$$

<sup>6</sup>We can use (3.144), because the shifted harmonic oscillator has, except from a constant offset the same eigenenergies.

This means that the spatial distribution of  $\psi_n^{(1)}$  around  $\bar{x}(t)$  is the same as of  $\psi_n$  around  $\bar{x} = 0$ . The entire distribution oscillates without deformation. The momentum distribution follows from the Fourier transform,

$$\begin{aligned}\phi_n^{(1)}(p, t) &= \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-(i/\hbar)px} \psi_n^{(1)}(x, t) \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int du e^{-(i/\hbar)pu} e^{-(i/\hbar)um\omega_{ho}} \frac{g}{\omega_{ho}^2} \sin \omega_{ho}t e^{i\gamma(p,t)} \psi_n \\ &= e^{i\gamma(p,t)} \phi_n(p + m\omega_{ho} \frac{g}{\omega_{ho}^2} \sin \omega_{ho}t),\end{aligned}\tag{3.163}$$

where the abbreviation  $\gamma = \gamma^*$  contains all unitary transformations of (3.161), that do not depend on  $x$ . We obtain,

$$\boxed{|\phi_n^{(1)}(p, t)|^2 = |\phi_n(p - \bar{p}(t))|^2 \quad \text{where} \quad \bar{p}(t) \equiv -m \frac{g}{\omega_{ho}} \sin \omega_{ho}t}.\tag{3.164}$$

### 3.6.4.2 Discussion of the kick dynamics

For the acceleration of the harmonic oscillator to resemble a 'kick', the time during which the perturbation is active must be much smaller than a trap oscillation period,  $\omega_{ho}\Delta t \ll 1$ . In this case, we may expand the oscillatory motion (3.162) and (3.164),

$$\bar{x} = \frac{g}{\omega_{ho}^2} \quad \text{and} \quad \bar{p} = -mg\Delta t \equiv -\hbar k,\tag{3.165}$$

which is consistent with the initial request (3.150). It is also clear that, for a given force  $mg$ , the maximum momentum that can be transmitted is limited,  $\hbar k < mg/\omega_{ho}$ .

As long as the kick-approximation  $\omega_{ho}\Delta t \ll 1$  holds, we may simply describe the dynamics during the application of the force, via a time-dependent kick operator,

$$e^{ik(t)\hat{x}} = D(\alpha(t)),\tag{3.166}$$

where the acquired momentum increases linearly with time according to  $k(t) = k \frac{\max(\min(t, \Delta t), 0)}{\Delta t}$ . I.e. the populations of the vibrational states evolve like (3.130) into a coherent state with increasing amplitude  $|\alpha(t)|^2$ . At the end of the kick, on a much slower time-scale  $\omega_{ho}^{-1}$ , the wavefunctions will start to oscillate all in phase, according to (3.162).

The time-dependence of the states  $|\alpha(t)\rangle$ , as shown in Exc. 3.6.6.7 is given by <sup>7</sup>,

$$\begin{aligned}|\alpha(t)\rangle &= e^{-(i/\hbar)\hat{H}t} |\alpha(0)\rangle = \sum_n e^{-(i/\hbar)E_n t} e^{-|\alpha(0)|^2/2} \frac{\alpha(0)^n}{\sqrt{n!}} |n\rangle \\ &= e^{-i\omega_{ho}t/2} \sum_n e^{-|\alpha(0)|^2/2} \frac{(\alpha(0)e^{-i\omega_{ho}t})^n}{\sqrt{n!}} |n\rangle = e^{-i\omega_{ho}t/2} |\alpha(0)e^{-i\omega_{ho}t}\rangle.\end{aligned}\tag{3.167}$$

With (3.144) we find,

$$\begin{aligned}\hat{x}(t) &= e^{-(i/\hbar)\hat{H}t} \hat{x}(0) e^{(i/\hbar)\hat{H}t} = \hat{x}(0) \cos \omega_{ho}t + \frac{\hat{p}(0)}{m\omega_{ho}} \sin \omega_{ho}t \quad \text{and} \\ \hat{p}(t) &= e^{-(i/\hbar)\hat{H}t} \hat{p}(0) e^{(i/\hbar)\hat{H}t} = m\omega_{ho}\hat{x}(0) \sin \omega_{ho}t + \hat{p}(0) \cos \omega_{ho}t,\end{aligned}\tag{3.168}$$

<sup>7</sup>Be careful:  $D(\alpha)$  is only a displacement operator for imaginary  $\alpha$ .

or with (3.167),

$$\begin{aligned} \langle \alpha(t) | \hat{x} | \alpha(t) \rangle &= \langle \alpha(0) | \hat{x} | \alpha(0) \rangle \cos \omega_{ho} t + \frac{1}{m\omega_{ho}} \langle \alpha(0) | \hat{p} | \alpha(0) \rangle \sin \omega_{ho} t \\ \langle \alpha(t) | \hat{p} | \alpha(t) \rangle &= m\omega_{ho} \langle \alpha(0) | \hat{x} | \alpha(0) \rangle \sin \omega_{ho} t + \langle \alpha(0) | \hat{p} | \alpha(0) \rangle \cos \omega_{ho} t \end{aligned} \quad (3.169)$$

We note, that the position and momentum wavefunctions  $\langle x|n\rangle$  and  $\langle p|n\rangle$  of the excited vibrational states are complicated Hermite polynomials, but we don't have to write them down explicitly to get to the last result. We will derive some further properties in 3.6.6.8.

### 3.6.4.3 Simulation of the displacement of a harmonic oscillator

The Hamiltonian of a harmonic oscillator subject to an external force can be cast into the form,

$$\begin{aligned} \hat{H}(t) &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m}{2} \omega_{ho}^2 \hat{x}^2 + mg\hat{x} = \hbar\omega_{ho} \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + mg \frac{a_{ho}}{\sqrt{2}} (\hat{a} + \hat{a}^\dagger) \\ &= \begin{pmatrix} \ddots & & & & \\ & \ddots & & & \\ & & (n - \frac{1}{2})\hbar\omega_{ho} & mg \frac{a_{ho}}{\sqrt{2}} \sqrt{n} & \\ & & mg \frac{a_{ho}}{\sqrt{2}} \sqrt{n} & (n + \frac{1}{2})\hbar\omega_{ho} & \ddots \\ & & & & \ddots & \ddots \end{pmatrix}. \end{aligned} \quad (3.170)$$

The temporal evolution of the state is given by,

$$|\psi(t)\rangle = e^{-(i/\hbar)\hat{H}t} |\psi(0)\rangle = e^{-(i/\hbar)\hat{H}t} \sum_n a_n |n\rangle \xrightarrow{a_n = \delta_{n,0}} e^{-(i/\hbar)\hat{H}t} |0\rangle, \quad (3.171)$$

when the oscillator is initially in the state  $|0\rangle$ . Note that, without perturbation,  $|\psi(t)\rangle = \sum_n e^{-i\omega_{ho}(\hat{n}+1/2)t} a_n |n\rangle$ .

Various quantities now are interesting to plot as a function of time. Firstly, we calculate the populations  $|\langle n | \psi(t) \rangle|^2$  of the various states and the total energy from,

$$\begin{aligned} \langle n | \psi(t) \rangle &= \langle n | e^{-(i/\hbar)\hat{H}t} \sum_m a_m |m\rangle \\ E_{tot}(t) &= \sum_n \hbar\omega_{ho} \left( n + \frac{1}{2} \right) |\langle n | \psi(t) \rangle|^2 \end{aligned} \quad (3.172)$$

Secondly, we get for the temporal evolution of the spatial wavefunction,

$$\langle x | \psi(t) \rangle = \sum_n \langle x | n \rangle \langle n | \psi(t) \rangle = \sum_n \langle x | n \rangle \langle n | e^{-(i/\hbar)\hat{H}t} \sum_m a_m |m\rangle, \quad (3.173)$$

where  $|\langle x | n \rangle \langle n | \psi(t) \rangle|^2$  is the spatial representation of the wavefunction of the  $n$ -th eigenstate derived in (3.94),

$$\langle x | n \rangle = \frac{e^{-x^2/2a_{ho}^2} H_n(x/a_{ho})}{\sqrt{a_{ho}\sqrt{\pi}2^n n!}}, \quad (3.174)$$

weighed with instantaneous population (3.172) of this state. We thus obtain for the total wavefunction,

$$\langle x|\psi(t)\rangle = \sum_n \frac{e^{-x^2/2a_{ho}^2} H_n(x/a_{ho})}{\sqrt{a_{ho}\sqrt{\pi}2^n n!}} \langle n|e^{-(i/\hbar)\hat{H}t}|n\rangle. \quad (3.175)$$

Furthermore, we may calculate the expectation values of the position and the momentum of the harmonic oscillator from the total wavefunction  $\langle x|\psi(t)\rangle$ ,

$$\begin{aligned} \langle \psi(t)|\hat{x}|\psi(t)\rangle &= \int \langle \psi(t)|\hat{x}|x\rangle \langle x|\psi(t)\rangle dx = \int x|\psi(x,t)|^2 dx \\ \langle \psi(t)|\hat{p}|\psi(t)\rangle &= \int \langle \psi(t)|\hat{p}|p\rangle \langle p|\psi(t)\rangle dp = \int p|\phi(p,t)|^2 dx, \end{aligned} \quad (3.176)$$

where  $\phi(p,t)$  is the Fourier transform of  $\psi(x,t)$  according to (2.99). In practice, it is however easier to calculate them from the populations  $\langle n|\psi(t)\rangle$ ,

$$\begin{aligned} \langle \psi(t)|\hat{x}|\psi(t)\rangle &= \frac{a_{ho}}{\sqrt{2}} \sum_n \langle \psi(t)|\hat{a} + \hat{a}^\dagger|n\rangle \langle n|\psi(t)\rangle \\ \langle \psi(t)|\hat{p}|\psi(t)\rangle &= \frac{\hbar}{ia_{ho}\sqrt{2}} \sum_n \langle \psi(t)|\hat{a} - \hat{a}^\dagger|n\rangle \langle n|\psi(t)\rangle \end{aligned}. \quad (3.177)$$

The temporal evolution of the forced harmonic oscillator defined by (3.171) can be numerically propagated. In cases where the force varies in time, the propagation can be done iteratively by subdividing time in intervals  $t_k - t_{k-1}$  for  $k \in \mathbb{N}$  sufficiently small that the force can be considered constant within them,

$$|\psi(t_k)\rangle = e^{-(i/\hbar)\hat{H}(t_k - t_{k-1})} |\psi(t_{k-1})\rangle. \quad (3.178)$$

The results of such a simulation are illustrated in Fig. 3.19.

### 3.6.5 Quantization of the electromagnetic field

The quantization of light (also called *second quantization*) triggered by Max Planck's treatments of black-body radiation in 1905 resolved the problem of the ultraviolet divergence and explained the photoelectric effect. Twenty years later the quantization of the atom by Niels Bohr (also called *first quantization*) explained the internal structure of the atom.

The operator for the electric field of a laser mode is given by,

$$\hat{\mathcal{E}} = \imath\mathcal{E}_1 [\hat{a}e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t} - \hat{a}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega t}], \quad (3.179)$$

where  $\mathcal{E}_1 = \sqrt{\hbar\omega/2\varepsilon_0 V}$  is the electric field generated by a single photon in the mode volume  $V$ . Exc. 3.6.6.9 asks to calculate the eigenvalues  $\langle \hat{\mathcal{E}} \rangle$  and  $\Delta \hat{\mathcal{E}}$ .

It is sometimes convenient to represent the light field by its quadratures. With the definition  $\hat{a} \equiv \hat{x}_1 + \imath\hat{x}_2$ , where  $\hat{x}_{1,2}$  are non-commuting observables ( $[\hat{x}_1, \hat{x}_2] = \imath/2$ ), we can write the field as,

$$\hat{\mathcal{E}} = -2\mathcal{E}_1 [\hat{x}_1 \sin(\mathbf{k}\cdot\mathbf{r} - \omega t) + \hat{x}_2 \cos(\mathbf{k}\cdot\mathbf{r} - \omega t)]. \quad (3.180)$$

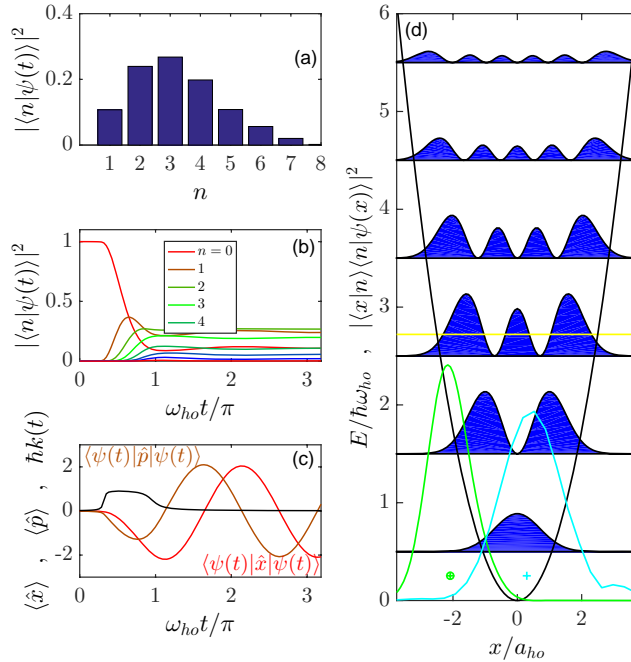


Figure 3.19: (code) Evolution of a harmonic oscillator subject to time-dependent forcing. (a) Histogram of the final population of the vibrational states. (b) Time evolution of the vibrational state populations. (c) Time evolution of the applied force (black) and of the expectation values of position (red) and momentum (brown). (d) Spatial wavefunctions  $|\langle n|\psi(x)\rangle|^2$  (Hermite polynomials) (blue) of the lowest vibrational states of the harmonic potential (black). The green Gaussian is the coherent sum of the spatial wavefunctions  $|\sum_n \langle n|\psi(x)\rangle|^2$ , and the cyan Gaussian the coherent sum of the momentum wavefunctions  $|\sum_n \langle n|\psi(p)\rangle|^2$ . The horizontal yellow line is the total energy of the system. You may also run a movie of the simulation clicking on [\(watch movie\)](#)! Furthermore, a presentation about the topic of recoil on trapped atoms is available at [\(watch talk\)](#)!

Heisenberg's uncertainty relations requires,

$$\Delta x_1 \Delta x_2 \geq \frac{1}{4}. \quad (3.181)$$

For coherent states,  $\Delta x_1 = \Delta x_2 = \frac{1}{2}$ .

### 3.6.6 Exercises

#### 3.6.6.1 Ex: Sum of displacements operators

Prove formula (3.117).

#### 3.6.6.2 Ex: Harmonic oscillator and coherent states

- Verify whether the Glauber states of a harmonic oscillator are orthogonal.
- Show that  $\langle \alpha|\hat{n}|\alpha\rangle = |\alpha|^2$ ,  $\langle \alpha|\hat{n}^2|\alpha\rangle = |\alpha|^4 + |\alpha|^2$ , and  $\Delta \hat{n} = |\alpha|$ .

c. What is the population of the state  $|n\rangle$  of a harmonic oscillator in a Glauber state?

### 3.6.6.3 Ex: Annihilation operator acting on Fock and Glauber states

Show that the annihilation operator  $\hat{a}$  does not reduce the photon number of a Glauber state in contrast to a Fock state.

### 3.6.6.4 Ex: Schrödinger cat state

Calculate the probability of finding  $n$  photons in Schrödinger's cat state  $|\psi\rangle = 2^{-1/2}(|\alpha\rangle \pm |-\alpha\rangle)$ .

### 3.6.6.5 Ex: Transition elements for arbitrary Lamb-Dicke parameters

Calculate the general expression for  $\langle m|e^{ik\hat{x}}|n\rangle$  with the abbreviation  $\alpha \equiv ik a_{ho}/\sqrt{2}$  for arbitrary values of the Lamb-Dicke parameter using the following results of the discussion of the displacement operator  $D(\alpha) = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = e^{-|\alpha|^2/2} e^{\alpha\hat{a}^\dagger} e^{-\alpha^*\hat{a}}$  for Glauber states. The relations

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \quad \text{and} \quad \langle n|\alpha\rangle = e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}}$$

describe the relation between Fock and Glauber states. Furthermore,

$$D(-\alpha) = D^\dagger(\alpha) \quad \text{and} \quad D^\dagger(\alpha)\hat{a}^\dagger D(\alpha) = \hat{a}^\dagger + \alpha^* .$$

### 3.6.6.6 Ex: Resonantly excited harmonic oscillator

Write down the Hamiltonian of a harmonic oscillator subject to an oscillating homogeneous force, and numerically simulate the evolution of the vibrational states starting from the ground state.

### 3.6.6.7 Ex: Shifted harmonic oscillator

Consider a HO of mass  $m$ , angular frequency  $\omega$ , and electric charge  $q$  immersed in a uniform electric field oriented parallel to the axis  $\hat{e}_x$  of the oscillator.

- Get the energies of the stationary states of the HO and show how to get the corresponding eigenstates.
- Calculate the expectation values  $\langle x \rangle$  and  $\langle p \rangle$  for the displaced oscillator now using Glauber states (or arbitrary superpositions of states) and taking advantage of the formulas (3.83), (3.116), and (2.165).
- Now, the electric field is suddenly turned off. Calculate the time evolution of the oscillator.

**3.6.6.8 Ex: Spatial wavefunction of a particle in a coherent state**

a. Derive the following relations for the harmonic oscillator having received a recoil momentum,

$$\langle \psi_n^{(1)} | \hat{x} | \psi_n^{(1)} \rangle = 0 \quad \text{and} \quad \langle \psi_n^{(1)} | \hat{p} | \psi_n^{(1)} \rangle = \hbar k .$$

b. Calculate the temporal evolution of the oscillator after having received the recoil via,

$$\langle x | e^{-i\hat{H}t/\hbar} e^{-ik\hat{x}} | n \rangle .$$

c. Calculate the spatial wavefunction of a particle in a coherent state  $\langle x | \alpha \rangle = \sum_n e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}} \langle x | n \rangle$ .

**3.6.6.9 Ex: Glauber state**

Calculate  $\langle \hat{E} \rangle$  and  $\Delta \hat{E}$ .

**3.6.6.10 Ex: Beam splitter**

A beam splitter is a device dividing an input mode (e.g. a laser beam) into two output modes 1 and 2. Assuming that a beam splitter sends every single photon with equal probability to one of the two output modes and that the input mode be a Fock state, what would be the photon statistics in the output mode? **Help:** Create the total output state  $|n_1, n_2\rangle$  from vacuum by successive application of the photon creation operator  $\hat{a}_1^\dagger + \hat{a}_2^\dagger$ .

**3.6.6.11 Ex: Glauber state**

Derive the wavefunction for a harmonic oscillator in a coherent state using the exponential generating function of Hermite polynomials,

$$e^{2xt-t^2} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x) .$$

**3.7 (Quasi-)probability distribution functions**

As we have seen in the last sections, quantum observables are intrinsically affected by quantum noise, which leads to a spreading of their representation in phase space. For the case of Glauber states of a harmonic oscillator we illustrated in Fig. 3.14 the uncertainty of conjugate variables by circles around their expectation values whose areas are determined by the Heisenberg uncertainty relation. These circles represent phase space probability distribution functions. These are distribution functions measuring the probability to encounter the observables at specific points in phase space.

States other than Glauber states are possible, for instance Fock or cat states. Some of these states may exhibit quantum correlations, which we would like to identify in probability distributions. Quantum correlation in systems with small Hilbert spaces, such as the two-level atom, are conveniently represented by a density operator or by the Bloch vector introduced in Eq. (2.48). Large or infinite Hilbert spaces require

different approaches. We have seen in Sec. 3.6.1 how to expand the state of a harmonic oscillator on a Fock state basis. On the other hand, we have seen that Glauber states are more 'natural' states for a harmonic oscillator, so that we would like to visualize expansions of arbitrary states into a coherent state basis.

The following sections are devoted to introducing various such distribution functions [616] and to calculating them for a selection of particular states, such as the Fock and the Glauber state, the thermal state, and the Schrödinger cat state. We will restrict the discussion to pure states, postponing a discussion of the representation of statistical mixtures to Sec. 15.2, where we will also extend the discussion to quantum correlations in light fields resulting from a Jaynes-Cummings type interaction of an atom with a light mode.

### 3.7.1 The density operator

We define the *density operator* for a pure state as,

$$\hat{\rho} \equiv |\psi\rangle\langle\psi|. \quad (3.182)$$

A detailed discussion of the density operator for non pure states, that is, statistical mixtures will be given in Sec. 14.1. The definition (3.182) is independent from a chosen basis, but a proper representation can be found by simply expanding the state  $|\psi\rangle$  on a proper basis.

### 3.7.2 The Wigner function

The *Wigner function* represents something like the spectrum of two-dimensional phase-space correlation function. For a pure state and a one-dimensional system it is defined by,

$$W(x, p) \equiv \frac{1}{\pi} \int_{-\infty}^{\infty} \langle\psi|x+y\rangle\langle x-y|\psi\rangle e^{2ipy/\hbar} dy. \quad (3.183)$$

**Example 24 (Wigner function of a free particle in 3D):** For example, for a free particle described by the wavefunction in three-dimensional space,

$$\langle\mathbf{r}|\psi\rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}},$$

the Wigner function is,

$$\begin{aligned} W(\mathbf{r}, \mathbf{p}) &= \frac{1}{\pi^3} \int_{-\infty}^{\infty} \frac{1}{\sqrt{V}} e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{x})} \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{x})} e^{(2i/\hbar)\mathbf{p}\cdot\mathbf{x}} d^3x \\ &= \frac{1}{\pi^3 V} \int_{-\infty}^{\infty} e^{-2i(\mathbf{k}-\mathbf{p}/\hbar)\cdot\mathbf{x}} d^3x = \frac{1}{V} \delta^3(\mathbf{p} - \hbar\mathbf{k}). \end{aligned}$$

For a harmonic oscillator, the Wigner function can be embedded into a formalism that will be detailed in the following sections.



### 3.7.3 $P$ , $Q$ , and Wigner functions for the harmonic oscillator

The most common distribution function in a coherent state basis are the so-called *P-function* (or *Glauber-Sudarshan representation*), the *Q-function* (or *Husimi representation*), and the (already introduced) Wigner function. Defining the two-dimensional complex inverse Fourier transform by,

$$(\mathcal{F}^{-1}\chi)(\alpha) = \frac{1}{\pi^2} \int \chi(\lambda) e^{\lambda^* \alpha - \lambda \alpha^*} d^2\lambda \quad (3.184)$$

with  $d^2\lambda = d\text{Re } \lambda d\text{Im } \lambda = dr_\lambda dp_\lambda$ ,

these three coherent distribution functions are expressed by inverse Fourier transforms of the following characteristic functions <sup>8</sup>,

$\chi_N(\lambda) = \langle \psi   e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}}   \psi \rangle$	,	$P = \mathcal{F}^{-1} \chi_N$
$\chi_S(\lambda) = \langle \psi   e^{\lambda \hat{a}^\dagger - \lambda^* \hat{a}}   \psi \rangle$	,	$W = \mathcal{F}^{-1} \chi_S$
$\chi_A(\lambda) = \langle \psi   e^{-\lambda^* \hat{a}} e^{\lambda \hat{a}^\dagger}   \psi \rangle$	,	$Q = \mathcal{F}^{-1} \chi_A$

Here, the index  $N$  denotes *normal order*,  $S$  *symmetric order*, and  $A$  *antisymmetric order*.  $D(\alpha) = e^{\lambda \hat{a}^\dagger - \lambda^* \hat{a}}$  is the displacement operator defined in (3.109). We see that the distribution functions  $\chi_{N,S,A}$  are related to each other. Using the *Baker-Hausdorff formula* (3.108) we derive in Exc. 3.7.5.1 the so-called disentangling theorem [264],

$$e^{-|\lambda|^2/2} \chi_N(\lambda) = \chi_S(\lambda) = e^{|\lambda|^2/2} \chi_A(\lambda). \quad (3.185)$$

Thus,  $Q$ -function corresponds to a smoothed Wigner function, which in turn corresponds to a smoothed  $P$ -function. The inverse complex Fourier transformation converts the products in (3.185) into convolutions. Exploiting the useful integral formula,

$$\frac{1}{\pi} \int e^{-a|\lambda|^2 + b\lambda + c\lambda^*} d^2\lambda = \frac{1}{a} e^{bc/a}, \quad (3.186)$$

we find,

$$W = P \star \frac{2}{\pi} e^{-2|\lambda|^2} \quad \text{and} \quad Q = W \star \frac{2}{\pi} e^{-2|\lambda|^2} = P \star \frac{1}{\pi} e^{-|\lambda|^2}. \quad (3.187)$$

The distribution functions can be interpreted as follows:  $P(\alpha)$  is the probability of finding the coherent state  $|\alpha\rangle$  within the statistical mixture given by,

$$\hat{\rho} = \int P(\alpha) |\alpha\rangle \langle \alpha| d^2\alpha, \quad (3.188)$$

<sup>8</sup>For statistical mixtures, such as for example thermal states, we need to generalize the definition of the characteristic functions to,

$$\chi_N(\lambda) = \text{Tr } \hat{\rho} e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \quad , \quad \chi_S(\lambda) = \text{Tr } \hat{\rho} e^{\lambda \hat{a}^\dagger - \lambda^* \hat{a}} \quad , \quad \chi_A(\lambda) = \text{Tr } \hat{\rho} e^{-\lambda^* \hat{a}} e^{\lambda \hat{a}^\dagger} .$$

and  $Q(\alpha)$  is the expectation value of the density operator (3.182):

$$Q(\alpha) = \frac{1}{\pi} \langle \alpha | \hat{\rho} | \alpha \rangle . \quad (3.189)$$

The various states that a light field can adopt can now be expressed either by photon number distribution in a Fock state basis, or by two-dimensional weighting functions  $P, Q, W$  in a coherent state basis. Here, are some examples for these representations.

### 3.7.3.1 Characteristic functions for arbitrary HO states in the Fock basis

If a state of a harmonic oscillator can be expanded into Fock states,

$$|\psi\rangle = \sum_n c_n |n\rangle , \quad (3.190)$$

the normally ordered characteristic function (3.185) will be composed of terms like  $\langle m | e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} | n \rangle$ . To evaluate these terms, we begin calculating,

$$\hat{a}^k |n\rangle = \sqrt{\frac{n!}{(n-k)!}} |n-k\rangle \quad \text{for } k \leq n \quad \text{and} \quad \hat{a}^k |n\rangle = 0 \quad \text{for } k \geq n , \quad (3.191)$$

and,

$$e^{-\lambda^* \hat{a}} |n\rangle = \sum_{k=0}^{\infty} \frac{(-\lambda^* \hat{a})^k}{k!} |n\rangle = \sum_{k=0}^n \frac{(-\lambda^*)^k}{\sqrt{k!}} \sqrt{\binom{n}{k}} |n-k\rangle . \quad (3.192)$$

Hence, assuming  $m \geq n$ ,

$$\begin{aligned} \langle m | e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} | n \rangle &= \sum_{k=0}^n \frac{(-\lambda^*)^k \lambda^{m-n+k}}{\sqrt{k!(m-n+k)!}} \sqrt{\binom{n}{k} \binom{m}{m-n+k}} \\ &= \sqrt{\frac{n!}{m!}} \lambda^{m-n} \sum_{k=0}^n \binom{m}{k+m-n} \frac{(-|\lambda|^2)^k}{k!} = \sqrt{\frac{n!}{m!}} \lambda^{m-n} L_n^{m-n}(|\lambda|^2) , \end{aligned} \quad (3.193)$$

where  $L_n^{m-n}$  are Laguerre polynomials. Now, exploiting the fact that

$$\begin{aligned} \langle m | e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} | n \rangle &= (\langle n | e^{-\lambda \hat{a}^\dagger} e^{\lambda^* \hat{a}} | m \rangle)^\dagger = \overline{\langle n | e^{-\lambda \hat{a}^\dagger} e^{\lambda^* \hat{a}} | m \rangle} \\ &= \sqrt{\frac{m!}{n!}} (-\lambda^*)^{n-m} L_n^{n-m}(|\lambda|^2) , \end{aligned} \quad (3.194)$$

and with the expansion (3.190) we obtain for the normally-ordered characteristic function,

$$\begin{aligned} \chi_N(\lambda) &= \sum_{m,n} c_m^* c_n \langle m | e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} | n \rangle \\ &= \sum_{m \geq n} (1 - \frac{1}{2} \delta_{m,n}) \left( c_m^* c_n \langle m | e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} | n \rangle + \overline{c_m^* c_n \langle m | e^{-\lambda \hat{a}^\dagger} e^{\lambda^* \hat{a}} | n \rangle} \right) . \end{aligned} \quad (3.195)$$

finally yielding,

$$\chi_N(\lambda) = \sum_{m \geq n} \left(1 - \frac{1}{2} \delta_{m,n}\right) \left[ c_m^* c_n \lambda^{m-n} + c_m c_n^* (-\lambda^*)^{m-n} \right] \sqrt{\frac{n!}{m!}} L_n^{m-n}(|\lambda|^2). \quad (3.196)$$

Remembering that the symmetrically ordered function is given by  $\chi_S(\lambda) = e^{-|\lambda|^2} \chi_N(\lambda)$  we may obtain the Wigner function by a numerical two-dimensional FFT,

$$W(\alpha) = \frac{1}{\pi^2} \int e^{-|\lambda|^2} \chi_N(\lambda) e^{\lambda^* \alpha - \lambda \alpha^*} d^2 \lambda. \quad (3.197)$$

We will use this result in Sec. 15.2.2 to characterize correlations in an optical mode emanating from a Jaynes-Cummings type coupling to an atom. In Exc. 3.7.5.2 we will try to find an analytic solution for this integral.

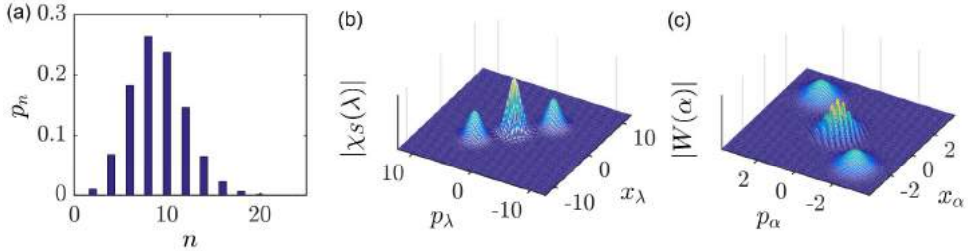


Figure 3.20: (code) Starting from a cat-state photon distribution, as shown in (a), we calculate the symmetrically ordered characteristic function (b) from the expression (3.195), and the Wigner function (c) by an FFT.

### 3.7.4 Representation of particular states in the Fock and Glauber basis

#### 3.7.4.1 Representations of Glauber states

We have seen earlier that coherent states  $|\beta\rangle$  can be expanded on a Fock state basis  $|n\rangle$ . For the state function, the density operator, and the photon number distribution we have,

$$\begin{aligned} |\beta\rangle &= e^{-|\beta|^2/2} \sum_n \frac{\beta^n}{\sqrt{n!}} |n\rangle \\ \hat{\rho} &= e^{-|\beta|^2} \sum_{m,n} \frac{\beta^n \beta^{*m}}{\sqrt{m!n!}} |n\rangle \langle m| \\ P_n &= |\langle n|\beta\rangle|^2 = e^{-|\beta|^2} \frac{|\beta|^{2n}}{n!} \end{aligned} \quad (3.198)$$

Expanding a coherent state on a basis of Glauber states, we will derive in Exc. 3.7.5.3 the  $P$ -function, the density matrix, the  $Q$ -function, and the Wigner function,

$$\begin{aligned}
 |\psi\rangle &= |\beta\rangle \\
 P_{|\beta\rangle}(\alpha) &= \delta^{(2)}(\alpha - \beta) \\
 \hat{\rho} &= \int \delta^{(2)}(\alpha - \beta) |\alpha\rangle\langle\alpha| d^2\alpha = |\beta\rangle\langle\beta| \\
 Q_{|\beta\rangle}(\alpha) &= \frac{1}{\pi} e^{-|\alpha-\beta|^2} \\
 W_{|\beta\rangle}(\alpha) &= \frac{2}{\pi} e^{-2|\alpha-\beta|^2}
 \end{aligned} \tag{3.199}$$

**Example 25 (State of a laser):** Following [597], the correct *state of a laser* beam is not simply a coherent state, but rather,

$$\hat{\rho} = \int |\alpha e^{i\varphi}\rangle\langle\alpha e^{i\varphi}| \frac{d\varphi}{2\pi} . \tag{3.200}$$

After averaging, this state can be written as a superposition of Fock states,

$$\hat{\rho} = \sum_n P_n |n\rangle\langle n| , \tag{3.201}$$

but without a specific phase,

$$\hat{\rho} \neq \sum_{m,n} c_m^* c_n |m\rangle\langle n| . \tag{3.202}$$

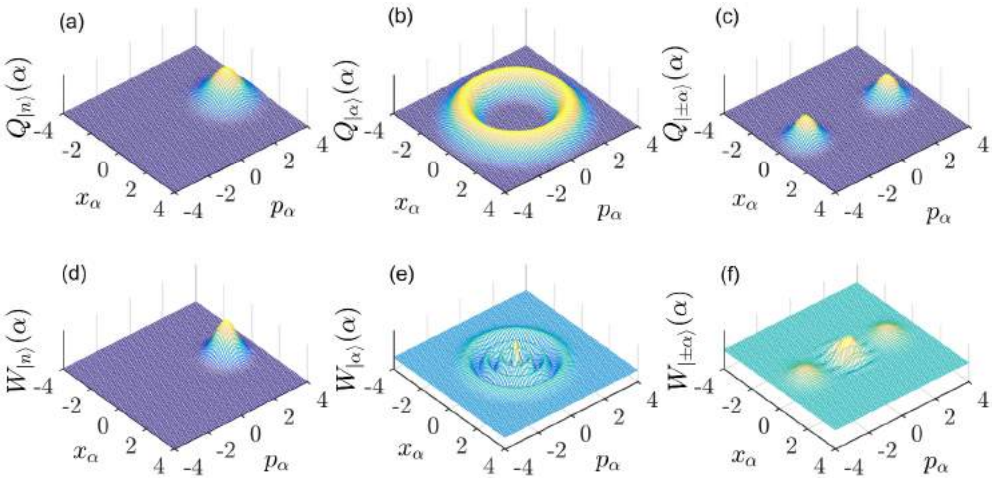


Figure 3.21: (code) (a-c)  $Q$  functions and (d-f) Wigner functions of a Glauber state (a,d), a Fock state (b,e), and a Schrödinger cat state (c,f).

### 3.7.4.2 Representations of Schrödinger cat states

Schrödinger cat states are correlated states of many particles (or quasi-particles). The expansion of the *Schrödinger cat state*  $|\beta_0\rangle \pm |\beta_1\rangle$  on a Fock state basis yields, as we have seen in Exc. 3.6.6.4,

$$\begin{aligned} |\psi_{\pm}\rangle &= \sum_n \frac{e^{-|\beta_0|^2/2} \beta_0^n \pm e^{-|\beta_1|^2/2} \beta_1^n}{\sqrt{2n!}} |n\rangle \\ P_n &= |\langle n|\psi_{\pm}\rangle|^2 \longrightarrow e^{-|\beta_0|^2} \frac{|\beta_0|^{2n}}{n!} \frac{|1 \pm (-1)^n|^2}{2} \quad \text{for } \beta_0 = -\beta_1 \end{aligned} \quad (3.203)$$

Expanding a Schrödinger cat state on a basis of Glauber states, we will derive in Exc. 3.7.5.4 the  $P$ -function, the density matrix, the  $Q$ -function, and the Wigner function,

$$\begin{aligned} |\psi_{\pm}\rangle &= \frac{1}{C} (|\beta_0\rangle \pm |\beta_1\rangle) \quad \text{with} \quad C = \sqrt{2 \pm 2e^{-|\beta_0 - \beta_1|^2}} \\ P_{|\beta_0\rangle|\beta_1\rangle}(\alpha) &= \delta^{(2)}(\alpha - \beta_0) + \delta^{(2)}(\alpha - \beta_1) \\ \hat{\rho} &= |\psi_{\pm}\rangle\langle\psi_{\pm}| \\ Q_{|\beta_0\rangle|\beta_1\rangle}(\alpha) &= \frac{1}{\pi} e^{-|\alpha - \beta_0|^2} + \frac{1}{\pi} e^{-|\alpha - \beta_1|^2} \\ W_{|\beta_0\rangle|\beta_1\rangle}(\alpha) &= \frac{2}{C^2\pi} \left( e^{-2|\alpha - \beta_0|^2} + e^{-2|\alpha - \beta_1|^2} \right. \\ &\quad \left. \pm 2e^{-|\beta_0|^2/2 - |\beta_1|^2/2} \text{Re} e^{-2(\beta_1 - \alpha)(\beta_0^* - \alpha^*) + \beta_0^* \beta_1} \right) \end{aligned} \quad (3.204)$$

We know from microscopic systems, for instance a two-level atom, that they can live in superposition states  $|1\rangle + |2\rangle$ . In contrast, the Schrödinger cat states discussed above occur in continuous Schrödinger fields involving many particles. Macroscopic quantum interferences (i.e. interferences that are detectable with macroscopic apparatuses, for example in heterodyne schemes) are named *fuzzy Schrödinger cats*, if the interfering states are conspicuously separated in phase space.

At this point, we have to emphasize the fundamental difference between Schrödinger cats and superpositions of modes,

$$\begin{aligned} |\psi\rangle &= |\alpha\rangle + |\beta\rangle && \neq |\alpha\rangle|\beta\rangle \\ \hat{\rho} &= |\alpha\rangle\langle\alpha| + |\beta\rangle\langle\beta| + |\alpha\rangle\langle\beta| + |\beta\rangle\langle\alpha| && \neq |\alpha\beta\rangle\langle\alpha\beta| \end{aligned} \quad (3.205)$$

Schrödinger cats exhibit interferences in phase space, whereas for mode superpositions, interferences only appear when a parameter is varied (e.g., the length of an interferometer arm).

Schrödinger cat states are very sensitive to dissipation and easily converted into statistical mixtures. For example,  $|\alpha\rangle \pm |-\alpha\rangle$  contains only odd (even) photon numbers in the distribution function  $P_n$ . After some time  $\sim \tau_{cav}/N$ , the distribution is converted into a Poisson distribution. The higher the particle number  $N$ , the faster the decoherence will be. Consequently, *truly macroscopic* cat states have never been observed.

### 3.7.4.3 Representations of Fock states

On the Fock state basis  $|n\rangle$ , a number state is characterized by,

$$\boxed{\begin{aligned} |n\rangle &= (\hat{a}^\dagger)^n |0\rangle \\ \hat{\rho} &= |n\rangle\langle n| \\ P_k &= \delta_{nk} \end{aligned}}. \quad (3.206)$$

This state can be expanded into Glauber states  $|\alpha\rangle$  by following procedure. For large  $n$  we first calculate the  $P$ -distribution function,

$$P_{|n\rangle}(\alpha) = \delta^{(1)}(|\alpha| - \sqrt{n}), \quad (3.207)$$

because it allows us to derive the density matrix via the formula (3.188),

$$\begin{aligned} \hat{\rho}_{|n\rangle} &= \int \delta^{(1)}(|\alpha| - \sqrt{n}) |\alpha\rangle\langle\alpha| d^2\alpha \\ &= \int_0^\infty \int_0^{2\pi} \delta^{(1)}(|\alpha| - \sqrt{n}) |\alpha\rangle\langle\alpha| |\alpha| d|\alpha| d\varphi_\alpha = \sqrt{n} \int_0^{2\pi} |\alpha\rangle\langle\alpha| d\varphi_\alpha. \end{aligned} \quad (3.208)$$

The  $Q$ -distribution function becomes, inserting the density operator obtained in (3.208),

$$\begin{aligned} Q_{|n\rangle}(\alpha) &= \frac{1}{\pi} \langle\alpha|\hat{\rho}_{|n\rangle}|\alpha\rangle \\ &= \frac{1}{\pi} n \int_0^{2\pi} |\langle\alpha|\beta\rangle|^2 d\varphi_\beta = \frac{1}{\pi} n \int_0^{2\pi} e^{-|\alpha-\beta|e^{i\varphi_\beta}|^2} d\varphi_\beta \triangleq \frac{|\alpha|^{2n}}{\pi n!} e^{-|\alpha|^2}, \end{aligned} \quad (3.209)$$

and finally the Wigner function is,

$$W_{|n\rangle}(\alpha) = \frac{2}{\pi} e^{-2|\alpha|^2} (-1)^n \sum_{m=0}^n \binom{n}{m} \frac{(-4|\alpha|^2)^m}{m!} = \frac{2}{\pi} e^{-2|\alpha|^2} (-1)^n L_n(4|\alpha|^2), \quad (3.210)$$

where  $L_m(4|\alpha|^2)$  are Laguerre polynomials. In Exc. 3.7.5.5 we will learn how to derive the above distribution functions directly from the characteristic functions. In summary, we have,

$$\boxed{\begin{aligned} |\psi\rangle &= |n\rangle \\ P_{|n\rangle}(\alpha) &= \delta^{(1)}(|\alpha| - \sqrt{n}) \\ \hat{\rho} &= \sqrt{n} \int_0^{2\pi} |\alpha\rangle\langle\alpha| d\varphi_\alpha \\ Q_{|n\rangle}(\alpha) &= \frac{|\alpha|^{2n}}{\pi n!} e^{-|\alpha|^2} \\ W_{|n\rangle}(\alpha) &= \frac{2}{\pi} e^{-2|\alpha|^2} (-1)^n L_n(4|\alpha|^2) \end{aligned}}. \quad (3.211)$$

### 3.7.4.4 Representations of thermal states

A light mode in a thermal mixture can not be represented by a pure state, but requires a density matrix description beyond (3.182). We have not introduced the concept of statistical mixtures, yet, which will be done in Sec. 14.1. Therefore, the following formulas are only given for the sake of completeness,

$$\hat{\rho}_{therm} = \sum_n \frac{\bar{n}^n}{(1 + \bar{n})^{1+n}} |n\rangle\langle n|. \quad (3.212)$$

The coherent distribution  $P$ -function is,

$$\begin{aligned} P_{therm}(\alpha) &= \frac{1}{\pi\bar{n}} e^{-|\alpha|^2/\bar{n}} \\ \hat{\rho} &= \frac{1}{\pi\bar{n}} \int e^{-|\alpha|^2/\bar{n}} |\alpha\rangle\langle\alpha| d^2\alpha \\ Q_{therm}(\alpha) &= \frac{1}{\pi(\bar{n}+1)} e^{-|\alpha|^2/(\bar{n}+1)} \\ W_{therm}(\alpha) &= \frac{1}{\pi(\bar{n}+1/2)} e^{-|\alpha|^2/(\bar{n}+1/2)} \end{aligned} \quad (3.213)$$

### 3.7.5 Exercises

#### 3.7.5.1 Ex: Relationship between the characteristic functions

Derive the relationship (3.185) between the characteristic functions of the Glauber state basis.

#### 3.7.5.2 Ex: Wigner function for arbitrary HO states in the Fock basis

Search an analytic solution for the integral (3.196).

#### 3.7.5.3 Ex: $P$ -, $Q$ -, and Wigner distribution functions for Glauber states

Starting from the characteristic functions  $\chi_{A,S,N}(\lambda)$  derive for a coherent state  $|\beta\rangle$  (a) the Husimi representation, (b) the Glauber-Sudarshan representation, and (c) the Wigner representation.

#### 3.7.5.4 Ex: $P$ -, $Q$ -, and Wigner distribution functions for cat states

Starting from the characteristic functions  $\chi_{A,S,N}(\lambda)$  derive for a normalized cat state  $C^{-1}(|\beta_0\rangle + |\beta_1\rangle)$  (a) the Husimi representation, (b) the Glauber-Sudarshan representation, and (c) the Wigner representation.

#### 3.7.5.5 Ex: $P$ -, $Q$ -, and Wigner distribution functions for Fock states

Starting from the characteristic functions  $\chi_{A,S,N}(\lambda)$  derive for a number state  $|n\rangle$  (a) the Husimi representation, (b) the Glauber-Sudarshan representation, and (c) the Wigner representation.

**3.7.5.6 Ex: Wigner distribution function of a Fock state**

Calculate the Wigner function for a harmonic oscillator in a Fock state from its wavefunction  $\langle x|n\rangle$ .

**3.7.5.7 Ex: Calculating with Wirtinger derivatives**

Prove the following identities [264],

$$\hat{a}^\dagger - \alpha^* = \frac{\partial}{\partial \underline{\alpha}} \quad \text{and} \quad \hat{a}^\dagger - \alpha = \frac{\partial}{\partial \underline{\alpha}^*} .$$

Note, that with the bosonic operators we can construct the observables,

$$\hat{x} + i\hat{p} = \sqrt{2}\hat{a} \quad , \quad \partial_x - i\partial_p = 2\frac{\partial}{\partial \underline{\alpha}} \quad , \quad \partial_x + i\partial_p = 2\frac{\partial}{\partial \underline{\alpha}^*} .$$

In two dimensions [238],  $d^2\alpha = d(\text{Re } \alpha)d(\text{Im } \alpha) = dx dp$ .

**3.7.5.8 Ex: Characteristic functions**

- Evaluate the expression  $\left. \frac{\partial^{m+n} \chi_X(\lambda)}{\partial \lambda^{*m} \partial (-\lambda)^n} \right|_{\lambda=0}$  for  $X = N, S, A$ .
- Consider the particular case of a coherent state.

**3.7.5.9 Ex: Moments of Glauber states**

Prove the following relations:

$$\begin{aligned} \langle \hat{a}_j^{\dagger m} \hat{a}_k^n \rangle &= \int P(\alpha) \alpha_j^n \alpha_k^{*m} d\alpha \\ \langle \hat{a}_j^m \hat{a}_k^{\dagger n} \rangle &= \int Q(\alpha) \alpha_j^m \alpha_k^{*n} d\alpha \\ \langle \{ \hat{a}_j^{\dagger m} \hat{a}_k^n \}_S \rangle &= \int W(\alpha) \alpha_j^m \alpha_k^{*n} d\alpha , \end{aligned}$$

where the index  $S$  denotes *symmetric ordering*. Symmetric or *Weyl ordering* means that all products  $\hat{r}\hat{p}$  must be replaced by the symmetric expressions, such as  $(\hat{r}\hat{p} + \hat{p}\hat{r})/2$ .

**3.8 Squeezed states of the harmonic oscillator****3.8.1 The squeezing operator**

Let us consider a Hamiltonian of the following form,

$$\boxed{\hat{H}_{sqz} = \hbar\omega \hat{a}^\dagger \hat{a} + \frac{i}{2} \hbar \xi \hat{a}^{\dagger 2} + \frac{i}{2} \hbar \xi^* \hat{a}^2} . \quad (3.214)$$

leading to the equation of motion,

$$\dot{\hat{a}} = -i\omega \hat{a} + 2g \hat{a}^\dagger . \quad (3.215)$$



The non-linear, i.e. quadratic, appearance of the field operators suggests that the interaction should include correlation pair production, as is the case for parametric processes or four-wave mixing. We will see later that cavities are good for producing squeezing. However, the unused ports of a cavity let vacuum fluctuations come in, which partially overrule squeezing.

For now, we study, in analogy with the displacement operator (3.109), the propagator  $e^{-i\hat{H}_{sqz}t/\hbar}$ , i.e the operator given by,

$$\boxed{\hat{S}(\xi) \equiv e^{\xi\hat{a}^\dagger/2 - \xi^*\hat{a}^2/2}}, \quad (3.216)$$

which we will call the *squeezing operator* because, applied to the vacuum state,  $|\xi\rangle = S(\xi)|0\rangle$ , this operator will compress the uncertainty of one quadrature component, as we will see shortly.

In analogy with the calculation (3.110), using the commutation rules, it is possible to verify the unitarity of this operator [441] (see Exc. 3.8.4.1). In particular, using the relationship (2.165) and the abbreviation  $\hat{A} \equiv \frac{\xi}{2}\hat{a}^\dagger - \frac{\xi^*}{2}\hat{a}^2$ , we can show [665] (see Exc. 3.8.4.2),

$$\begin{aligned} \hat{S}^\dagger(\xi)\hat{a}\hat{S}(\xi) &= e^{\hat{A}}\hat{a}e^{-\hat{A}} = \hat{a} + [\hat{A}, \hat{a}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{a}]] + \frac{1}{3!}[\hat{A}, [\hat{A}, [\hat{A}, \hat{a}]]] \dots \quad (3.217) \\ &= \hat{a} + \xi\hat{a}^\dagger + \frac{1}{2!}\xi\xi^*\hat{a} + \frac{1}{3!}\xi\xi^*\xi\hat{a}^\dagger + \dots = \hat{a} \cosh|\xi| + \frac{|\xi|}{\xi^*}\hat{a}^\dagger \sinh|\xi|, \end{aligned}$$

and similarly for  $\hat{a}^\dagger$ , such that with  $\xi \equiv re^{i\varphi}$ ,

$$\boxed{\begin{aligned} \hat{S}^\dagger(\xi)\hat{a}\hat{S}(\xi) &= \hat{a} \cosh r + e^{-i\varphi}\hat{a}^\dagger \sinh r \\ \hat{S}^\dagger(\xi)\hat{a}^\dagger\hat{S}(\xi) &= \hat{a}^\dagger \cosh r + e^{i\varphi}\hat{a} \sinh r \end{aligned}}. \quad (3.218)$$

The formulas (3.218) describe a *Bogolubov transform*, as they can be cast into the form,

$$\boxed{\hat{b} \equiv u\hat{a} + v\hat{a}^\dagger, \quad \hat{b}^\dagger \equiv u^*\hat{a}^\dagger + v^*\hat{a}}, \quad (3.219)$$

for complex numbers  $u$  and  $v$ . By postulating the same commutation relation for new operators,  $[\hat{b}, \hat{b}^\dagger] = 1$ , we immediately get the condition,

$$|u|^2 - |v|^2 = 1. \quad (3.220)$$

Comparing with the hyperbolic identity  $\cosh^2 r - \sinh^2 r = 1$ , we can parametrize the constants as,

$$u = \cosh r \quad \text{and} \quad v = e^{i\varphi} \sinh r. \quad (3.221)$$

This is interpreted as a linear symplectic transformation in phase space between pairs of annihilation and creation operators satisfying the same commutation relation  $[\hat{a}, \hat{a}^\dagger] = 1$ .

### 3.8.1.1 Relation between squeezing and displacement operator

The squeezing operator *does not commute* with the displacement operator. However, from (3.218) we can derive the following simple relation,

$$\hat{S}(\xi)\hat{D}(\alpha) \neq \hat{D}(\alpha)\hat{S}(\xi) = \hat{S}(\xi)\hat{D}(\alpha \cosh r + \alpha^* e^{i\theta} \sin r). \quad (3.222)$$

Solve the Exc. 3.8.4.3.

Squeezed coherent states are generated by coherent displacement of a *squeezed vacuum*,

$$|\alpha, \xi\rangle = \hat{S}(\xi)|0, \xi\rangle = \hat{D}(\alpha)\hat{S}(\xi)|0\rangle. \quad (3.223)$$

On the other hand, from (3.222),

$$\begin{aligned} \hat{D}(\alpha)\hat{S}(\xi)|0\rangle &= \hat{S}(\xi)\hat{D}(\alpha \cosh r + \alpha^* e^{i\varphi} \sinh r)|0\rangle \\ &= \hat{S}(\xi)|\alpha \cosh r + \alpha^* e^{i\varphi} \sinh r\rangle. \end{aligned} \quad (3.224)$$

### 3.8.1.2 Squeezing of the uncertainty relation

The real and imaginary parts of the transformed operators, defined by  $\hat{b} = \hat{x}_b + i\hat{y}_b$ , are Hermitian and satisfy the Heisenberg uncertainty relation (2.88),

$$[\hat{x}_b, \hat{y}_b] = \frac{i}{2} \quad \text{and} \quad \Delta\hat{x}_b\Delta\hat{y}_b \geq \frac{1}{2i}\langle[\hat{x}_b, \hat{y}_b]\rangle = \frac{1}{4}. \quad (3.225)$$

However, let us take a look at the uncertainties separately. They relate to the Glauber mode via,

$$\begin{aligned} \hat{x}_b &= \frac{1}{2}(\hat{b} + \hat{b}^\dagger) = \frac{1}{2}(\hat{a} \cosh r + \hat{a}^\dagger e^{i\varphi} \sinh r) + \frac{1}{2}(\hat{a}^\dagger \cosh r + \hat{a} e^{-i\varphi} \sinh r) \\ &= \hat{x}_a \cosh r + \frac{1}{2} \sinh r (\hat{a}^\dagger e^{i\varphi} + \hat{a} e^{-i\varphi}) \xrightarrow{\varphi=0} \hat{x}_a e^r \\ \hat{y}_b &= \frac{1}{2i}(\hat{b} - \hat{b}^\dagger) = \frac{1}{2i}(\hat{a} \cosh r + \hat{a}^\dagger e^{i\varphi} \sinh r) - \frac{1}{2i}(\hat{a}^\dagger \cosh r + \hat{a} e^{-i\varphi} \sinh r) \\ &= \hat{y}_a \cosh r + \frac{1}{2i} \sinh r (\hat{a}^\dagger e^{i\varphi} - \hat{a} e^{-i\varphi}) \xrightarrow{\varphi=0} \hat{y}_a e^{-r}. \end{aligned} \quad (3.226)$$

The individual fluctuations are (assuming  $\varphi = 0$ ),

$$\begin{aligned} \Delta\hat{x}_b^2 &= \langle\hat{x}_b^2\rangle - \langle\hat{x}_b\rangle^2 = e^{2r} (\langle\hat{x}_a^2\rangle - \langle\hat{x}_a\rangle^2) \\ &= \frac{1}{4}e^{2r} (1 + \langle\hat{a}^2\rangle + \langle\hat{a}^\dagger\rangle^2 + 2\langle\hat{a}^\dagger\hat{a}\rangle - \langle\hat{a}\rangle^2 - \langle\hat{a}^\dagger\rangle^2 - 2\langle\hat{a}^\dagger\rangle\langle\hat{a}\rangle). \end{aligned} \quad (3.227)$$

With  $\langle\hat{a}\rangle = 0$ ,

$$\begin{aligned} \Delta\hat{x}_b^2 &= e^{2r} \left( \frac{1}{2}\text{Re} \langle\hat{a}^2\rangle + \frac{1}{4} + \frac{1}{2}\langle\hat{a}^\dagger\hat{a}\rangle \right) \\ \Delta\hat{y}_b^2 &= e^{-2r} \left( -\frac{1}{2}\text{Re} \langle\hat{a}^2\rangle + \frac{1}{4} + \frac{1}{2}\langle\hat{a}^\dagger\hat{a}\rangle \right). \end{aligned} \quad (3.228)$$

Looking at the coherent vacuum,  $\hat{a}|\alpha\rangle = 0$ , hence,

$$\Delta\hat{x}_b = \frac{1}{2}e^r \quad \text{and} \quad \Delta\hat{y}_b = \frac{1}{2}e^{-r}, \quad (3.229)$$

and the squeezed state is a the uncertainty minimum.

### 3.8.2 Squeezed state in the Fock basis

The numbers of photons in the squeezed state is [441],

$$\langle n|\alpha, \xi\rangle = \frac{(\zeta/2)^{n/2}}{\sqrt{n! \cosh r}} e^{-\frac{1}{2}(|\alpha|^2 + \alpha^*\zeta)} H_n \left( \frac{\alpha + \alpha^*\zeta}{\sqrt{2\zeta}} \right), \quad (3.230)$$

with the abbreviation  $\zeta \equiv e^{i\theta} \tanh r$ . For squeezed vacuum  $\alpha = 0$ , noting that  $H_n(0) = (-2)^{n/2}(n-1)!!$  for even  $n$  and  $H_n(0) = 0$  for odd  $n$ , we find,

$$\langle n|0, \xi \rangle = \frac{(-\zeta)^{n/2}(n-1)!!}{\sqrt{n!} \cosh r} \quad (3.231)$$

for even photon number. Odd photon numbers are excluded. Hence,

$$\begin{array}{l} |\alpha, \xi \rangle = \sum_n |n\rangle \langle n|\alpha, \xi \rangle \\ \hat{\rho} = |\alpha, \xi \rangle \langle \alpha, \xi| \\ P_n = |\langle n|\alpha, \xi \rangle|^2 \end{array} \quad (3.232)$$

In the photon representation we can easily see that the squeezed vacuum is (unlike the coherent and the Fock vacuum) not empty,

$$\begin{aligned} \langle \alpha, \xi | \hat{n} | \alpha, \xi \rangle &= |\alpha|^2 + \sinh^2 |\xi| \xrightarrow{\alpha \rightarrow 0} \sinh^2 |\xi| \\ \Delta_{\alpha, \xi} \hat{n} &= |\alpha| + 2 \cosh^2 |\xi| \sinh^2 |\xi| \xrightarrow{\alpha \rightarrow 0} 2 \cosh^2 |\xi| \sinh^2 |\xi|. \end{aligned} \quad (3.233)$$

Squeezed vacuum contains contributions from many  $|n\rangle$ .

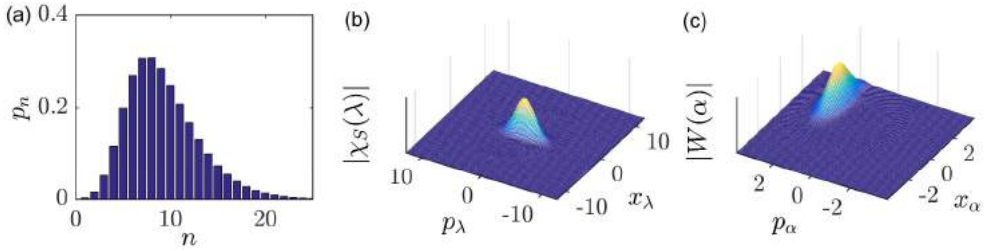


Figure 3.22: (code) Starting from a squeezed state photon distribution with  $r = 0.5$ , as shown in (a), we calculate the symmetrically ordered characteristic function (b) from the expression (3.196), and the Wigner function (c) by an FFT.

For the squeezed vacuum state the photon number distribution displays odd-even-oscillations. This can be explained by the mathematical form of the squeezing operator, that resembles the operator for two-photon generation and annihilation processes. Photons in a squeezed vacuum state are more likely to appear in pairs.

### 3.8.3 Squeezed state in the Glauber basis

The *squeezed state* contains non-classical quantum correlations, as we will show by calculating  $g^{(1)}$  and  $g^{(2)}$  for squeezed states,

$$g^{(2)}(0) = \frac{\langle \hat{b}^\dagger \hat{b} \hat{b}^\dagger \hat{b} \rangle}{\langle \hat{b}^\dagger \rangle^2 \langle \hat{b} \rangle^2} = 1 + \frac{\cosh 2r}{\sinh^2 r}. \quad (3.234)$$

The distribution functions in the coherent representation are,

$$\begin{aligned}
 |\psi\rangle &= \\
 P_{|\beta\rangle}(\alpha) &= \\
 \hat{\rho} &= \\
 Q_{|\beta\rangle}(\alpha) &= \frac{\operatorname{sech} r}{\pi} e^{-(|\alpha|^2+|\beta|^2)+(\alpha^*\beta+\alpha\beta^*)} \operatorname{sech} r - \frac{1}{2} [e^{i\theta}(\alpha^{*2}-\beta^{*2})+e^{-i\theta}(\alpha^2-\beta^2)] \tanh r \\
 W_{|\beta\rangle}(\alpha) &= \frac{1}{2\pi} \exp\left(-\frac{(\alpha+\alpha^*)^2}{2e^{-2r}} + \frac{(\alpha-\alpha^*)^2}{2e^{2r}}\right)
 \end{aligned}
 \tag{3.235}$$

### 3.8.4 Exercises

#### 3.8.4.1 Ex: Unitarity of the squeezing operator

Calculate  $\langle \hat{E} \rangle$  and  $\Delta \hat{E}$ .

#### 3.8.4.2 Ex: Transformation by the squeezing operator

Demonstrate the relationship (3.217).

#### 3.8.4.3 Ex: Squeezed states

Squeezed states may be introduced by the application of the operator  $\hat{S}(\xi) \equiv e^{\frac{\xi^*}{2}\hat{a}^2 - \frac{\xi}{2}\hat{a}^{\dagger 2}}$  on a Glauber state  $|\alpha\rangle$ , where  $\xi$  is the squeezing parameter.

Calculate  $\langle \alpha, \xi | \hat{n} | \alpha, \xi \rangle$  and show with  $\alpha \rightarrow 0$ , that the squeezed vacuum is not empty.

#### 3.8.4.4 Ex: Studying the squeezing operator

Using the Baker-Campbell-Hausdorff braiding identity,

$$e^{\hat{x}} e^{\hat{y}} e^{-\hat{x}} = e^{\hat{y} + [\hat{x}, \hat{y}] + \frac{1}{2!} [\hat{x}, [\hat{x}, \hat{y}]] + \dots}$$

evaluate the expression  $e^{\hat{a}^{\dagger 2}/2} e^{\hat{a}^2/2} e^{-\hat{a}^{\dagger 2}/2}$ .

## 3.9 Further reading

A. Görlitz et al., *Observing the Position Spread of Atomic Wave Packets* [DOI]

### 3.9.1 on the Fourier grid method

R. Meyer, *Trigonometric Interpolation Method for One-Dimensional Quantum-Mechanical Problems* [DOI]

O. Dulieu, *Coupled channel bound states calculations for alkali dimers using the Fourier grid method* [DOI]

- J. Stare et al., *Fourier Grid Hamiltonian Method for Solving the Vibrational Schroedinger Equation in Internal Coordinates Theory and Test Applications* [\[DOI\]](#)
- C. Clay Marston et al., *The Fourier grid Hamiltonian method for bound state eigenvalues and eigenfunctions* [\[DOI\]](#)

### 3.9.2 on the harmonic oscillator

- I. Bouchoule et al., *Neutral atoms prepared in Fock states of a one-dimensional harmonic potential* [\[DOI\]](#)

# Chapter 4

## Rotations / Central potentials

Rotations are, on the same rights as translations, symmetry operations in space. They are of fundamental importance for the discussion of composite particles, such as atoms because they help us to formulate appropriate boundary conditions facilitating the solution of the three-dimensional Schrödinger equation.

### 4.1 Particle in a central potential

Many potentials do not have Cartesian symmetry, but fortunately, many problems have *some* kind of symmetry, cylindrical, spherical or periodic. Those with cylindrical or spherical symmetry can be solved by separating the curvilinear coordinates, as we will show in the following. Particularly important are spherical potentials caused by central forces, for example, the Coulomb force between the proton and the electron in the hydrogen atom.

#### 4.1.1 Transformation to relative coordinates

The hydrogen atom represents a *two-body problem*. We consider the two masses  $m_{1,2}$  of a proton and an electron separated by a distance  $\mathbf{r}$  and interacting through a potential  $V(\mathbf{r})$ . The Hamiltonian is

$$\hat{H} = \frac{-\hbar^2}{2m_1} \nabla_{\mathbf{r}_1}^2 + \frac{-\hbar^2}{2m_2} \nabla_{\mathbf{r}_2}^2 + V(\mathbf{r}_1 - \mathbf{r}_2) , \quad (4.1)$$

where  $\mathbf{r}_{1,2}$  are the positions of the proton and the electron. With the ansatz  $\Xi(t, \mathbf{r}_1, \mathbf{r}_2) = \Xi(\mathbf{r}_1, \mathbf{r}_2)e^{-iE_{tot}t/\hbar}$ , the time-dependent Schrödinger equation

$$\hat{H}\Xi(t, \mathbf{r}_1, \mathbf{r}_2) = i\hbar \frac{d}{dt}\Xi(t, \mathbf{r}_1, \mathbf{r}_2) , \quad (4.2)$$

becomes stationary,

$$\left[ \frac{-\hbar^2}{2m_1} \nabla_{\mathbf{r}_1}^2 + \frac{-\hbar^2}{2m_2} \nabla_{\mathbf{r}_2}^2 + V(\mathbf{r}_1 - \mathbf{r}_2) \right] \Xi(\mathbf{r}_1, \mathbf{r}_2) = E_{tot}\Xi(\mathbf{r}_1, \mathbf{r}_2) . \quad (4.3)$$

Now we transform into the center-of-mass system making for the total wavefunction the ansatz  $\Xi(\mathbf{r}_1, \mathbf{r}_2) = e^{-i\mathbf{P}\cdot\mathbf{R}/\hbar}\Psi(\mathbf{r})$  with  $\mathbf{R} \equiv \frac{m_1}{M}\mathbf{r}_1 + \frac{m_2}{M}\mathbf{r}_2$  and  $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$  and introducing the abbreviation  $M = m_1 + m_2$ . This corresponds to a product of a plane

wave, describing the linear motion of the center of the masses, and a radial wave function, which describes the relative motion of the atom. The kinetic energy of one mass is:

$$\begin{aligned} & \frac{-\hbar^2}{2m_1} \nabla_{r_1}^2 e^{-i\mathbf{P}\cdot\mathbf{R}/\hbar} \Psi(\mathbf{r}) \\ &= \frac{-\hbar^2}{2m_1} \left[ e^{-i\mathbf{P}\cdot\mathbf{R}/\hbar} \nabla_{r_1}^2 \Psi(\mathbf{r}) + 2\left(-\frac{im_1\mathbf{P}}{\hbar M}\right) e^{-i\mathbf{P}\cdot\mathbf{R}/\hbar} \nabla_{r_1} \Psi(\mathbf{r}) + \Psi(\mathbf{r}) \left(-\frac{im_1}{\hbar^2 M} \mathbf{P}\right)^2 e^{-i\mathbf{P}\cdot\mathbf{R}/\hbar} \right] \\ &= e^{-i\mathbf{P}\cdot\mathbf{R}/\hbar} \left[ \frac{-\hbar^2}{2m_1} \nabla_{r_1}^2 \Psi(\mathbf{r}) + \frac{i\hbar\mathbf{P}}{M} \nabla_{r_1} \Psi(\mathbf{r}) - \frac{m_1\mathbf{P}^2}{2M^2} \Psi(\mathbf{r}) \right]. \end{aligned} \quad (4.4)$$

Hence, for two atoms,

$$\begin{aligned} & E_{tot} \Xi(\mathbf{r}_1, \mathbf{r}_2) - V(\mathbf{r}) \Xi(\mathbf{r}_1, \mathbf{r}_2) \\ &= e^{-i\mathbf{P}\cdot\mathbf{R}/\hbar} \left[ \frac{-\hbar^2}{2m_1} \nabla_{r_1}^2 \Psi(\mathbf{r}) + \frac{-\hbar^2}{2m_2} \nabla_{r_2}^2 \Psi(\mathbf{r}) + \frac{i\hbar\mathbf{P}}{M} (\nabla_{r_1} + \nabla_{r_2}) \Psi(\mathbf{r}) + \frac{\mathbf{P}^2}{2M} \Psi(\mathbf{r}) \right]. \end{aligned} \quad (4.5)$$

Using  $\nabla_{r_1} = -\nabla_{r_2} = \nabla_r$ , we see that the third term cancels, such that,

$$\frac{P^2}{2M} \Psi(\mathbf{r}) + \frac{-\hbar^2}{2m_1} \nabla_r^2 \Psi(\mathbf{r}) + \frac{-\hbar^2}{2m_2} \nabla_r^2 \Psi(\mathbf{r}) + V(\mathbf{r}) \Psi(\mathbf{r}) = E_{tot} \Psi(\mathbf{r}). \quad (4.6)$$

Subtracting the energy of the center-of-mass motion with  $E = E_{tot} - \frac{P^2}{2M}$  and introducing the abbreviation  $m^{-1} = m_1^{-1} + m_2^{-1}$ , we finally get,

$$\boxed{\left[ \frac{-\hbar^2}{2m} \nabla_r^2 + V(\mathbf{r}) \right] \Psi(\mathbf{r}) = E \Psi(\mathbf{r})}. \quad (4.7)$$

### 4.1.2 Particle in a cylindrical potential

The equation (4.7) is three-dimensional because  $\Psi(\mathbf{r})$  is a *scalar field* and the momentum operator in Cartesian coordinates is given by,

$$\nabla_r^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \quad (4.8)$$

However, in some situations, the symmetry of the system allows to reduce dimensionality similarly to the cases of the box potential and the three-dimensional harmonic oscillator. Let us now discuss the cases of cylindrical and spherical symmetry.

Electrons in magnetic fields are subject to the Lorentz force, which keeps them in a rotating motion. We can rewrite the momentum operator in cylindrical coordinates,

$$x = \rho \cos \varphi, \quad y = \rho \sin \varphi, \quad z = z, \quad (4.9)$$

as

$$\nabla_r^2 = \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2}. \quad (4.10)$$

Now, with the assumption that the potential only depends on  $\rho$ ,  $V(\mathbf{r}) = V(\rho)$ , we can try the ansatz,

$$\Psi(\mathbf{r}) = R(\rho) \xi(\varphi) \zeta(z), \quad (4.11)$$

and obtain,

$$\frac{1}{R(\rho)} \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + V(\rho) \right) \right] R(\rho) - \frac{\hbar^2}{2m} \frac{1}{\zeta(z)} \frac{\partial^2}{\partial z^2} \zeta(z) - \frac{\hbar^2}{2m\rho^2} \frac{1}{\xi(\varphi)} \frac{\partial^2}{\partial \varphi^2} \xi(\varphi) = E. \quad (4.12)$$

First, we separate the axial motion,

$$-\frac{\zeta''}{\zeta} = \text{const} \equiv \frac{2mE_z}{\hbar^2} \equiv k_z^2, \quad (4.13)$$

the solution of this equation being a superposition of two plane waves counterpropagating along the axis  $z$ ,  $\zeta(z) = Ae^{ik_z z} + Be^{-ik_z z}$ . Now, we separate the azimuthal motion,

$$\frac{\rho^2}{R(\rho)} \frac{\partial R^2(\rho)}{\partial \rho^2} + \frac{\rho}{R(\rho)} \frac{\partial R(\rho)}{\partial \rho} + \frac{2m\rho^2}{\hbar^2} [E - V(\rho)] - \rho^2 k_z^2 = -\frac{\xi''}{\xi} = \text{const} \equiv m_\varphi^2. \quad (4.14)$$

The solution of the right-hand part of the equation is  $\xi(\varphi) = Ce^{im_\varphi \varphi} + De^{-im_\varphi \varphi}$ . Finally, we have the radial equation,

$$\frac{1}{R(\rho)} \frac{\partial R(\rho)^2}{\partial \rho^2} + \frac{1}{\rho R(\rho)} \frac{\partial R(\rho)}{\partial \rho} - \frac{2m}{\hbar^2} [E - V(\rho)] - k_z^2 - \frac{m_\varphi^2}{\rho^2} = 0, \quad (4.15)$$

with the effective potential  $V_{eff} = V(\rho) + \frac{\hbar^2 m_\varphi^2}{2m\rho^2}$ . For a homogeneous potential,  $V(\rho) = V_0$ , the solution will be a superposition of Bessel functions.

**Example 26 (Rigid rotor in cylindrical coordinates):** To give an example, we disregard the potential,  $V(\rho) = 0$ , and we consider for the particle an orbit with constant radius,  $\rho = \text{const}$  such that  $R(\rho) = \delta(\rho - \rho_0)$ . In this case, we only need to treat the orbital motion described by the right part of Eq. (4.14). For the solution of this equation,  $\xi(\varphi) = Ae^{im_\varphi \varphi}$ , to be well-defined, we need  $\xi(\varphi) = \xi(\varphi + 2\pi)$ . This implies,

$$m_\varphi = 0, \pm 1, \pm 2, ..$$

and

$$E_\varphi = \frac{\hbar^2 m_\varphi^2}{2m\rho^2}.$$

The allowed energies  $E_{m_\varphi} = E_\varphi$  can be obtained by letting the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2I} \frac{\partial^2}{\partial \varphi^2},$$

with the moment of inertia  $I = m\rho^2$  actuate on the azimuthal wavefunction  $\xi(\varphi)$ . We now define the operator,

$$\hat{l}_z = \frac{\hbar}{i} \frac{\partial}{\partial \varphi}.$$

This operator acts on the wavefunction  $\xi$  as follows,

$$\hat{l}_z \xi(\varphi) = \hbar m_\varphi \xi(\varphi).$$

It is easy to show that wavefunctions with different values  $m_l$  are orthogonal.

Note: 1. The state  $m_\varphi = 0$  has zero energy; that is, it has no zero-point energy.

2. The particle is delocalized within a ring of radius  $r$ :  $\Delta l_z \Delta \sin \varphi \geq \frac{\hbar}{2} |\langle \cos \varphi \rangle|$ .



### 4.1.3 Hamiltonian in spherical coordinates

We can rewrite the momentum operator in spherical coordinates,

$$x = r \sin \vartheta \cos \varphi \quad , \quad y = r \sin \vartheta \sin \varphi \quad , \quad z = r \cos \vartheta \quad , \quad (4.16)$$

as <sup>1</sup>,

$$\nabla_r^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \hat{\mathbf{L}}^2 \quad \text{where} \quad \frac{\hat{\mathbf{L}}^2}{\hbar^2} \equiv \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left( \sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{\sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2} \quad , \quad (4.17)$$

is an abbreviation called *Legendre operator*. For an isotropic potential,  $V(\mathbf{r}) = V(r)$ , we can try the ansatz,

$$\Psi(\mathbf{r}) = R(r)Y(\vartheta, \varphi) \quad (4.18)$$

to solve the Schrödinger equation (2.57),

$$\frac{r^2}{R(r)} \left[ -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + V(r) - E \right] R(r) = \frac{-1}{2m} \frac{\hat{\mathbf{L}}^2 Y(\vartheta, \varphi)}{Y(\vartheta, \varphi)} = \text{const} \equiv -\frac{\hbar^2}{2m} \ell(\ell+1) \quad , \quad (4.19)$$

where we choose a separation constant,  $\ell(\ell+1)$ , the significance of which we shall soon learn. Considering only the angular part,

$$\boxed{\hat{\mathbf{L}}^2 Y(\vartheta, \varphi) = \hbar^2 \ell(\ell+1) Y(\vartheta, \varphi)} \quad , \quad (4.20)$$

and making another separation ansatz,

$$Y(\vartheta, \varphi) = \Theta(\vartheta)\Phi(\varphi) \quad , \quad (4.21)$$

we obtain,

$$\sin^2 \vartheta \left( \frac{1}{\Theta(\vartheta)} \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \sin \vartheta \frac{\partial}{\partial \vartheta} \Theta(\vartheta) + \ell(\ell+1) \right) = -\frac{1}{\Phi(\varphi)} \frac{\partial^2}{\partial \varphi^2} \Phi(\varphi) = \text{const} \equiv m^2 \quad , \quad (4.22)$$

where we choose a separation constant,  $m^2$ . Introducing another abbreviation,

$$\hat{L}_z \equiv \frac{\hbar}{i} \frac{\partial}{\partial \varphi} \quad , \quad (4.23)$$

the azimuthal equation takes the form

$$\boxed{\hat{L}_z \Phi(\varphi) = \hbar m \Phi(\varphi)} \quad . \quad (4.24)$$

As in the case of the cylindrical potential, the solution of the *azimuthal equation* is, using the normalization,

$$\Phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \quad , \quad (4.25)$$

with the *magnetic quantum number*  $m = 0, \pm 1, \pm 2, \dots$

<sup>1</sup>We may also write:  $\mathbf{p}^2 = (\hat{\mathbf{e}}_r \cdot \mathbf{p})^2 + (\hat{\mathbf{e}}_r \times \mathbf{p})^2 = p_r^2 + \frac{\mathbf{L}^2}{r^2}$ , where  $p_r^2$  is the radial part of the Laplace operator and  $\frac{\mathbf{L}^2}{r^2}$  the angular part.

The *polar equation*,

$$\frac{1}{\Theta(\vartheta)} \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \sin \vartheta \frac{\partial}{\partial \vartheta} \Theta(\vartheta) + \ell(\ell + 1) = \frac{m^2}{\sin^2 \vartheta} , \quad (4.26)$$

is called Legendre's differential equation and can be solved by a power series in  $\cos^k \vartheta$ . For  $m = 0$ , the solutions are the *Legendre polynomials*,  $P_\ell(\cos \vartheta)$  with

$$P_\ell(z) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dz^\ell} [(z^2 - 1)^\ell] . \quad (4.27)$$

The first polynomials are,

$$P_0(z) = 1 \quad , \quad P_1(z) = z \quad , \quad P_2(z) = \frac{1}{2}(3z^2 - 1) \quad , \quad P_3(z) = \frac{1}{2}(5z^3 - 3z) . \quad (4.28)$$

For  $m > 0$ , the solutions are the associated polynomials,

$$P_\ell^m(z) = (-1)^m (1 - z^2)^{m/2} \frac{d^m}{dz^m} P_\ell(z) = \frac{(-1)^m}{2^\ell \ell!} (1 - z^2)^{m/2} \frac{d^{\ell+m}}{dz^{\ell+m}} [(z^2 - 1)^\ell] \quad (4.29)$$

$$P_\ell^{-m}(z) = (-1)^m \frac{(\ell - m)!}{(\ell + m)!} P_\ell^m(z) .$$

The polar function must still be normalized,

$$\Theta_\ell^m(\vartheta) = P_\ell^m(\cos \vartheta) \sqrt{\frac{2\ell + 1}{2} \frac{(\ell - m)!}{(\ell + m)!}} . \quad (4.30)$$

The functions  $Y_{\ell m}(\vartheta, \varphi)$  are the *spherical harmonics*. They form an orthonormal system,

$$\int_0^\pi \int_0^{2\pi} Y_{\ell' m'}^*(\vartheta, \varphi) Y_{\ell m}(\vartheta, \varphi) \sin \vartheta d\vartheta d\varphi = \delta_{\ell' \ell} \delta_{m' m} . \quad (4.31)$$

Finite solutions only exist when the *angular momentum quantum number* is  $\ell = 0, 1, \dots$  and for  $|m| \leq \ell$ .

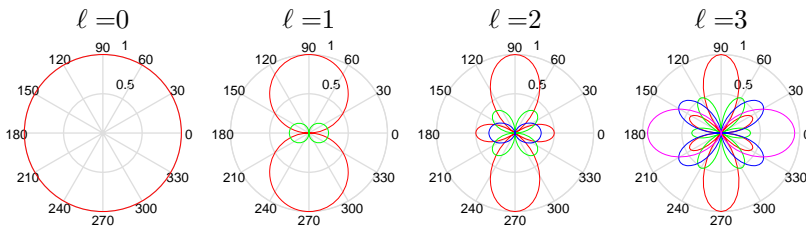


Figure 4.1: (code) Angular wavefunctions. Shown are the Legendre polynomials  $P_\ell^m(\cos \vartheta)$  for  $\ell = 0, 1, 2, 3$  and  $m = 0, \dots, \ell$ . Red:  $m = 0$ , green:  $|m| = 1$ , blue:  $|m| = 2$ , and magenta:  $|m| = 3$ .

The solutions of the angular part of the Schrödinger equation for the hydrogen atom are finally,

$$Y_{\ell m}(\vartheta, \varphi) = \frac{1}{\sqrt{2\pi}} P_{\ell}^m(\cos \vartheta) \sqrt{\frac{2\ell+1}{2} \frac{(\ell-m)!}{(\ell+m)!}} e^{im\varphi}. \quad (4.32)$$

The spherical harmonics are simultaneously eigenfunctions of the operators  $\mathbf{L}^2$ , as can be seen from Eq. (4.20), and of the operator  $L_z$  according to Eq. (4.24). The quantities represented by the quantum operators  $\hat{H}, \hat{\mathbf{L}}^2, \hat{L}_z$  are conserved in the hydrogen system. The conservation of the angular momentum is due to the spherical symmetry of the Coulomb potential.

We will verify the parity of the spherical harmonics in Exc. 4.1.5.1.

#### 4.1.4 Separation of radial motion

In Sec. 4.1.3 we derived, after having separated the motion of the center-of-mass (that is, of the heavy nucleus) and the angular coordinates, the radial equation (4.19) describing the radial component of the electronic motion,

$$\frac{1}{R(r)} \left[ -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + V(r) - E \right] R(r) = -\frac{\hat{\mathbf{L}}^2}{2mr^2}, \quad (4.33)$$

Now, we make the substitution  $R(r) = u(r)/r$  and the radial equation becomes,

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + \frac{\hat{\mathbf{L}}^2}{2mr^2} + V(r) \right] u(r) = Eu(r). \quad (4.34)$$

This equation is very similar to a one-dimensional Schrödinger equation, but there is an additional potential term called *centrifugal potential*,

$$V_{\ell}(r) \equiv \frac{\hat{\mathbf{L}}^2}{2mr^2}. \quad (4.35)$$

For example, for the potential of an electron orbiting a proton, we have,

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \frac{Ze^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} - E \right] u_{E\ell}(r) = 0. \quad (4.36)$$

We will discuss this equation intensely in the context of the hydrogen atom.

In Exc. 4.1.5.2 we derive the radial Gross-Pitaevskii equation for a Bose-Einstein condensate trapped in a spherical potential. In the Exc. 4.1.5.3 we will study particles inside a central potential of zero depth, in the Excs. 4.1.5.4 and 4.1.5.5 we consider 3D spherical box potentials and in Exc. 4.1.5.6 a spherical harmonic potential.

**Example 27 (Rigid rotor in spherical coordinates):** We continue the discussion of the rigid rotor, now in spherical coordinates. In the case that the orbit of the particle is fixed to a radius  $R$ , we can neglect the kinetic energy due

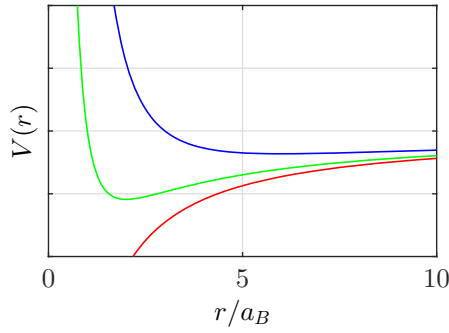


Figure 4.2: (code) Sum of a Coulomb potential and centrifugal potential for  $\ell = 0$  (lower curve),  $\ell = 1$  (center curve), and  $\ell = 2$  (upper curve).

to the radial motion and the potential, both being constant. In this case the radial Schrödinger equation is,

$$\left[ \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \right] u_{E\ell} = E_{\ell} u_{E\ell} .$$

The energies of the *rigid rotor* are

$$E_{\ell} = \frac{\hbar^2 \ell(\ell+1)}{2I} ,$$

with the *momentum of inertia*  $I = mR^2$ .

## 4.1.5 Exercises

### 4.1.5.1 Ex: Parity of the spherical harmonic functions

We consider the parity transformation  $\mathbf{P}$  with  $(x, y, z) \xrightarrow{\mathbf{P}} (-x, -y, -z)$ . Use spherical coordinates to show that  $Y_{\ell m} \xrightarrow{\mathbf{P}} (-1)^{\ell} Y_{\ell m}$ , and therefore that a spherical surface function has even parity when  $\ell$  is even, and odd parity, when  $\ell$  is odd.

### 4.1.5.2 Ex: Bose-Einstein condensate in an isotropic potential

The time-dependent Gross-Pitaevskii equation describing the wavefunction of a Bose-Einstein condensate reads,

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{trp}(r) + g|\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t) ,$$

where the factor  $g$  depends on the force of the interatomic interaction and  $V_{trp}$  is the potential trapping the atoms. Derive the stationary Gross-Pitaevskii equation via the transform  $\psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-i\mu t/\hbar}$ , where the constant  $\mu$  is called the chemical potential. For  $V(\mathbf{r}) = V(r)$  the wavefunction will have radial symmetry,  $\psi(\mathbf{r}) = \frac{\phi(r)}{r}$ . Rewrite the Gross-Pitaevskii equation for the function  $\phi$ .

**4.1.5.3 Ex: Motion of a free particle in spherical coordinates**

Obtain the eigenfunctions of a free particle as the limiting case of its motion in a central force field with  $V(r) \rightarrow 0$ . Compare the derived eigenfunctions – associated with the complete set of observables  $\hat{H}$ ,  $\hat{L}^2$ , and  $\hat{L}_z$  – to those described by plane waves – associated with the motion characterized by the observables  $\hat{p}_x$ ,  $\hat{p}_y$ ,  $\hat{p}_z$ , and  $\hat{H} = \hat{\mathbf{P}}^2/2m$  –, which also constitute a complete set of observables.

**4.1.5.4 Ex: Particle in a spherical box**

Find the energy levels and wavefunctions of a particle confined in a spherical box described by potential energy,  $V(r) = 0$  for  $r < a$  and  $V(r) = \infty$  for  $r \geq a$  considering the angular momentum  $\ell = 0$ .

**4.1.5.5 Ex: Finite spherical 3D potential well**

- Derive the possible energy levels and associated wavefunctions for a particle trapped in a spherical 3D potential well of depth  $V_0$  and radius  $a$ . Note that this problem is analogous to *Mie scattering* of scalar waves.
- Discuss the case of a well surrounded by infinitely high walls.

**4.1.5.6 Ex: Particle in a spherical harmonic potential**

A quantum particle of mass  $m$  is subject to a potential

$$V = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) .$$

- Obtain the energy levels of this particle. That is, determine the eigenvalues of

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi .$$

- Consider the fundamental level and the first two excited levels. Set up a table showing for each of these three levels the energy value, the degeneracy, and the respective states in terms of the quantum numbers.
- Using

$$\nabla^2\psi = \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \right] \psi$$

and remembering  $\hat{\mathbf{L}}^2 Y_{\ell m}(\theta, \phi) = \hbar^2 \ell(\ell + 1) Y_{\ell m}$ , write down the differential equation of item (a) for the radial part of the wavefunction (it is not necessary to solve it). Identify in this equation the effective potential  $V_{eff}(r)$ .

- Solve the differential equation of the previous item for the case where  $\ell = 0$  and determine the corresponding eigenvalue. To do this, allow for a solution of the type  $e^{-\alpha r^2}$  and determine  $\alpha$ .

**4.2 Quantum treatment of hydrogen**

According to Rutherford's and Bohr's planetary atomic model we may imagine an atom as a very heavy nucleus having a positive electric charge surrounded by a very

light negatively charged charge electronic cloud. Since the nucleus is very small compared to the electronic cloud, we treat it as an entity with mass  $M$  and charge  $Ze$ , where  $Z$  is the number of protons and corresponds to the order of the element in the periodic system.

The canonical procedure for calculating all properties of an atom is to establish its Hamiltonian, that is, to determine the kinetic energies of all components and all interaction energies between them, and to solve the Schrödinger equation. For each component we write the kinetic energy,

$$T_{ncl} = \frac{P^2}{2M} \quad \text{and} \quad T_{ele} = \sum_{i=1}^Z \frac{p_i^2}{2m} . \quad (4.37)$$

Here,  $(\mathbf{R}, \mathbf{P})$  are the nuclear coordinates and  $(\mathbf{r}_i, \mathbf{p}_i)$  those of the electrons. The energies that corresponds to the interactions, that is, Coulombian attraction or repulsion, between the components of the atom are,

$$V_{ncl-ele} = - \sum_{i=1}^Z \frac{Ze^2}{4\pi\epsilon_0|\mathbf{R} - \mathbf{r}_i|} \quad \text{and} \quad V_{ele-ele} = \sum_{i \neq j=1}^Z \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} . \quad (4.38)$$

There are also interactions due to the spin of the particles, which we will deal with later.

Obviously, the solution to this many-body problem is very complicated. For this reason, we will in this chapter, based on the Schrödinger equation, calculate the complete spectrum of the simplest possible atom, hydrogen. This atom consists of a proton and an electron, only.

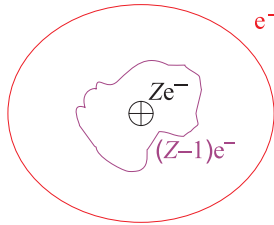


Figure 4.3: The hydrogen model applies to other atoms having a single valence electron occupying a sufficiently large space, that it sees the nucleus together with rest of the electrons shielding the nucleus as a single positive charge.

### 4.2.1 Bohr's model

Let us now turn our attention to the radial part of the Schrödinger equation describing a particle in a radial potential. We expect that the quantum solutions for the hydrogen atom are similar to the predictions of Bohr's model. Following this model, the orbit is stable when the attraction force is equal to the centrifugal force. But in addition, Bohr postulated, that only certain energies are allowed. For the hydrogen atom he found,

$$E_n = - \frac{1}{2} \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{r_n} = - \frac{Z^2\hbar^2}{2ma_B^2} \frac{1}{n^2} = - \frac{Z^2e^2}{4\pi\epsilon_0} \frac{1}{2a_B n^2} = - \frac{Z^2}{n^2} 13.6 \text{ eV} , \quad (4.39)$$

with the *Bohr radius*

$$a_B \equiv 4\pi\epsilon_0 \frac{\hbar^2}{me^2} . \quad (4.40)$$

With this equation he was able to explain the spectral observations. Electrons can only jump from one level to another, while emitting or absorbing a photon. The series observed in the hydrogen spectrum  $(E_n - E_m)/\hbar$  are the Lyman ( $m = 1$ ), the Balmer ( $m = 2$ ), the Paschen ( $m = 3$ ) and the Brackett series ( $m = 4$ ).

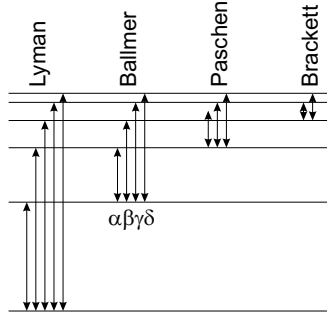


Figure 4.4: The hydrogen transitions.

The discussion of the hydrogen atom within quantum mechanics can start from the radial Schrödinger equation (4.36) with the Coulomb attraction potential,

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \frac{Ze^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} - E \right] u_{E\ell}(r) = 0 . \quad (4.41)$$

In order to facilitate comparison with Bohr's classical model, let us express the energy in terms of Bohr's energy,  $E \equiv E_n = E_1/n^2$ , and write the radius in units of  $a_B$ , that is,  $\tilde{r} \equiv Zr/a_B$ . This yields,

$$u_{n\ell}''(\tilde{r}) + \left( -\frac{\ell(\ell+1)}{\tilde{r}^2} + \frac{2}{\tilde{r}} - \frac{1}{n^2} \right) u_{n\ell}(\tilde{r}) = 0 . \quad (4.42)$$

To ensure that for large radii,  $r \rightarrow \infty$ , the solution is finite, we need an asymptotic behavior like  $u_{n\ell}(\tilde{r} \rightarrow \infty) = e^{-\tilde{r}/n}$ . To ensure that for small radii,  $r \rightarrow 0$ , the solution is finite, we need  $u_{n\ell}(\tilde{r} \rightarrow 0) = \tilde{r}^{\ell+1}$ . We derive the asymptotic solutions in Exc. 4.2.3.1. The resulting differential equation only has solutions for an integer and positive *main quantum number*  $n$  and when  $\ell = 0, 1, \dots, n-1$ . That is, in the relation  $E = E_1/n^2$  the parameter  $n$  is integer and positive, such that energy levels remain degenerate in  $\ell$  and  $m$ . This means that Bohr's postulate of discrete (i.e. quantized) energy levels is valid (uff!)

Substituting the ansatz,

$$u_{n\ell}(\tilde{r}) = D_{n\ell} \tilde{r}^{\ell+1} e^{-\tilde{r}/n} L(\tilde{r}) , \quad (4.43)$$

it's easy to show (see Exc. 4.2.3.2), that the differential equation (4.42) reduces to,

$$\tilde{r}L''(\tilde{r}) + 2 \left[ (\ell+1) - \frac{1}{n}\tilde{r} \right] L'(\tilde{r}) + 2 \left[ 1 - \frac{1}{n}(\ell+1) \right] L(\tilde{r}) = 0 . \quad (4.44)$$

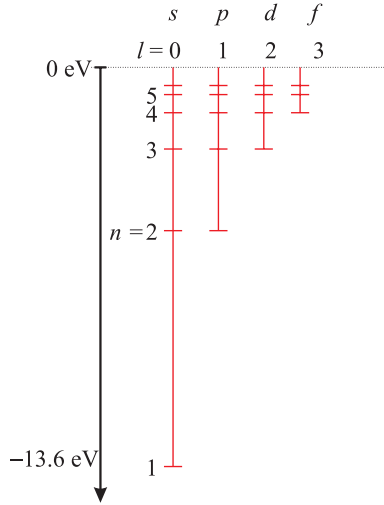


Figure 4.5: Level scheme.

Still with the abbreviation  $\rho \equiv 2\tilde{r}/n = 2Zr/na_B$  the ansatz

$$u_{n\ell}(\rho) = D_{n\ell} \rho^{\ell+1} e^{-\rho/2} L(\rho), \quad (4.45)$$

leads to the differential equation <sup>2</sup>

$$\rho L''(\rho) + [2(\ell + 1) - \rho] L'(\rho) + [n - \ell - 1] L(\rho) = 0. \quad (4.46)$$

The solutions of this differential equation,  $L_{n-\ell-1}^{(2\ell+1)}(\rho)$ , are the *Laguerre polynomials*. These polynomials are listed in mathematical tables. Using the properties of these polynomials it is possible to show that the radial functions are orthogonal and can be normalized (see Exc. 4.2.3.3). Fig. 4.6 shows the curves for the lowest orbitals.

Finally, we can write the complete solutions of the Schrödinger equation  $\hat{H}\psi = E\psi$ ,

$$\psi_{n\ell m}(r, \theta, \phi) = \frac{u_{n\ell}(r)}{r} Y_{\ell m}(\theta, \phi) \quad \text{and} \quad E_n = -\frac{\hbar^2}{2ma_B^2} \frac{Z^2}{n^2}, \quad (4.47)$$

where  $n = 1, 2, 3, \dots$  and  $\ell = 0, 1, \dots, n-1$  and  $m = -\ell, -\ell+1, \dots, \ell$ . Of course, each energy level  $n$  is,

$$\sum_{\ell=0}^{n-1} (2\ell + 1) = n^2 \quad (4.48)$$

<sup>2</sup> *Laguerre's associated differential equation* is,

$$\rho \partial_\rho^2 L_\nu^{(\alpha)} + (\alpha + 1 - \rho) \partial_\rho L_\nu^{(\alpha)} + \nu L_\nu^{(\alpha)} = 0.$$

The Laguerre polynomials are generated by

$$L_\nu^{(\alpha)}(\rho) = \frac{e^\rho \rho^{-\alpha}}{\alpha!} \frac{d^\nu}{d\rho^\nu} (e^{-\rho} \rho^{\nu+\alpha}).$$



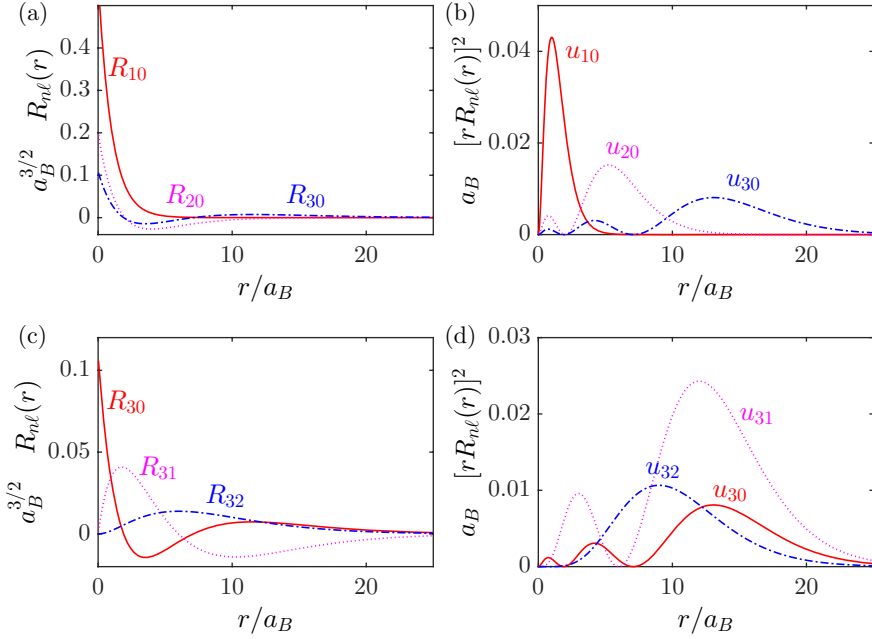


Figure 4.6: (code) (a,c) Radial wavefunctions  $R_{n\ell}(r)$  and (b,d) square of the radial wavefunctions  $u_{n\ell}(r)$  for various quantum numbers  $n$  and  $\ell$ .

times degenerate.

From the normalization condition,

$$\begin{aligned}
 1 &= \int_{\mathbb{R}^3} |\psi_{n\ell m}(r, \theta, \phi)|^2 d^3r \\
 &= \int_0^\infty |u_{n\ell}(r)|^2 dr \int_{\mathbb{R}^2} |Y_{\ell m}(\theta, \phi)|^2 \sin \theta d\theta d\phi = \int_0^\infty |u_{n\ell}(r)|^2 dr,
 \end{aligned} \tag{4.49}$$

we obtain the constants,

$$D_{n\ell} = \sqrt{\left(\frac{2Z}{na_B}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}}, \tag{4.50}$$

and the radial wavefunctions finally read,

$$R_{n\ell}(r) = D_{n\ell} \left(\frac{2\tilde{r}}{n}\right)^\ell e^{-\tilde{r}/n} L_{n-\ell-1}^{(2\ell+1)}\left(\frac{2\tilde{r}}{n}\right) = D_{n\ell} \rho^\ell e^{-\rho/2} L_{n-\ell-1}^{(2\ell+1)}(\rho), \tag{4.51}$$

using the previously introduced abbreviations.

Here is a list of the first wavefunctions of the hydrogen atom,

$$\begin{aligned}
 \psi_{100} &= \frac{1}{\sqrt{\pi}} \left( \frac{Z}{a_B} \right)^{3/2} e^{-\tilde{r}} \\
 \psi_{200} &= \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_B} \right)^{3/2} (2 - \tilde{r}) e^{-\tilde{r}/2} \\
 \psi_{210} &= \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_B} \right)^{3/2} \tilde{r} e^{-\tilde{r}/2} \cos \theta \\
 \psi_{21\pm 1} &= \frac{1}{8\sqrt{\pi}} \left( \frac{Z}{a_B} \right)^{3/2} \tilde{r} e^{-\tilde{r}/2} \sin \theta e^{\pm i\varphi} \\
 \psi_{300} &= \frac{1}{81\sqrt{3\pi}} \left( \frac{Z}{a_B} \right)^{3/2} (27 - 18\tilde{r} + 2\tilde{r}^2) e^{-\tilde{r}/3} \\
 \psi_{31\pm 1} &= \frac{\sqrt{2}}{81\sqrt{3\pi}} \left( \frac{Z}{a_B} \right)^{3/2} (6 - \tilde{r}) \tilde{r} e^{-\tilde{r}/3} \sin \theta e^{\pm i\varphi} \\
 \psi_{320} &= \frac{1}{81\sqrt{6\pi}} \left( \frac{Z}{a_B} \right)^{3/2} \tilde{r}^2 e^{-\tilde{r}/3} (3 \cos^2 \theta - 1),
 \end{aligned} \tag{4.52}$$

where we use the abbreviation  $\tilde{r} \equiv Zr/a_B$ . Using these wavefunctions we can now calculate important eigenvalues such as, for example,

$$\begin{aligned}
 \langle 1 \rangle_{n\ell m} &= 1 \\
 \langle \delta^{(3)}(\tilde{r}) \rangle_{n\ell m} &= \frac{\delta_{\ell,0}}{\pi n^3} \\
 \langle \tilde{r} \rangle_{n\ell m} &= n^2 \left[ 1 + \frac{1}{2} \left( 1 - \frac{\ell(\ell+1)}{n^2} \right) \right] \\
 \langle \tilde{r}^2 \rangle_{n\ell m} &= n^4 \left[ 1 + \frac{3}{2} \left( 1 - \frac{\ell(\ell+1) - \frac{1}{3}}{n^2} \right) \right] \\
 \langle \tilde{r}^3 \rangle_{n\ell m} &= n^6 \left[ \frac{35}{8} - \frac{35}{8n^2} - \frac{15}{4n^2} (\ell+2)(\ell-1) + \frac{3}{8n^4} (\ell+2)(\ell+1)\ell(\ell-1) \right] \\
 \langle \tilde{r}^4 \rangle_{n\ell m} &= n^8 \left[ \frac{63}{8} + \frac{35}{8n^2} (2\ell^2 + 2\ell - 3) + \frac{5}{8n^4} 5\ell(\ell+1)(3\ell^2 + 3\ell - 10) + \frac{12}{n^8} \right] \\
 \left\langle \frac{1}{\tilde{r}} \right\rangle_{n\ell m} &= \frac{1}{n^2} \\
 \left\langle \frac{1}{\tilde{r}^2} \right\rangle_{n\ell m} &= \frac{1}{n^3(\ell + \frac{1}{2})} \\
 \left\langle \frac{1}{\tilde{r}^3} \right\rangle_{n\ell m} &= \frac{n}{n^4\ell(\ell + \frac{1}{2})(\ell + 1)} \\
 \left\langle \frac{1}{\tilde{r}^4} \right\rangle_{n\ell m} &= \frac{\frac{3}{2}n^2 - \frac{1}{2}\ell(\ell + 1)}{n^5(\ell + \frac{3}{2})(\ell + 1)(\ell + \frac{1}{2})\ell(\ell - \frac{1}{2})}.
 \end{aligned} \tag{4.53}$$

These results will become important later. In Exc. 4.2.3.4 we will calculate the eigenvalue  $\langle r \rangle$  for several orbitals  $|\psi_{n\ell m}\rangle$ .

## 4.2.2 The virial theorem

Originally derived for classical mechanics, the *virial theorem* also holds for quantum mechanics, as shown for the first time by *Fock*. We evaluate the commutator between the Hamiltonian

$$\hat{H} = \hat{\mathbf{p}}^2/2m + V(\hat{\mathbf{r}}) , \quad (4.54)$$

and the product of the position operator  $\hat{\mathbf{r}}$  with the momentum operator  $\hat{\mathbf{p}} = -i\hbar\nabla$  of the particle:

$$[\hat{H}, \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}] = [\hat{H}, \hat{\mathbf{r}}] \cdot \hat{\mathbf{p}} + \hat{\mathbf{r}} \cdot [\hat{H}, \hat{\mathbf{p}}] = -i\hbar \frac{\hat{\mathbf{p}}^2}{m} + i\hbar \hat{\mathbf{r}} \cdot \nabla V , \quad (4.55)$$

using the theorems of Ehrenfest. Therefore, we find for the operator  $\hat{Q} = \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}$  the commutator,

$$\frac{i}{\hbar} [\hat{H}, \hat{Q}] = 2E_{kin} - \hat{\mathbf{r}} \cdot \nabla V . \quad (4.56)$$

The left side of this equation is precisely  $-d\hat{Q}/dt$ , following the Heisenberg equation of motion. The eigenvalue  $\langle d\hat{Q}/dt \rangle$  of the temporal derivative vanishes in steady state, therefore we obtain the virial theorem,

$$2\langle E_{kin} \rangle = \langle \hat{\mathbf{r}} \cdot \nabla V \rangle . \quad (4.57)$$

**Example 28 (Virial theorem applied to a central potential):** For example, for a central potential  $V(r) \propto r^s$  we obtain,

$$2\langle E_{kin} \rangle = \langle \hat{\mathbf{r}} \cdot \hat{\mathbf{e}}_r \frac{\partial V}{\partial r} \rangle = \langle r \frac{\partial V}{\partial r} \rangle = s\langle V \rangle .$$

In Exc. 4.2.3.5 we calculate the eigenvalues  $\langle r^{-1} \rangle$  and  $\langle p^2 \rangle$  and we verify the virial theorem. Finally, in Exc. 4.2.3.6 we calculate transition matrix elements between different orbitals.

## 4.2.3 Exercises

### 4.2.3.1 Ex: Asymptotes of Laguerre's polynomials

Derive the asymptotic solutions of equation (4.42).

### 4.2.3.2 Ex: Laguerre equation

Show that the equation (4.42) transforms with the ansatz (4.43) into equation (4.44).

### 4.2.3.3 Ex: Laguerre functions

Using the orthogonality relation of associated Laguerre polynomials,

$$\int_0^\infty \rho^\alpha e^{-\rho} L_n^{(\alpha)}(\rho) L_m^{(\alpha)}(\rho) d\rho = \frac{\Gamma(n+\alpha+1)}{n!} \delta_{n,m}$$

$$\int_0^\infty \rho^{\alpha+1} e^{-\rho} L_n^{(\alpha)}(\rho)^2 d\rho = \frac{(n+\alpha)!}{n!} (2n+\alpha+1) ,$$

and the recursion formula,

$$\begin{aligned} nL_n^{(\alpha+1)}(\rho) &= (n - \rho)L_{n-1}^{(\alpha+1)}(\rho r) + (n + \alpha)L_{n-1}^{(\alpha)}(\rho) \\ \rho L_n^{(\alpha+1)}(\rho) &= (n + \alpha)L_{n-1}^{(\alpha)}(\rho) - (n - \rho)L_n^{(\alpha)}(\rho) , \end{aligned}$$

- calculate the normalization constant  $D_{n,l}$  for a hydrogen-like atom with atomic number  $Z$ ;
- calculate the mean value

$$\langle r \rangle_{nlm} = \frac{n^2 a_B}{Z} \left[ 1 + \frac{1}{2} \left( 1 - \frac{\ell(\ell+1)}{n^2} \right) \right] ;$$

- calculate the mean value

$$\left\langle \frac{1}{r} \right\rangle_{nlm} = \frac{Z}{n^2 a_B} .$$

#### 4.2.3.4 Ex: Orbital radii in Bohr's model

Using the results of 4.2.3.3, obtain the expectation values  $\langle r \rangle$  for the states  $\psi_{100}$ ,  $\psi_{210}$  and  $\psi_{320}$  of the hydrogen atom. Compare the results with those of Bohr's model.

#### 4.2.3.5 Ex: The virial theorem and Bohr's model

Calculate, for the state  $\psi_{320}$  of the hydrogen atom, the expectation values  $\langle \frac{1}{r} \rangle$ ,  $\langle \frac{\mathbf{L}^2}{r^2} \rangle$ , and  $\langle \mathbf{p}^2 \rangle$ .

From the results, obtain the expectation values for the kinetic and potential energies,  $\langle T \rangle$  and  $\langle V \rangle$ , and show that, consistent with the virial theorem,  $\langle T \rangle = -(1/2)\langle V \rangle$ . Compare the results with Bohr's model.

#### 4.2.3.6 Ex: Transition matrix elements

Using the following (non-normalized) wavefunctions of hydrogen,  $\psi_{100}(\mathbf{r}) = e^{-\tilde{r}}$ ,  $\psi_{210}(\mathbf{r}) = \tilde{r}e^{-\tilde{r}/2} \cos \theta$  and  $\psi_{21\pm 1}(\mathbf{r}) = \tilde{r}e^{-\tilde{r}/2} \sin \theta e^{\pm i\phi}$ , calculate the matrix elements (a)  $\langle \psi_{100} | \tilde{z} | \psi_{210} \rangle$ , (b)  $\langle \psi_{100} | \tilde{z} | \psi_{211} \rangle$ , (c)  $\langle \psi_{100} | \tilde{x} - i\tilde{y} | \psi_{210} \rangle$ , and (d)  $\langle \psi_{100} | \tilde{x} - i\tilde{y} | \psi_{211} \rangle$  using the formulae:

$$\begin{aligned} \int_0^\infty x^4 e^{-3x/2} dx &= \frac{256}{81} \quad , \quad \int_0^\pi \sin^3 x dx = \frac{4}{3} \quad , \\ \int_0^\pi \cos x \sin^2 x dx &= 0 \quad , \quad \int_0^\pi \cos^2 x \sin x dx = \frac{2}{3} \quad . \end{aligned}$$

Try to interpret the results.

## 4.3 Angular momentum

### 4.3.1 The orbital angular momentum operator

The definition of *orbital angular momentum* is adopted from classical mechanics:

$$\hat{\mathbf{I}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}} = -i\hbar \hat{\mathbf{r}} \times \hat{\nabla} = -i\hbar \begin{vmatrix} \hat{\mathbf{e}}_x & \hat{\mathbf{e}}_y & \hat{\mathbf{e}}_z \\ x & y & z \\ \partial_x & \partial_y & \partial_z \end{vmatrix}. \quad (4.58)$$

To better understand the properties of the angular momentum operator in quantum mechanics we will derive in the Excs. 4.3.4.1 and 4.3.4.2 some of its properties.

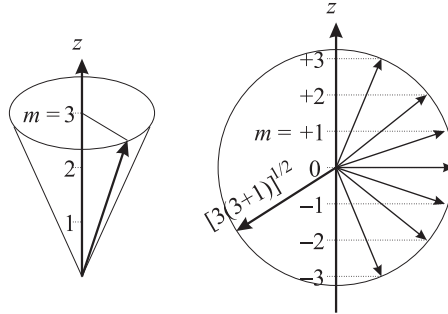


Figure 4.7: Illustration of angular momentum in quantum mechanics.

#### 4.3.1.1 Constants of motion

The preceding chapter dealt with the resolution of the radial and angular equations for the case of a radial potential. The radial equation allowed to calculate the eigenenergies of the Hamiltonian  $\hat{H}$ ,

$$\hat{H}|\psi\rangle = E_{n\ell}|\psi\rangle. \quad (4.59)$$

We also found the common eigenvalues and eigenfunctions of operators  $\hat{\mathbf{I}}^2$  and  $\hat{l}_z$  [see Eqs. (4.20) and (4.24)]. We now use the notation  $|\ell, m\rangle \equiv Y_{\ell m}(\theta, \phi)$  for the eigenfunctions,

$$\hat{\mathbf{I}}^2|\ell, m\rangle = \hbar^2\ell(\ell+1)|\ell, m\rangle \quad \text{and} \quad \hat{l}_z|\ell, m\rangle = \hbar m|\ell, m\rangle. \quad (4.60)$$

With this we have,

$$\begin{aligned} [\hat{H}, \hat{\mathbf{I}}^2]|\psi\rangle &= \hat{H}\hbar^2\ell(\ell+1)|\psi\rangle - \hat{\mathbf{I}}^2 E|\psi\rangle = 0 \\ \text{and} \quad [\hat{H}, \hat{l}_z]|\psi\rangle &= \hat{H}\hbar m|\psi\rangle - \hat{l}_z E|\psi\rangle = 0. \end{aligned} \quad (4.61)$$

Therefore, the operators  $\hat{\mathbf{I}}^2$  and  $\hat{l}_z$  are constants of motion,

$$[\hat{H}, \hat{l}_z] = 0 = [\hat{H}, \hat{\mathbf{I}}^2]. \quad (4.62)$$

Exc. 4.3.4.3 asks to show explicitly, at the example of an isotropic three-dimensional harmonic oscillator, that  $\hat{\mathbf{I}}^2$  and  $\hat{l}_z$  are constants of motion.

### 4.3.2 SU(2) algebra of angular momentum and spin

So far, we have solved the angular eigenvalue equation in the spatial representation for an orbital angular momentum,  $\hat{\mathbf{I}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$ . But it is not clear, whether *every* angular momentum has this representation, which is derived from classical notions. In fact, we will see that the electron has an intrinsic spin with no orbiting charges. What we must show now is, that for any spin  $\hat{\mathbf{j}}$  satisfying

$$\boxed{\hat{\mathbf{j}} \times \hat{\mathbf{j}} = i\hbar\hat{\mathbf{j}}}, \quad (4.63)$$

or  $[\hat{j}_m, \hat{j}_n] = i\hbar\epsilon_{kmn}\hat{j}_k$  using the Levi-Civita symbol, we obtain a consistent algebra.

Since  $\hat{\mathbf{j}}^2$  and  $\hat{j}_z$  commute (we show this from Eq. (4.63) in Exc. 4.3.4.4), they have common eigenfunctions  $|j, m\rangle$ . We can write the eigenvalues as,

$$\hat{\mathbf{j}}^2|j, m\rangle = \hbar^2 j(j+1)|j, m\rangle \quad \text{and} \quad \hat{j}_z|j, m\rangle = \hbar m|j, m\rangle, \quad (4.64)$$

where, for now, we only know that  $m$  is real and  $j \geq 0$ . But since  $\langle j, m|\hat{\mathbf{j}}^2|j, m\rangle \geq \langle j, m|\hat{j}_z^2|j, m\rangle$ , it is clear that  $j(j+1) \geq m^2$ .

#### 4.3.2.1 Rising and lowering operator

Now we introduce the *rising operator*  $\hat{j}_+$  and the *lowering operator*  $\hat{j}_-$  via

$$\hat{j}_{\pm} \equiv \hat{j}_x \pm i\hat{j}_y \quad \text{such that} \quad \hat{j}_- = \hat{j}_+^\dagger. \quad (4.65)$$

It is easy to check the following relationships

$$[\hat{j}_z, \hat{j}_{\pm}] = \pm\hbar\hat{j}_{\pm} \quad \text{and} \quad [\hat{\mathbf{j}}^2, \hat{j}_{\pm}] = 0 \quad \text{and} \quad \hat{j}_{\mp}\hat{j}_{\pm} = \hat{\mathbf{j}}^2 - \hat{j}_z^2 \mp \hbar\hat{j}_z. \quad (4.66)$$

With this we find

$$\begin{aligned} \hat{j}_z\hat{j}_{\pm}|j, m\rangle &= ([\hat{j}_z, \hat{j}_{\pm}] + \hat{j}_{\pm}\hat{j}_z)|j, m\rangle = \hbar(m \pm 1)\hat{j}_{\pm}|j, m\rangle \\ \text{and} \quad \hat{\mathbf{j}}^2\hat{j}_{\pm}|j, m\rangle &= \hat{j}_{\pm}\hat{\mathbf{j}}^2|j, m\rangle = \hbar^2 j(j+1)\hat{j}_{\pm}|j, m\rangle. \end{aligned} \quad (4.67)$$

That is,  $\hat{j}_{\pm}|j, m\rangle$  is a eigenstate of  $\hat{\mathbf{j}}^2$  and  $\hat{j}_z$  with the eigenvalues  $j$  and  $m \pm 1$ , respectively, if  $\hat{j}_{\pm}|j, m\rangle \neq 0$ . Hence,

$$\hat{j}_+|j, m\rangle \propto |j, m+1\rangle. \quad (4.68)$$

In order not to violate the condition  $m^2 \leq j(j+1)$ , we need to fix  $\hat{j}_{\pm}|j, \pm j\rangle = 0$ . Therefore, for a specified  $j$ , the  $m$  can have only one of the  $2j+1$  possible values  $m = -j, -j+1, \dots, j$ . Since  $2j+1$  is an integer,  $j$  can only have values  $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ . Thus, the eigenvalue equation of the observables  $\hat{\mathbf{j}}^2, \hat{\mathbf{j}}$  is solved since we could have chosen instead of  $\hat{j}_z$  any one of the components of  $\hat{\mathbf{j}}$ , knowing that the others do not commute with the chosen one.

All spin components  $\hat{j}_z$  and the scalar  $\hat{\mathbf{j}}^2$  can only have discrete eigenvalues. The smallest unit is  $\hbar/2$ . With the normalization  $\langle j, m|j', m'\rangle = \delta_{j,j'}\delta_{m,m'}$  we have,

$$\langle j, m|\hat{j}_{\mp}\hat{j}_{\pm}|j, m\rangle = \langle j, m|(\hat{\mathbf{j}}^2 - \hat{j}_z^2 \mp \hbar\hat{j}_z)|j, m\rangle = \hbar^2[j(j+1) - m(m \pm 1)], \quad (4.69)$$

and

$$\hat{j}_{\pm}|j, m\rangle = \hbar\sqrt{j(j+1) - m(m \pm 1)}|j, m \pm 1\rangle. \quad (4.70)$$

In Exc. 4.3.4.5 we calculate the uncertainty of the angular momentum components, in Exc. 4.3.4.6 we write the operator  $\hat{j}_x$  in a matrix form, and in Excs. 4.3.4.7 and 4.3.4.8 we calculate projections of the spin of the electron in different directions of the quantization axis.

### 4.3.3 The electron spin

Every angular momentum  $\hat{\mathbf{I}}$  generates a *magnetic dipole moment*  $\vec{\mu}_\ell \propto \hat{\mathbf{I}}$ , which interacts with external magnetic fields,  $V(\vec{\mathcal{B}}) = \vec{\mu}_\ell \cdot \vec{\mathcal{B}}$ . *Inhomogeneous* magnetic fields exert forces on dipole moments,  $\mathbf{F} = -\nabla(\vec{\mu}_\ell \cdot \vec{\mathcal{B}})$ , which are detected by the *Stern-Gerlach experiment*. This experiment reveals not only the quantization of angular momentum, but also the presence of semi-integral values for the magnetic quantum number.

In 1925 Uhlenbeck and Goudsmit proposed that the electron could have an intrinsic angular momentum with the quantum number  $s = 1/2$ . This angular momentum, called *spin*, would not correspond to any orbiting mass or charge distribution within the classical radius of the electron of the type  $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ . The spin is a purely quantum phenomenon because it disappears when  $\hbar \rightarrow 0$ . It is believed nowadays that the electron is actually point-like with no detectable deviation from Coulomb's law at any distance. The spin of the electron does not follow from the Schrödinger equation, but can be included, ad hoc. On the other hand, it is interesting that it is a necessary consequence of the stringent relativistic derivation of quantum mechanics by *Paul Dirac*.

To characterize the spin, we can use the whole SU(2) formalism of the quantum mechanics of angular momentum:

$$\hat{\mathbf{s}} \times \hat{\mathbf{s}} = i\hbar\hat{\mathbf{s}}, \quad (4.71)$$

and

$$\begin{aligned} \hat{\mathbf{s}}^2|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle &= \hbar^2\frac{3}{4}|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle, & \hat{s}_z|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle &= \pm\frac{\hbar}{2}|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle, \\ \text{and } \hat{s}_{\pm} &= \hbar\hat{\sigma}_{\pm} = \hbar|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle\langle\tfrac{1}{2}, \mp\tfrac{1}{2}|. \end{aligned} \quad (4.72)$$

The operators  $\hat{\sigma}_{\pm}$  are the *Pauli spin matrices*.

### 4.3.4 Exercises

#### 4.3.4.1 Ex: Properties of the angular orbital momentum

Show that  $\hat{\mathbf{L}} \times \hat{\mathbf{L}} = i\hbar\hat{\mathbf{L}}$  and  $[\hat{l}_x, \hat{l}_y] = i\hbar\hat{l}_z$ .

#### 4.3.4.2 Ex: Levi-Civita tensor

Demonstrate  $[\hat{l}_k, \hat{r}_m] = i\hbar r_n \epsilon_{kmn}$  where the Levi-Civita tensor is defined by  $\epsilon_{kmn} = 1$  when  $(kmn)$  is an even permutation of  $(123)$ ,  $\epsilon_{kmn} = -1$  for an odd permutation, and  $\epsilon_{kmn} = 0$  when two of the indices are equal.

**4.3.4.3 Ex: Angular orbital momentum of a harmonic oscillator**

Show for an isotropic three-dimensional harmonic oscillator:  $[\hat{H}, \hat{\mathbf{I}}^2] = [\hat{H}, \hat{l}_z] = 0$ . Make explicit calculations, that is, show

$$\left[ \frac{p^2}{2m}, \hat{l}_z \right] = 0 = \left[ \frac{m}{2} \omega^2 r^2, \hat{l}_z \right] \quad \text{and} \quad \left[ \frac{p^2}{2m}, \hat{\mathbf{I}}^2 \right] = 0 = \left[ \frac{m}{2} \omega^2 r^2, \hat{\mathbf{I}}^2 \right].$$

**4.3.4.4 Ex: Commutation of the absolute value and the components of the orbital angular momentum**

Show  $[\hat{\mathbf{j}}^2, \hat{\mathbf{j}}] = 0$ .

**4.3.4.5 Ex: Uncertainty of angular momentum components**

Show that if  $\hat{j}_z$  is precise, then  $\hat{j}_x$  and  $\hat{j}_y$  are imprecise.

**4.3.4.6 Ex: Matrix representation of the components of the angular momentum**

Calculate the matrix elements of  $\hat{j}_x$  and  $\hat{j}_x^2$  in the base where  $\hat{j}_z$  is observable. Give the general formula and examples for  $j = \frac{1}{2}$  and  $j = 1$ .

**4.3.4.7 Ex: Spin-1/2-particle in a magnetic field**

Consider a spin-1/2-particle whose magnetic moment is  $\vec{\mu} = \gamma \mathbf{S}$  (where  $\gamma$  is a constant). We can describe the quantum state of this particle in terms of the space generated by the eigenvectors  $|+\rangle$  and  $|-\rangle$  of the operator  $\hat{S}_z$ , which measures the spin projection in  $z$ -direction:

$$\hat{S}_z |+\rangle = \frac{\hbar}{2} |+\rangle \quad , \quad \hat{S}_z |-\rangle = -\frac{\hbar}{2} |-\rangle$$

Initially ( $t = 0$ ) the particle is in the state  $\psi(t = 0) = |+\rangle$  and is subject to a uniform magnetic field  $\mathbf{B} = B \hat{\mathbf{e}}_y$ , so that:

$$\hat{H} = -\vec{\mu} \cdot \mathbf{B} = -\gamma B \hat{S}_y .$$

- What are the possible measurements of the spin projection on the  $y$ -axis?
- Find the eigenvectors of  $\hat{S}_y$ .
- Get  $|\psi(t)\rangle$  at  $t > 0$  in terms of the eigenvectors  $|+\rangle$  and  $|-\rangle$  defined above.
- Obtain the mean expectation values of the observables  $\hat{S}_x$ ,  $\hat{S}_y$  and  $\hat{S}_z$  as a function of time.

**4.3.4.8 Ex: Spin expectation value for a two-level system**

Consider an arbitrary state of a two-level system  $|\vartheta, \varphi\rangle = \cos \frac{\vartheta}{2} |+\rangle + e^{i\varphi} \sin \frac{\vartheta}{2} |-\rangle$  and calculate the expectation values of the ladder operators  $\hat{s}_{\pm}$  and of the spin operator  $\hat{\mathbf{s}}$ . Also calculate the expectation values of  $\hat{s}_{\pm}^2$ ,  $\hat{s}_{\pm} \hat{s}_{\mp}$ ,  $\hat{s}_{\alpha}^2$  with  $\alpha = x, y, z$ . Finally, calculate the uncertainties of  $\hat{s}_{\alpha}^2$  and check the uncertainty relation.



## 4.4 Coupling of angular momenta

### 4.4.1 Singlet and triplet states with two electrons

In this section we first consider the spin states of two electrons, which can be combined into two groups with well-defined total spin. With this we can understand the energy spectrum of helium, which is very much dominated by Pauli's principle and quantum statistics. The introduced concepts can be extended to atoms with many electrons.

Angular momentum is an important quantum number in the treatment of the internal structure of atoms. The two electrons in the helium electronic shell each contribute a spin of  $S = \frac{1}{2}$ , which couple to a total angular momentum. Let us consider, for simplicity, two free electrons. The state of the two-particle system is an element of the product space of the two Hilbert spaces in which the individual electrons are described. We will now apply the formalism of Sec. 2.3.8 explicitly to a pair of electrons. The states that the two electrons can occupy are:

$$|\gamma_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \equiv |\uparrow\uparrow\rangle \quad , \quad (4.73)$$

$$|\gamma_2\rangle = |\uparrow\downarrow\rangle \quad , \quad |\gamma_3\rangle = |\downarrow\uparrow\rangle \quad , \quad |\gamma_4\rangle = |\downarrow\downarrow\rangle .$$

The Pauli matrices act on the spin of the individual electrons. They can be extended to the product Hilbert space as follows,

$$\begin{aligned} \frac{\hbar}{2}\hat{\sigma}_x \otimes \mathbb{I}_2 &= \frac{\hbar}{2} \begin{pmatrix} 0 & \mathbb{I}_2 \\ \mathbb{I}_2 & 0 \end{pmatrix} \quad , \quad \frac{\hbar}{2}\mathbb{I}_2 \otimes \hat{\sigma}_x = \frac{\hbar}{2} \begin{pmatrix} \hat{\sigma}_x & 0 \\ 0 & \hat{\sigma}_x \end{pmatrix} \\ \frac{\hbar}{2}\hat{\sigma}_y \otimes \mathbb{I}_2 &= \frac{\hbar}{2} \begin{pmatrix} 0 & i\mathbb{I}_2 \\ -i\mathbb{I}_2 & 0 \end{pmatrix} \quad , \quad \frac{\hbar}{2}\mathbb{I}_2 \otimes \hat{\sigma}_y = \frac{\hbar}{2} \begin{pmatrix} \hat{\sigma}_y & 0 \\ 0 & \hat{\sigma}_y \end{pmatrix} \\ \frac{\hbar}{2}\hat{\sigma}_z \otimes \mathbb{I}_2 &= \frac{\hbar}{2} \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix} \quad , \quad \frac{\hbar}{2}\mathbb{I}_2 \otimes \hat{\sigma}_z = \frac{\hbar}{2} \begin{pmatrix} \hat{\sigma}_z & 0 \\ 0 & \hat{\sigma}_z \end{pmatrix} . \end{aligned} \quad (4.74)$$

With these operators we can now build other operators. We first consider the three components of the total angular momentum,

$$\hat{S}_k = \frac{\hbar}{2}(\hat{\sigma}_k \otimes \mathbb{I}_2 + \mathbb{I}_2 \otimes \hat{\sigma}_k) \quad \text{such that} \quad (4.75)$$

$$\hat{S}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \quad , \quad \hat{S}_y = \frac{i\hbar}{2} \begin{pmatrix} 0 & -1 & -1 & 0 \\ 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \quad , \quad \hat{S}_z = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} .$$

The operator for the square of the absolute value of the total angular momentum is calculated as follows:

$$\hat{\mathbf{S}}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} . \quad (4.76)$$

Now, we look for the eigenvalues of the total angular momentum. The equation for the eigenvalues of  $\hat{S}_z$ ,

$$\hat{S}_z|\gamma_k\rangle = M_S|\gamma_k\rangle, \quad (4.77)$$

is already diagonal in the introduced basis  $\{\gamma_k\}$  with the eigenvalues,

$$M_S = \hbar, 0, 0, -\hbar. \quad (4.78)$$

For  $\hat{\mathbf{S}}^2$  the situation is more interesting: The states  $|\gamma_1\rangle$  and  $|\gamma_4\rangle$  are eigenstates of  $\mathbf{S}^2$  for the eigenvalue  $2\hbar^2$ , but the states  $|\gamma_2\rangle$  and  $|\gamma_3\rangle$  are *not* eigenstates. On the other hand, we know that the linear combination of two eigenstates with the same eigenvalue is also a eigenstate. Therefore, the states

$$|\tilde{\gamma}_1\rangle \equiv |\gamma_1\rangle, \quad |\tilde{\gamma}_4\rangle \equiv |\gamma_4\rangle, \quad |\tilde{\gamma}_a\rangle \equiv \frac{1}{\sqrt{2}}(|\gamma_2\rangle - |\gamma_3\rangle), \quad |\tilde{\gamma}_s\rangle \equiv \frac{1}{\sqrt{2}}(|\gamma_2\rangle + |\gamma_3\rangle), \quad (4.79)$$

are *still* eigenstates of  $\hat{S}_z$ , but they *also* are eigenstates of  $\hat{\mathbf{S}}^2$ , since we can easily verify,

$$\hat{\mathbf{S}}^2|\gamma_s\rangle = 2\hbar^2|\gamma_s\rangle \quad \text{and} \quad \hat{\mathbf{S}}^2|\gamma_a\rangle = 0\hbar^2|\gamma_a\rangle, \quad (4.80)$$

using the matrices (4.75). In summary, for the eigenvalue  $\langle\hat{\mathbf{S}}^2\rangle = 2\hbar^2$  there exist the following three states:

$$\left. \begin{array}{l} |\gamma_1\rangle \quad M_s = 1 \\ |\gamma_4\rangle \quad M_s = -1 \\ |\gamma_s\rangle \quad M_s = 0 \end{array} \right\} \quad \text{triplet, } S = 1 \quad (4.81)$$

For  $\langle\mathbf{S}^2\rangle = 0$  there is only one state:

$$|\gamma_a\rangle \quad M_s = 0 \quad \text{singlet, } S = 0. \quad (4.82)$$

By exchanging the two electrons, the vectors  $|\gamma_1\rangle$  and  $|\gamma_4\rangle$  retain their shape, while the mixed vectors change their shape:  $\gamma_2 \longleftrightarrow \gamma_3$ . Under particle exchange  $|\gamma_a\rangle$  reverses its sign, that is, it is antisymmetric, while  $|\gamma_1\rangle$ ,  $|\gamma_4\rangle$  and  $|\gamma_c\rangle$  conserve their signs, that is, they are symmetrical.

In summary, the triplet states have the quantum number of the total angular momentum (with the expected value for  $\hat{\mathbf{S}}^2$  of  $\hbar^2 S(S+1) = 2\hbar^2$ ), and they are symmetrical about the exchange of particles. The singlet state has the quantum number of the total angular momentum  $S = 0$ , and it is antisymmetric about the exchange of particles. The transition from the original basis  $\{|\gamma_1\rangle, |\gamma_2\rangle, |\gamma_3\rangle, |\gamma_4\rangle\}$  to the new basis  $\{|\tilde{\gamma}_1\rangle, |\tilde{\gamma}_s\rangle, |\tilde{\gamma}_a\rangle, |\tilde{\gamma}_4\rangle\}$  described by Eqs. (4.79) is done by a unitary transformation,

$$|\tilde{\gamma}\rangle = U_{CGC}|\gamma\rangle \quad \text{with} \quad U_{CGC} = \begin{pmatrix} 1 & & & \\ & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \\ & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \\ & & & 1 \end{pmatrix}, \quad (4.83)$$

whose components are known as Clebsch-Gordan coefficients. A similar treatment can be done with bosons, as will be discussed in Sec. 10.1.

### 4.4.2 Coupling two spins

We now consider a perturbation of the system which, for some reason, only affects the first spin. In the absence of the second atom we would have,

$$\hat{H}_1 = \begin{pmatrix} 0 & \Omega^* \\ \Omega & 0 \end{pmatrix}. \quad (4.84)$$

Including the second atom,

$$\hat{H} = \hat{H}_1 \otimes \mathbb{I} = \begin{pmatrix} & & \Omega^* & \\ & & & \Omega^* \\ \Omega & & & \\ & \Omega & & \end{pmatrix}. \quad (4.85)$$

In this case, the perturbation Hamiltonian does not commute with the total angular momentum,

$$[\hat{\mathbf{S}}^2, \hat{H}] \neq 0. \quad (4.86)$$

Another type of perturbation affects both spin symmetrically (e.g., Dicke superradiance with two atoms in the same radiative mode or two counterpropagating modes in a ring cavity). The interaction Hamiltonian is now the sum of the individual perturbations,

$$\hat{H} = \hat{H}_1 \otimes \mathbb{I} + \mathbb{I} \otimes \hat{H}_1 = \begin{pmatrix} & \Omega^* & \Omega^* & \\ \Omega & & & \Omega^* \\ \Omega & & & \Omega^* \\ & \Omega & \Omega & \end{pmatrix}. \quad (4.87)$$

This Hamiltonian commutes with the total angular momentum,

$$[\hat{\mathbf{S}}^2, \hat{H}] = 0. \quad (4.88)$$

$S$  now is a good quantum number. Singlet states do not couple with triplets. This is the idea behind Dicke's superradiance. The absolute value of the total angular momentum is conserved. The quantum number  $\mathbf{S}$  is called *Dicke cooperativity* [196].

**Example 29 (Two atoms interacting through their dipole moments):** As an example of a system exhibiting coupling of the type described in (4.87) we consider two atoms  $j = 1, 2$  interacting through their dipole moments. First, without interaction the Hamiltonian will be,

$$\hat{H} = \hbar\omega_0 \hat{S}_z, \quad (4.89)$$

with  $\hat{S}_z$  given by (4.75).

Now, the atoms interact via their dipole moments with an electromagnetic field assumed to be the same for both atoms,

$$\begin{aligned} \hat{H}_{int} = & -\frac{q}{m} \mathbf{A}(\mathbf{r}_1) \cdot (p_x \hat{\mathbf{e}}_x \hat{\sigma}^x \otimes \mathbb{I} + p_y \hat{\mathbf{e}}_y \hat{\sigma}^y \otimes \mathbb{I}) \\ & -\frac{q}{m} \mathbf{A}(\mathbf{r}_2) \cdot (p_x \hat{\mathbf{e}}_x \mathbb{I} \otimes \hat{\sigma}^x + p_y \hat{\mathbf{e}}_y \mathbb{I} \otimes \hat{\sigma}^y), \end{aligned} \quad (4.90)$$

with  $\mathbf{r}_1 \simeq \mathbf{r}_2$ . By the rules (4.74) we find in matrix notation a Hamiltonian equivalent to (4.87). Using the abbreviations  $\Omega_x \equiv \frac{q}{m} A_x p_x$ ,  $\Omega_y \equiv \frac{q}{m} A_y p_y$ ,  $\Omega_{\pm} \equiv \Omega_x \pm i\Omega_y$ , and  $\Omega \equiv \sqrt{\Omega_x^2 + \Omega_y^2}$ ,

$$\hat{H} = \begin{pmatrix} 0 & \Omega_- & \Omega_- & 0 \\ \Omega_+ & 0 & 0 & \Omega_- \\ \Omega_+ & 0 & 0 & \Omega_- \\ 0 & \Omega_+ & \Omega_+ & 0 \end{pmatrix}. \quad (4.91)$$

Note, that the Hamiltonian is Hermitian, although it consists of sums of operators  $\hat{\sigma}_{1,2}^{\pm}$ . Thus, the coupling is inherently different from a beamsplitter-type couplings generated by terms expressions like  $\hat{\sigma}_{1+}^+ \hat{\sigma}_{2-}^-$ .

Using MAPLE we find the eigenvector and eigenvalue matrices,

$$U = \begin{pmatrix} \frac{\Omega_-}{\Omega_+} & -\frac{\Omega_-}{\Omega_+} & 0 & \frac{\Omega_-}{\Omega_+} \\ -\sqrt{\frac{\Omega_-}{\Omega_+}} & 0 & -1 & \sqrt{\frac{\Omega_-}{\Omega_+}} \\ -\sqrt{\frac{\Omega_-}{\Omega_+}} & 0 & 1 & \sqrt{\frac{\Omega_-}{\Omega_+}} \\ 1 & 1 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \hat{E} = \begin{pmatrix} -2\Omega & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\Omega \end{pmatrix}. \quad (4.92)$$

Now we get to the evolution of the various states,

$$U e^{i\hat{E}t} U^{-1} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -\sqrt{\frac{\Omega_-}{\Omega_+}} \sin 2\Omega t \\ \cos 2\Omega t \\ \cos 2\Omega t \\ \sqrt{\frac{\Omega_+}{-\Omega_-}} \sin 2\Omega t \end{pmatrix} \quad \text{and} \quad U e^{i\hat{E}t} U^{-1} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}. \quad (4.93)$$

That is, the Hamiltonian (4.89) does not mix antisymmetric singlet states and symmetric triplet states.

### 4.4.3 Decoupled and coupled bases

Electrically charged orbiting particles produce a magnetic field. This field can influence the motion of other particles. In the same way, the spin of an electron can influence its own orbital motion. That is, angular momenta can couple and interact in a complicated way. Even to describe the behavior of an atom as simple as hydrogen in an external field, we need to construct the eigenstates of the total angular momentum resulting from a coupling of the electron's intrinsic spin and its orbital motion.

On the other side, we have hitherto considered predominantly hydrogen and hydrogen-like atoms, that is, atoms with a nucleus and a single (valence) electron. But in fact atoms can have more than 100 electrons, which complicates the exact description. In atoms with many electrons, one of the most common coupling schemes is when the angular momenta of all electrons couple to a *total angular momentum*,  $\hat{\mathbf{L}} = \sum_k \hat{\mathbf{l}}_k$ , which then couples to the *total spin*,  $\hat{\mathbf{S}} = \sum_k \hat{\mathbf{s}}_k$ , to form the complete total angular momentum,  $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ . We generally assign total momenta to capital letters.

Adopting an unbiased notation we study some properties of the total angular momentum,  $\hat{\mathbf{j}} \equiv \hat{\mathbf{j}}_1 + \hat{\mathbf{j}}_2$ . In Exc. 4.4.5.1 we find that the addition of angular momenta produces a quantity which is also an angular momentum, but not the subtraction.

The angular momenta of two particles or two angular momenta of different origins in a single particle represent independent degrees of freedom,  $[\mathbf{j}_1, \mathbf{j}_2] = 0$ . Without interaction between angular momenta the Hilbert spaces are orthogonal:

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \begin{pmatrix} \mathcal{H}_1 & 0 \\ 0 & \mathcal{H}_2 \end{pmatrix}. \quad (4.94)$$

The eigenfunctions act on a space of dimension,  $\dim \mathcal{H}_1 \cdot \dim \mathcal{H}_2$ :

$$|j_1, m_{j1}; j_2, m_{j2}\rangle. \quad (4.95)$$

That is, there is a complete set of commuting operators  $\{\hat{\mathbf{J}}_1^2, \hat{j}_{1z}, \hat{\mathbf{J}}_2^2, \hat{j}_{2z}\}$ . Therefore, we can specify quantum numbers  $j_1, j_2, m_{j1}$ , and  $m_{j2}$  simultaneously. On the other hand, the group  $\{\hat{\mathbf{J}}_1^2, \hat{\mathbf{J}}_2^2, \hat{\mathbf{J}}^2, \hat{j}_z\}$  also represents a complete set of commuting operators, as shown in Exc. 4.4.5.2. It has the basis

$$|(j_1, j_2)j, m_j\rangle. \quad (4.96)$$

To describe the two angular momenta simultaneously, we must opt between the decoupled picture  $|j_1, m_{j1}; j_2, m_{j2}\rangle$  and the coupled picture  $|(j_1, j_2)j, m_j\rangle$ . For now, the choice of the picture makes no difference, but we will see later that there may be an energy associated with the coupling<sup>3</sup>. In this case, as we will show, the choice of the coupled base is more natural, because the energy commutes like  $[\hat{H}, \hat{\mathbf{J}}^2] = 0 = [\hat{H}, \hat{j}_z]$ , but  $[\hat{H}, \hat{\mathbf{J}}_1^2] \neq 0 \neq [\hat{H}, \hat{\mathbf{J}}_2^2]$ .

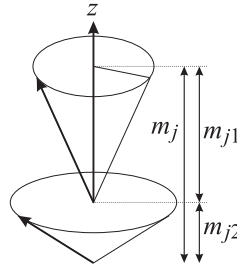


Figure 4.8: Illustration of the coupling of two angular momenta.

#### 4.4.3.1 Allowed values of total angular momentum

Since we do not specify an interaction energy between the spins or between spins and external fields, all states are energetically degenerate. In the decoupled image the degeneracy is easily calculated,

$$\# = \sum_{m_{j1}=-j_1}^{j_1} \sum_{m_{j2}=-j_2}^{j_2} 1 = (2j_1 + 1)(2j_2 + 1). \quad (4.97)$$

<sup>3</sup>That is, the Hamiltonian of the system does not contain terms of type  $\hat{\mathbf{j}}_1 \cdot \hat{\mathbf{j}}_2$ , but may have terms proportional to  $\hat{\mathbf{j}}_1 + \hat{\mathbf{j}}_2$ .

Now we need to find the possible values of  $j$  and  $m_j$  in the coupled picture. The values of  $m_j$  follow immediately from  $\hat{\mathbf{j}}_1 + \hat{\mathbf{j}}_2 = \hat{\mathbf{j}}$ ,

$$m_j = m_{j_1} + m_{j_2} . \tag{4.98}$$

With  $|m_{j_1}| \leq j_1$  and  $|m_{j_2}| \leq j_2$  the values of  $m_j$  are limited to

$$|m_j| \leq j_1 + j_2 . \tag{4.99}$$

We often know the two angular momenta  $j_1$  and  $j_2$  and all their projections in the decoupled base,

$$|m_{j_1}| \leq j_1 \quad \text{and} \quad |m_{j_2}| \leq j_2 . \tag{4.100}$$

To find the quantum numbers in the coupled base, we arrange the states ordering them by their total magnetic quantum number  $m_j$ . We can, without losing generality, concentrate on the situation  $j_1 \geq j_2$ . The following table reproduces the possible combinations. The  $x$ -symbols represent Clebsch-Gordan coefficients:

$m_{j_1} + m_{j_2} = m_j$	$j$	$j$	$j-1$	$j-1$	$j$	$j-1$	$j-2$		$j$	$j-1$	$j$
	$j$	$j-1$	$j-1$	$j-2$	$j-2$	$j-2$			$-j+1$	$-j+1$	$-j$
$j_1$	$j_2$	$x$									
$j_1$	$j_2-1$		$x$	$x$							
$j_1-1$	$j_2$		$x$	$x$							
$j_1$	$j_2-2$				$x$	$x$	$x$				
$j_1-1$	$j_2-1$				$x$	$x$	$x$				
$j_1-2$	$j_2$				$x$	$x$	$x$				
$-j_1+1$	$-j_2$								$x$	$x$	
$-j_1$	$-j_2+1$								$x$	$x$	
$-j_1$	$-j_2$										$x$

The possible values for  $j$  are all those allowing for  $j \geq |m_j| = |m_{j_1} + m_{j_2}|$ , that is,

$$|j_1 - j_2| \leq j \leq j_1 + j_2 . \tag{4.101}$$

Each value of  $j$  has the degeneracy  $2j+1$ . Therefore, as will be verified in Exc. 4.4.5.3, the total degeneracy is,

$$\sum_{j=|j_1-j_2|}^{j_1+j_2} 2j+1 = (2j_1+1)(2j_2+1) . \tag{4.102}$$

**Example 30 (Spin states in the presence of L·S coupling):** As an example we consider two electrons occupying the  $(5p)^2$  orbital. That is, both electrons have  $s_i = \frac{1}{2}$  and  $\ell_i = 1$ . As illustrated in Fig. 4.9, the coupling first gives  $S = s_1 + s_2 = 0, 1$  and  $L = \ell_1 + \ell_2 = 0, 1, 2$ . Then we determine the possible values of the total angular momentum  $J = L + S = 0, 1, 2$  depending on the values of  $L$  and  $S$ .

#### 4.4.4 Clebsch-Gordan coefficients

Let us now describe how to add *two* angular momenta,  $\hat{\mathbf{j}}_1$  and  $\hat{\mathbf{j}}_2$ . Since they act on different degrees of freedom,

$$[\vec{\alpha}_1 \cdot \hat{\mathbf{j}}_1, \vec{\alpha}_2 \cdot \hat{\mathbf{j}}_2] = 0 \tag{4.103}$$

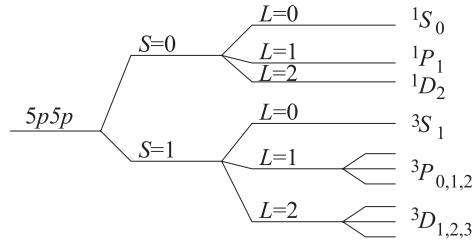


Figure 4.9: Possible spin states of two electrons occupying the  $(5p)^2$  orbital. Spin-orbit coupling  $\mathbf{L} \cdot \mathbf{S}$  leads to a splitting of the energy levels.

for arbitrary vectors  $\vec{\alpha}_1$  and  $\vec{\alpha}_2$ . We have a system of common eigenvectors,  $|\eta, j_1, j_2, m_1, m_2\rangle$ , where  $\eta$  are the eigenvalues of other observables commuting with  $\hat{\mathbf{j}}_1$  and  $\hat{\mathbf{j}}_2$ . These eigenvectors give the values  $\hbar^2 j_1(j_1 + 1)$  and  $\hbar^2 j_2(j_2 + 1)$  for the observables  $\hat{\mathbf{j}}_1^2$  and  $\hat{\mathbf{j}}_2^2$ , as well as  $\hbar m_1$  and  $\hbar m_2$  for the observables  $j_{z1}$  and  $j_{z2}$ . The number of states is  $(2j_1 + 1)(2j_2 + 1)$ . Now we want to construct the eigenstates of the total angular momentum  $\hat{\mathbf{j}} = \hat{\mathbf{j}}_1 + \hat{\mathbf{j}}_2$ . Since

$$[\hat{\mathbf{j}}, \hat{\mathbf{j}}_1^2] = 0 = [\hat{\mathbf{j}}, \hat{\mathbf{j}}_2^2], \quad (4.104)$$

there exist common eigenstates  $|j_1, j_2, j, m\rangle$  for the set of observables  $\hat{\mathbf{j}}_1^2$ ,  $\hat{\mathbf{j}}_2^2$ ,  $\hat{\mathbf{j}}^2$  and  $j_z$ . These eigenstates are linear combinations of the individual states,

$$\begin{aligned} |(j_1, j_2)j, m\rangle &= \sum_{m_1, m_2} |j_1, j_2, m_1, m_2\rangle \langle j_1, j_2, m_1, m_2 | (j_1, j_2)j, m\rangle \\ &= \sum_{m_1, m_2} |j_1, j_2, m_1, m_2\rangle \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix}. \end{aligned} \quad (4.105)$$

The matrix coefficient is called *Clebsch-Gordan coefficient*. The Clebsch-Gordans disappear when the conditions <sup>4</sup>

$$|j_1 - j_2| \leq j \leq j_1 + j_2 \quad \text{and} \quad m = -j_1 - j_2, -j_1 - j_2 + 1, \dots, j_1 + j_2 \quad (4.106)$$

are not satisfied.

The unitary transformation matrices between decoupled and coupled bases,

$$|(j_1, j_2)j, m\rangle = U_{CGC} |j_1, m_1; j_2, m_2\rangle, \quad (4.107)$$

are listed in tables of the Clebsch-Gordan coefficients.

**Example 31 (Clebsch-Gordans for the coupling of two spins  $\frac{1}{2}$ ):** For example, for the system consisting of two  $\frac{1}{2}$  spins we have,

$$\begin{pmatrix} |(\frac{1}{2}, \frac{1}{2})1, +1\rangle \\ |(\frac{1}{2}, \frac{1}{2})1, 0\rangle \\ |(\frac{1}{2}, \frac{1}{2})0, 0\rangle \\ |(\frac{1}{2}, \frac{1}{2})1, -1\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 \\ 0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} |(\frac{1}{2}, +\frac{1}{2}, \frac{1}{2}, +\frac{1}{2})\rangle \\ |(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, +\frac{1}{2})\rangle \\ |(\frac{1}{2}, +\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\rangle \\ |(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\rangle \end{pmatrix}.$$

<sup>4</sup>The Clebsch-Gordans are related to the  $(3j)$  de Wigner symbols.

In the Excs. 4.4.5.4 and 4.4.5.5 we write all possible states of two angular momenta in decoupled and coupled bases. In Excs. 4.4.5.6, 4.4.5.7, we derive the matrix representation of two spins in the decoupled and the coupled base. In 4.4.5.8, and 4.4.5.9 we practice the transformation between decoupled and coupled bases, and in Exc. 4.4.5.10 we verify a rule guaranteeing the unitarity of the Clebsch-Gordan transformation. Finally in 4.4.5.11, 4.4.5.12, and 4.4.5.13 we study  $\mathbf{L} \cdot \mathbf{S}$ -coupling.

#### 4.4.4.1 Coupling of three angular moments

Three angular momenta can be coupled in three different configurations: First  $j_1$  with  $j_2$ , then the total spin  $(j_1, j_2)j_{12}$  with the third one  $j_3$ . We use the notation  $[(j_1, j_2)j_{12}, j_3]J$  or  $[(j_1, j_3)j_{13}, j_2]J$  or  $[(j_2, j_3)j_{23}, j_1]J$ . The recoupling of three spins

$$\begin{array}{rcl}
 \mathbf{j}_1 & + & \mathbf{j}_2 = \mathbf{j}_{12} \\
 + & & + \\
 \mathbf{j}_3 & & \mathbf{j}_3 \\
 = & & = \\
 \mathbf{j}_{13} & + & \mathbf{j}_2 = \mathbf{J}
 \end{array} \tag{4.108}$$

is described by  $\{6j\}$ -symbols, for example,

$$[(j_1, j_2)j_{12}, j_3]J = \sum_{j_{13}} \{6j\} [(j_1, j_3)j_{13}, j_2]J . \tag{4.109}$$

#### 4.4.4.2 Notation for atomic states with LS-coupling

In an atom, the spins of the electrons often couple to a total spin,  $\mathbf{S} = \sum_k \mathbf{s}_k$ , and separately the orbital angular momenta to a total orbital angular momentum,  $\mathbf{L} = \sum_k \mathbf{l}_k$ . These two total spins now couple to a total angular momentum,  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ . When this **LS-coupling** happens, the following notation is used to characterize the electronic states in atoms:

$${}^{2S+1}L_J . \tag{4.110}$$

#### 4.4.4.3 jj-coupling

There is also the case that for each electron its spin couples to its own orbital angular momentum,  $\mathbf{j}_k = \mathbf{l}_k + \mathbf{s}_k$ , before coupling to the total angular momenta of other electrons,  $\mathbf{J} = \sum_k \mathbf{j}_k$ . This is called **jj-coupling**. In the case of two electrons the recoupling of the four involved spins

$$\begin{array}{rcl}
 \mathbf{l}_1 & + & \mathbf{l}_2 = \mathbf{L} \\
 + & & + \\
 \mathbf{s}_1 & + & \mathbf{s}_2 = \mathbf{S} \\
 = & & = \\
 \mathbf{j}_1 & + & \mathbf{j}_2 = \mathbf{J}
 \end{array} \tag{4.111}$$



is described by  $\{9j\} = \left\{ \begin{matrix} l_1 & l_2 & L \\ s_1 & s_2 & S \\ j_1 & j_2 & J \end{matrix} \right\}$ -symbols,

$$|[l_1, s_1]j_1, [l_2, s_2]j_2]J\rangle = \sum_{L,S} \{9j\} |[l_1, l_2]L, [s_1, s_2]S]J\rangle. \quad (4.112)$$

#### 4.4.5 Exercises

##### 4.4.5.1 Ex: Addition/subtraction of angular momenta

Show that  $\hat{\mathbf{j}}_1 + \hat{\mathbf{j}}_2$  is an angular momentum, but not  $\hat{\mathbf{j}}_1 - \hat{\mathbf{j}}_2$ .

##### 4.4.5.2 Ex: CSCO for coupled angular momenta

Be  $\hat{\mathbf{j}} = \hat{\mathbf{j}}_1 + \hat{\mathbf{j}}_2$ . Show that  $\{\hat{\mathbf{j}}_1^2, \hat{\mathbf{j}}_2^2, \hat{\mathbf{j}}^2, \hat{j}_z\}$  is a CSCO; that is, show that

a.  $\hat{\mathbf{j}}^2$  commutes with  $\hat{\mathbf{j}}_1^2$  and  $\hat{\mathbf{j}}_2^2$ ;

b.  $\hat{\mathbf{j}}^2$  does not commute with  $\hat{j}_{1z}$  or  $\hat{j}_{2z}$  and that we can not specify  $m_{j_1}$  or  $m_{j_2}$  together with  $j$ .

##### 4.4.5.3 Ex: Multiplicity of coupled angular momenta

Verify  $\# = (2j_1 + 1)(2j_2 + 1)$  within the coupled representation.

##### 4.4.5.4 Ex: Possible states of two (de-)coupled angular momenta

Find all possible states with the angular momenta  $j_1 = 1$  and  $j_2 = 1/2$  in decoupled and coupled pictures.

##### 4.4.5.5 Ex: Fine and hyperfine structure of the rubidium atom $^{85}\text{Rb}$

1. The rubidium atom  $^{85}\text{Rb}$  has one valence electron. In the first excited state this electron has the orbital angular momentum,  $L = 1$ . What are the possible states?

2. In the fundamental state of this atom the total electronic angular momentum  $J$  couples with the spin of the nucleus,  $I = 5/2$ , to form the total angular momentum  $\mathbf{F} = \mathbf{J} + \mathbf{I}$ . Determine the possible values for the angular momentum  $F$  and the magnetic quantum number  $m_F$ .

##### 4.4.5.6 Ex: Expansion of the hyperfine structure of the rubidium atom $^{87}\text{Rb}$

Determine for the states  $S_{1/2}$  and  $P_{3/2}$  of an atom with nuclear spin  $I = 3/2$  and hyperfine coupling  $\hat{\mathbf{J}} \cdot \hat{\mathbf{I}}$  how the eigenstates of the coupled base expand into the decoupled base. Do not consider external magnetic fields.

**4.4.5.7 Ex: Transition amplitudes between Zeeman sub-states**

- a. We consider the atom of  $^{87}\text{Rb}$  having the nuclear angular momentum  $I = 3/2$ . What are the possible hyperfine states  $F$  resulting from a coupling of  $I$  with the total electronic state angular momentum of the ground state  $^2S_{1/2}$ ? What are the possible Zeeman sub-states of  $F$ ?
- b. What are the possible hyperfine states  $F'$  resulting from a coupling of  $I$  with the total electronic angular momentum of the excited state  $^2P_{3/2}$ ,  $F' = 2$ ? What are the possible Zeeman sub-states of  $F'$ ?
- c. A transition between a ground hyperfine state and an excited hyperfine state can be described by a coupling of the total angular momentum  $F$  with the angular momentum of the photon  $\kappa$  forming the angular momentum of the excited state  $F'$ . To see this, we now consider the levels  $F = 1$  and  $F' = 2$ . Expand the coupled angular momentum  $|(F, \kappa)F', m_{F'}\rangle = |(1, 1)2, m_{F'}\rangle$  on a decoupled basis for every possible value  $m_{F'}$ . Use the table in Fig. 4.10 to determine the Clebsch-Gordan coefficients. **Note:** The Clebsch-Gordans only compare the oscillator strengths of transitions between Zeeman sub-states of a given set  $(F, F')$ . In order to compare the oscillator strengths to other transitions  $(F, F')$  it is necessary to calculate  $6j$ -coefficients.

**4.4.5.8 Ex: Gymnastics of angular momentum operators**

Consider the problem of adding angular momenta  $j_1 = 1$  and  $j_2 = 1/2$ :

- a. What are the possible values of  $m$  and  $j$ , in which  $\hat{j}^2|j, m\rangle = j(j+1)\hbar^2|j, m\rangle$  and  $j_z|j, m\rangle = m\hbar|j, m\rangle$ ?
- b. What are the degeneracy  $g_{j_1, j_2}(m)$ ?
- c. Find the base states  $\{|j, m\rangle\}$ , which are common to the operators  $\mathbf{j}_1^2, \mathbf{j}_2^2, \mathbf{j}, j_z$ , expanded in the base  $\{|j_1, m_1\rangle \otimes |j_2, m_2\rangle\}$  of the eigenstates of  $\mathbf{j}_1^2, \mathbf{j}_2^2, j_{1z}, j_{2z}$ .

**4.4.5.9 Ex: (Un-)coupled bases of the spherical harmonics**

Expand the triplet state  $^3P_J$  of strontium in a decoupled basis and write down the transformation matrix between the bases.

**4.4.5.10 Ex: Properties of Clebsch-Gordan coefficients**

Given the momenta  $j_1$  and  $j_2$ , and  $C_{m_1, m_2}$  denoting the Clebsch-Gordan coefficients, prove that  $\sum_{m_1, m_2} |C_{m_1, m_2}|^2 = 1$ .

**4.4.5.11 Ex: Spin-orbit coupling**

- a. Show that the operator  $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$  associated with the spin-orbit coupling, satisfies the relation  $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}} = \hat{L}_z \hat{S}_z + (\hat{L}_+ \hat{S}_- + \hat{L}_- \hat{S}_+)/2$ . Obtain the matrix representation of the operator  $\mathbf{L} \cdot \mathbf{S}$ , considering the bases:
- b.  $\{|m_L\rangle \otimes |m_S\rangle\}$  of the eigenstates which are common to the operators  $\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{L}_z, \hat{S}_z$ ;
- c.  $\{|J, M\rangle\}$ , which is associated with the operators  $\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{\mathbf{J}}^2, \hat{J}_z$ .
- d. Give the explicit matrices for the case  $L = 1$  and  $S = \frac{1}{2}$  in the representations (b) and (c) and verify that the two representations yield the same eigenvalue spectrum.

**4.4.5.12 Ex: Expansion of the spin-orbit coupling**

Consider the problem of adding the orbital angular momentum  $\ell$  and a spin  $1/2$ . Obtain the  $2\ell + 1$  states  $|\ell + 1/2, m_j\rangle$ , in addition to the  $2\ell$  states  $|\ell - 1/2, m_j\rangle$  (which constitute a common basis for the operators  $\mathbf{I}_1^2, \mathbf{s}_2^2, \mathbf{j}^2, j_z$ ), expanded in the base  $|m_1, m_2\rangle$  of the eigenstates of the operators  $\mathbf{I}^2, \mathbf{s}^2, l_z, s_z$ . You can simplify the procedure by deriving two recurrence relationships from which the desired states follow <sup>5</sup>.

**4.4.5.13 Ex: External product of two spins**

Derive the matrix representation of the spin-orbit coupling operator  $\mathbf{L} \cdot \mathbf{S}$  for  $L = 1$  and  $S = 1/2$  from the definition of the outer product.

**4.4.5.14 Ex: Coupling three spins**

Express the states of three coupled  $\frac{1}{2}$  spins in the uncoupled basis.

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<sup>5</sup>See Cohen-Tannoudji, Vol.2, Complement A.X.

## 4.5 Further reading

et al., [\[DOI\]](#)

Note: A square-root sign is to be understood over every coefficient, e.g., for  $-8/15$  read  $-\sqrt{8/15}$ .

Notation:

$J$	$J$	...
$M$	$M$	...
$m_1$	$m_2$	...
$m_1$	$m_2$	...
...	...	...
...	...	...

Coefficients

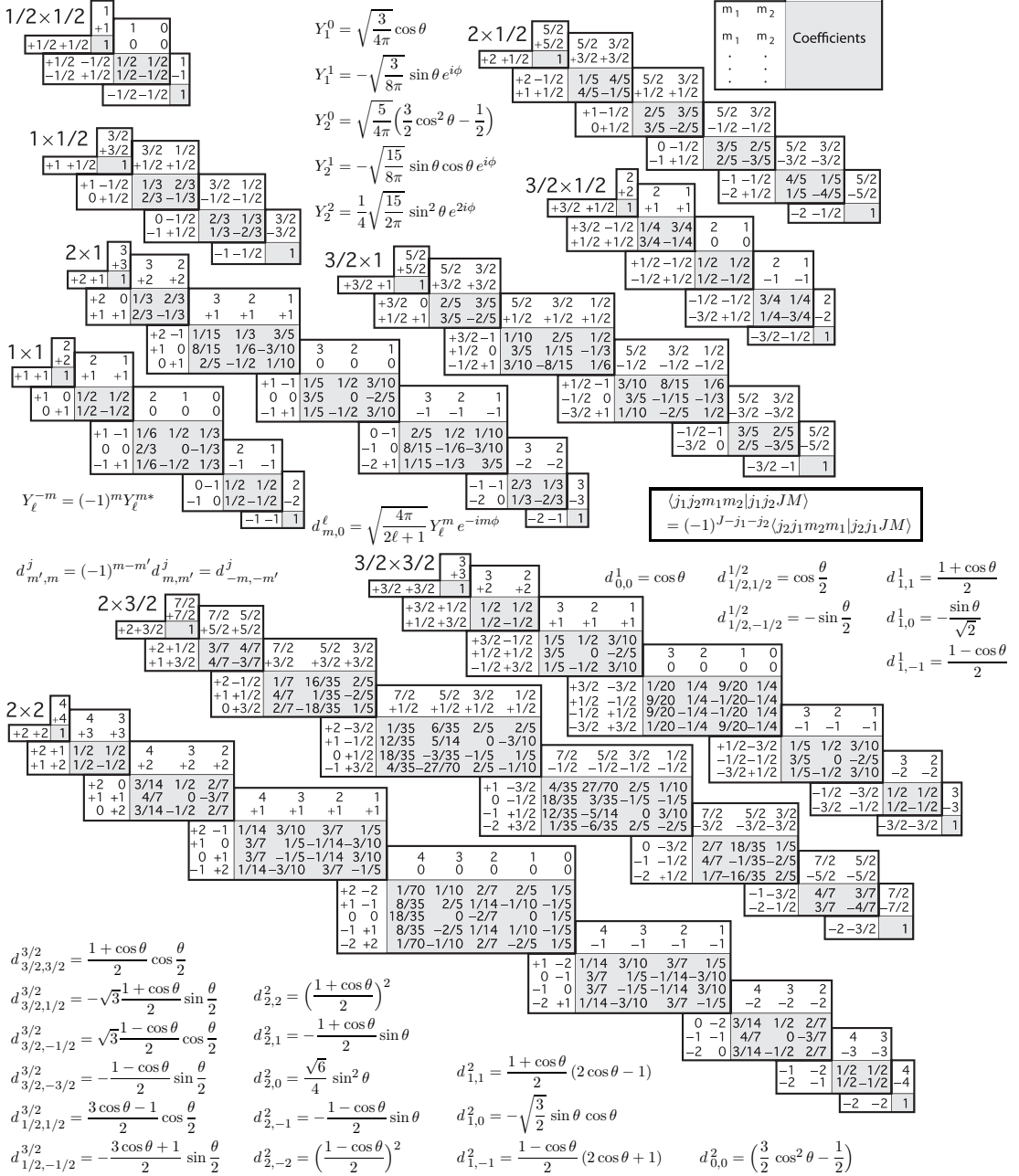


Figure 4.10: Clebsch-Gordan coefficients.

# Chapter 5

## Periodic systems

Many physical systems treat quantum particles in periodic potential. Examples are electrons in crystals or cold atoms in optical lattices. The periodicity gives rise to a wealth of new phenomena, such as Bragg scattering, the formation of energy bands, Mott insulators, or Bloch oscillations. Various theoretical approaches have been developed leading to a deep understanding of the features of crystals, metals, and optical lattices for atomic gases.

In the following sections we will mainly focus on the Bloch model, which is based on introducing periodic boundary conditions to the Schrödinger equation. In the Secs. 5.1 we will give a brief introduction into the Bloch model for electrons in solids, where the periodicity is imposed by the crystalline structure of the material. We will, however, not go into details leaving a comprehensive treatment to specialized textbooks [24, 398]. In the Secs. 5.2 we will concentrate on optical lattices for atomic gases formed by counterpropagating laser beams. The physical realization of these lattices, which can be realized with nearly perfect periodicity, have permitted the experimental observation of phenomena which had been elusive in solid state physics.

### 5.1 The Bloch model for electrons

The motion of an electron inside a crystal is ruled by a spatially periodic potential  $V(\mathbf{r})$  originating from the positively charged crystal atoms and the mean field produced by the quasi-free electrons,

$$V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R}) , \quad (5.1)$$

where  $\mathbf{R}$  is a vector connecting two arbitrarily chosen atoms of the lattice. With the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \quad (5.2)$$

we can write the Schrödinger equation,

$$[\hat{H} + V(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r}) . \quad (5.3)$$

Since  $V$  and  $\nabla$  are invariant under translations  $U_{tr}(\mathbf{R})\psi(\mathbf{r}) \equiv \psi(\mathbf{r} + \mathbf{R})$  by a fixed distance  $\mathbf{R}$ , where the translation operator has been defined in Eq. (2.171), we have,

$$\hat{H}U_{tr}(\mathbf{R})\psi(\mathbf{r}) = EU_{tr}(\mathbf{R})\psi(\mathbf{r}) . \quad (5.4)$$

That is, for a non-degenerate eigenvalue <sup>1</sup>,

$$\psi(\mathbf{r} + \mathbf{R}) = f(\mathbf{R})\psi(\mathbf{r}) . \quad (5.5)$$

This relation holds for all vectors  $\mathbf{R}$  of the lattice, such that,

$$f(\mathbf{R}_1 + \mathbf{R}_2)\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R}_1 + \mathbf{R}_2) = f(\mathbf{R}_1)\psi(\mathbf{r} + \mathbf{R}_2) = f(\mathbf{R}_1)f(\mathbf{R}_2)\psi(\mathbf{r}) . \quad (5.6)$$

The relationship  $f(\mathbf{R}_1 + \mathbf{R}_2) = f(\mathbf{R}_1)f(\mathbf{R}_2)$  is satisfied by the ansatz  $f(\mathbf{R}) \equiv e^{i\mathbf{k}\cdot\mathbf{R}}$ , where  $\mathbf{k}$  is an arbitrary vector of reciprocal space. We get the famous *Bloch theorem*,

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\mathbf{k}}(\mathbf{r})} , \quad (5.7)$$

which represents a necessary condition for any eigenfunction  $\psi_{\mathbf{k}}$  of the Schrödinger equation with periodic potential. Bloch's theorem simply postulates that, apart from a phase factor, the wavefunction has the same periodicity as the potential.

The *Bloch function*,

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r}) \equiv u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{with} \quad u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})} , \quad (5.8)$$

automatically satisfies Bloch's theorem. That is, the wave function of the electron  $\psi$  is a plane wave  $e^{i\mathbf{k}\cdot\mathbf{r}}$  modulated by a function  $u_{\mathbf{k}}$  having the same periodicity as the lattice [405]. Although the vector of the electronic wave is arbitrary, it is possible (and useful) to restrict its value to the first *Brillouin zone* defined by  $\mathbf{k} \in [-\pi/\mathbf{a}, \pi/\mathbf{a}]$ , where  $\mathbf{a}$  is an elementary vector of the lattice. The reason is that we can reduce a wavevector  $\mathbf{k}$  in a wavefunction trespassing the first Brillouin zone by an appropriate vector  $\mathbf{G}$  of *reciprocal lattice*,

$$\mathbf{k}' = \mathbf{k} + \mathbf{G} , \quad (5.9)$$

yielding,

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} = u_{\mathbf{k}}(\mathbf{r})e^{-i\mathbf{G}\cdot\mathbf{r}}e^{i\mathbf{k}'\cdot\mathbf{r}} . \quad (5.10)$$

We now define another function  $u_{\mathbf{k}'}(\mathbf{r}) \equiv u_{\mathbf{k}}(\mathbf{r})e^{-i\mathbf{G}\cdot\mathbf{r}}$ , which also satisfies the requirement (5.8), knowing that  $\mathbf{G} \cdot \mathbf{R} = n2\pi$ , we see,

$$u_{\mathbf{k}'}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{k}}(\mathbf{r} + \mathbf{R})e^{-i\mathbf{G}\cdot(\mathbf{r}+\mathbf{R})} = u_{\mathbf{k}}(\mathbf{r})e^{-i\mathbf{G}\cdot\mathbf{r}} = u_{\mathbf{k}'}(\mathbf{r}) . \quad (5.11)$$

Hence,

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}'}(\mathbf{r})e^{i\mathbf{k}'\cdot\mathbf{r}} = \psi_{\mathbf{k}'}(\mathbf{r}) . \quad (5.12)$$

### 5.1.1 Approximation for quasi-bound electrons

We now assume that the behavior of the electron near an atom is not influenced by atoms farther apart,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{i \in \text{lattice}} c_i(\mathbf{k})\phi(\mathbf{r} - \mathbf{R}_i) . \quad (5.13)$$

That is, we neglect superposition states of the electron at various sites of the lattice. The atom is subject to a potential  $U_{at}(\mathbf{r} - \mathbf{R}_i)$  located near the atom at the position

<sup>1</sup>This also holds true for degenerate eigenvalues if we choose suitable basis of eigenvectors.

$\mathbf{R}_i$ , and it is described by the eigenfunction  $\phi(\mathbf{r} - \mathbf{R}_i)$  (only defined for the site  $i$ ) with energy  $E_0$ ,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U_{at}(\mathbf{r} - \mathbf{R}_i) \right] \phi(\mathbf{r} - \mathbf{R}_i) = E_0 \phi(\mathbf{r} - \mathbf{R}_i) . \quad (5.14)$$

Even so, the function  $\psi_{\mathbf{k}}(\mathbf{r})$  must satisfy Bloch's theorem. This is the case when  $c_i(\mathbf{k}) = e^{i\mathbf{k} \cdot \mathbf{R}_i}$  and therefore,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{i \in \text{lattice}} e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi(\mathbf{r} - \mathbf{R}_i) . \quad (5.15)$$

**Example 32 (Ansatz for a quasi-bound electron wavefunction):** The ansatz (5.15) satisfies Bloch's theorem because,

$$\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_j) = \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi(\mathbf{r} - (\mathbf{R}_i - \mathbf{R}_j)) = e^{i\mathbf{k} \cdot \mathbf{R}_j} \sum_i e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \phi(\mathbf{r} - (\mathbf{R}_i - \mathbf{R}_j)) = e^{i\mathbf{k} \cdot \mathbf{R}_j} \psi_{\mathbf{k}}(\mathbf{r}) .$$

We now calculate the energy  $E(\mathbf{k})$  of an electron with the wavevector  $\mathbf{k}$  inserting the function  $\psi_{\mathbf{k}}(\mathbf{r})$  of (5.15) in the Schrödinger equation and obtain,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi(\mathbf{r} - \mathbf{R}_i) = E(\mathbf{k}) \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi(\mathbf{r} - \mathbf{R}_i) . \quad (5.16)$$

$U(\mathbf{r})$  is the potential energy of the electron illustrated in Fig. 5.1 together with the energy  $U_{at}(\mathbf{r} - \mathbf{R}_i)$  of a free electron.

Substituting the kinetic energy term of (5.16) by the kinetic energy of (5.14), we calculate,

$$\sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} [-U_{at}(\mathbf{r} - \mathbf{R}_i) + E_0 + U(\mathbf{r}) - E(\mathbf{k})] \phi(\mathbf{r} - \mathbf{R}_i) = 0 . \quad (5.17)$$

Now, multiplying this equation with  $\psi_{\mathbf{k}}^*(\mathbf{r}) = \sum_j e^{i\mathbf{k} \cdot \mathbf{R}_j} \phi^*(\mathbf{r} - \mathbf{R}_j)$  and integrating over the volume of the crystal, we obtain,

$$\begin{aligned} [E(\mathbf{k}) - E_0] \sum_{i,j} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \int \phi^*(\mathbf{r} - \mathbf{R}_j) \phi(\mathbf{r} - \mathbf{R}_i) dV \\ = \sum_{i,j} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \int \phi^*(\mathbf{r} - \mathbf{R}_j) [U(\mathbf{r}) - U_{at}(\mathbf{r} - \mathbf{R}_i)] \phi(\mathbf{r} - \mathbf{R}_i) dV . \end{aligned} \quad (5.18)$$

The functions  $\phi^*(\mathbf{r} - \mathbf{R}_j)$  and  $\phi(\mathbf{r} - \mathbf{R}_i)$  overlap only a little, even for adjacent atoms, such that we can neglect the terms  $i \neq j$  on the left side. The sum then corresponds to the number  $N$  of sites in the lattice. On the right side we can not neglect the terms involving other sites, because even if the wavefunctions of adjacent sites overlap little, the contribution of the potential difference  $|U(\mathbf{r}) - U_{at}(\mathbf{r} - \mathbf{R}_i)|$  is much lower for  $\mathbf{r} = \mathbf{R}_i$  than for  $\mathbf{r} = \mathbf{R}_j$ . On the other hand, as the wavefunctions  $\phi(\mathbf{r} - \mathbf{R}_i)$



disappear quickly when  $|\mathbf{r} - \mathbf{R}_i| > |\mathbf{R}_m - \mathbf{R}_i|$ , we can focus on adjacent sites (called  $\mathbf{R}_m$ ),

$$N[E(\mathbf{k}) - E_0] = N \int \phi^*(\mathbf{r} - \mathbf{R}_i)[U(\mathbf{r}) - U_{at}(\mathbf{r} - \mathbf{R}_i)]\phi(\mathbf{r} - \mathbf{R}_i)dV \quad (5.19)$$

$$+ N \sum_{m=\text{adjacent}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_m)} \int \phi^*(\mathbf{r} - \mathbf{R}_m)[U(\mathbf{r}) - U_{at}(\mathbf{r} - \mathbf{R}_i)]\phi(\mathbf{r} - \mathbf{R}_i)dV .$$

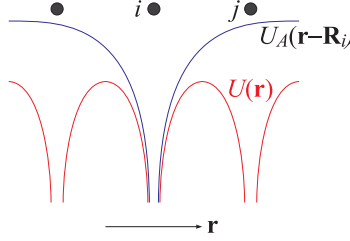


Figure 5.1: Potential energy  $U(\mathbf{r})$  of a crystal electron (red) and potential energy  $U_A(\mathbf{r} - \mathbf{R}_i)$  of the electron of a free atom (blue).

Now we further suppose that the eigenfunction  $\phi$  exhibits radial symmetry corresponding to an  $s$  orbital. We obtain for the eigenvalues from the Schrödinger equation,

$$E(\mathbf{k}) = E_0 - \alpha - \gamma \sum_{m \text{ adjacent of } i} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_m)} \quad (5.20)$$

$$\text{with } \alpha = \int \phi^*(\mathbf{r} - \mathbf{R}_i)[U_{at}(\mathbf{r} - \mathbf{R}_i) - U(\mathbf{r})]\phi(\mathbf{r} - \mathbf{R}_i)dV$$

$$\text{and } \gamma = \int \phi^*(\mathbf{r} - \mathbf{R}_m)[U_{at}(\mathbf{r} - \mathbf{R}_i) - U(\mathbf{r})]\phi(\mathbf{r} - \mathbf{R}_i)dV .$$

The interpretation is as follows: The combination of the atoms in a lattice produces an energy displacement  $\alpha$ . In addition, it generates a splitting into a continuous band of energies as a function of reduced wavevector  $\mathbf{k}$ ...

### 5.1.2 Approximation for quasi-free electrons

Here we assume an essentially homogeneous potential acting on the free electrons and consider the impact of the periodic lattice as a small perturbation. The periodic potential can be decomposed into a Fourier series by the vectors  $\mathbf{G}$  of the reciprocal lattice,

$$U(\mathbf{r}) = \sum_{\mathbf{G}} U_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} . \quad (5.21)$$

Consequently, we can make for Bloch functions (5.10) the following periodic ansatz,

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{with} \quad u_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V_c}} \sum_{\mathbf{G}} u_{\mathbf{G}}(\mathbf{k})e^{i\mathbf{G}\cdot\mathbf{r}} , \quad (5.22)$$

where  $V_c$  is the volume of the crystal.

Without periodic potential, the eigenfunctions would be those of a free particle,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{V_c} e^{i\mathbf{k}\cdot\mathbf{r}} \quad (5.23)$$

with the eigenenergies

$$E_0(\mathbf{k}) = V_0 + \frac{\hbar^2 k^2}{2m} . \quad (5.24)$$

Inserting the functions (5.21) and (5.22) in the Schrödinger equation, we obtain,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + \sum_{\mathbf{G}''} U_{\mathbf{G}''} e^{i\mathbf{G}''\cdot\mathbf{r}} \right] \frac{1}{\sqrt{V_c}} e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{G}'} u_{\mathbf{G}'}(\mathbf{k}) e^{i\mathbf{G}'\cdot\mathbf{r}} = E(\mathbf{k}) \frac{1}{\sqrt{V_c}} e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{G}} u_{\mathbf{G}}(\mathbf{k}) e^{i\mathbf{G}'\cdot\mathbf{r}} , \quad (5.25)$$

that is,

$$\frac{1}{\sqrt{V_c}} \sum_{\mathbf{G}'} \left[ -\frac{\hbar^2}{2m} (\mathbf{k} + \mathbf{G}')^2 - E(\mathbf{k}) \right] u_{\mathbf{G}'}(\mathbf{k}) e^{i(\mathbf{k}+\mathbf{G}')\cdot\mathbf{r}} + \frac{1}{\sqrt{V_c}} \sum_{\mathbf{G}''} U_{\mathbf{G}''} e^{i\mathbf{G}''\cdot\mathbf{r}} \sum_{\mathbf{G}'} u_{\mathbf{G}'}(\mathbf{k}) e^{i(\mathbf{k}+\mathbf{G}')\cdot\mathbf{r}} = 0 . \quad (5.26)$$

Now multiplying with  $\frac{1}{\sqrt{V_c}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$  and integrating over the volume of the crystal (knowing  $\frac{1}{V_c} \int_{V_c} e^{i\mathbf{G}\cdot\mathbf{r}} dV = \delta_{\mathbf{G},0}$ ), we obtain,

$$\left[ \frac{\hbar^2}{2m} (\mathbf{k} + \mathbf{G})^2 - E(\mathbf{k}) \right] u_{\mathbf{G}}(\mathbf{k}) + \sum_{\mathbf{G}'} U_{\mathbf{G}-\mathbf{G}'} u_{\mathbf{G}'}(\mathbf{k}) = 0 , \quad (5.27)$$

for any value of  $\mathbf{G}$ .

To estimate the dependence of the Fourier components  $u_{\mathbf{G}}(\mathbf{k})$  for  $\mathbf{G} \neq 0$  we insert the unperturbed eigenenergies into the equation (5.27) only considering, in the sum over  $\mathbf{G}'$ , the terms of the first perturbative order, that is, those containing  $U_0$  or  $u_0(\mathbf{k})$ ,

$$\frac{\hbar^2}{2m} [(\mathbf{k} + \mathbf{G})^2 - k^2] u_{\mathbf{G}}(\mathbf{k}) - U_0 u_{\mathbf{G}}(\mathbf{k}) + U_0 u_{\mathbf{G}}(\mathbf{k}) + U_{\mathbf{G}} u_0(\mathbf{k}) = 0 \quad (5.28)$$

$$u_{\mathbf{G}}(\mathbf{k}) = \frac{U_{\mathbf{G}} u_0(\mathbf{k})}{\frac{\hbar^2}{2m} [k^2 - (\mathbf{k} + \mathbf{G})^2]} . \quad (5.29)$$

Since the Fourier coefficients  $U_{\mathbf{G}}$  have, for  $\mathbf{G} \neq 0$ , small values, the function  $u_{\mathbf{G}}(\mathbf{k})$  is not negligible only for  $k^2 \simeq (\mathbf{k} + \mathbf{G})^2$  that is,

$$-2\mathbf{k} \cdot \mathbf{G} \simeq |\mathbf{G}|^2 . \quad (5.30)$$

We now want to find out the meaning of this condition ...

For the coefficients  $u_0(\mathbf{k})$  and  $u_{\mathbf{G}}(\mathbf{k})$  we obtain,

$$\left[ \frac{\hbar^2}{2m} k^2 - E(\mathbf{k}) \right] u_0(\mathbf{k}) + U_0 u_0(\mathbf{k}) + U_{-\mathbf{G}}(\mathbf{k}) u_{\mathbf{G}}(\mathbf{k}) = 0 \quad (5.31)$$

$$\left[ \frac{\hbar^2}{2m} k^2 - E(\mathbf{k}) \right] u_{\mathbf{G}}(\mathbf{k}) + U_{\mathbf{G}} u_0(\mathbf{k}) + U_0(\mathbf{k}) u_{\mathbf{G}}(\mathbf{k}) = 0 .$$

From this follows,

$$\left[ \frac{\hbar^2}{2m} k^2 + U_0 - E(\mathbf{k}) \right]^2 = U_{\mathbf{G}} U_{-\mathbf{G}} = 0 . \quad (5.32)$$

Since the potential  $U(\mathbf{r})$  is real,  $U_{-\mathbf{G}} = U_{\mathbf{G}}^*$ . Therefore, introducing the eigenenergies  $E_0(\mathbf{k})$  of free electrons (5.24),

$$E(\mathbf{k}) = E_0(\mathbf{k}) \pm |U_{\mathbf{G}}| . \quad (5.33)$$

Under the influence of the periodic perturbation potential we find at the surfaces of a Brillouin zone an energy splitting developing a forbidden gap in the spectrum. We can understand this observation as follows: In the crystal all electronic waves with wavevectors ending on a surface of a Brillouin zone are reflected by Bragg reflection. In the example of a one-dimensional lattice we understand that the superposition of an incident wave ( $k = n\pi/a$ ) with the reflected one ( $k = -n\pi/a$ ) produces a standing electronic probability density wave  $\rho$  being proportional to  $\rho_1 \propto \cos^2 n\pi/a$  or  $\rho_2 \propto \sin^2 n\pi/a$ . The charge density  $\rho_1$  is maximal at the location of the atom in this site, which corresponds to an increased interaction energy; the density  $\rho_2$  is minimal at the location of the atom. This explains the splitting.

The Bloch model can explain many properties of metals, semiconductors and insulators.

### 5.1.3 One-dimensional periodic potentials

In the following, we restrict ourselves to a one-dimensional potential,  $V(z) = V(z+a)$ , acting on (the center-of-mass of) atoms. How such potentials can be realized in practice will be shown in Sec. 5.2. For now, we just assume that we can write the potential as,

$$V(z) = -2V_0 \cos^2 Kz . \quad (5.34)$$

In the Fourier expansion,  $V(z) = \sum_K U_K e^{iKz}$ , this potential corresponds to the Fourier coefficients  $U_0 = -V_0$  and  $U_{\pm K} = -\frac{V_0}{2}$ ,

$$V(z) = -V_0 \left( 1 + \frac{1}{2} e^{2ik_L z} + e^{-2ik_L z} \right) . \quad (5.35)$$

We also expand the wavefunction into plane waves,

$$\psi(z) = \sum_q c_q e^{iqz} , \quad (5.36)$$

and we insert these expansions into Schrödinger's stationary equation  $\hat{H}\psi = \varepsilon\psi$ , yielding,

$$\left[ \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \sum_K U_K e^{iKz} \right] \sum_q c_q e^{iqz} = \varepsilon \sum_q c_q e^{iqz} . \quad (5.37)$$

Defining  $q = k + nK$ , where  $k \in [-K/2, K/2]$  and  $n \in \mathbb{Z}$ ,

$$\left[ \frac{\hbar^2}{2m} (nK + k)^2 - V_0 \right] c_{nK+k} - \frac{1}{2} V_0 c_{nK+k-K} - \frac{1}{2} V_0 c_{nK+k+K} = \varepsilon c_{nK+k} . \quad (5.38)$$

In matrix notation,

$$\hat{H}\mathbf{c} = \varepsilon\mathbf{c} . \quad (5.39)$$

where the matrix is around  $n = \dots, -1, 0, +1, \dots$ :

$$\hat{H} = \begin{pmatrix} \ddots & & & & & & \\ & \frac{\hbar^2}{2m}(k-K)^2 - V_0 & -\frac{1}{2}V_0 & & & & \\ & -\frac{1}{2}V_0 & \frac{\hbar^2}{2m}k^2 - V_0 & & & & \\ & & -\frac{1}{2}V_0 & \frac{\hbar^2}{2m}(k+K)^2 - V_0 & & & \\ & & & & \ddots & & \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} \vdots \\ c_{k-K} \\ c_k \\ c_{k+K} \\ \vdots \end{pmatrix} \quad (5.40)$$

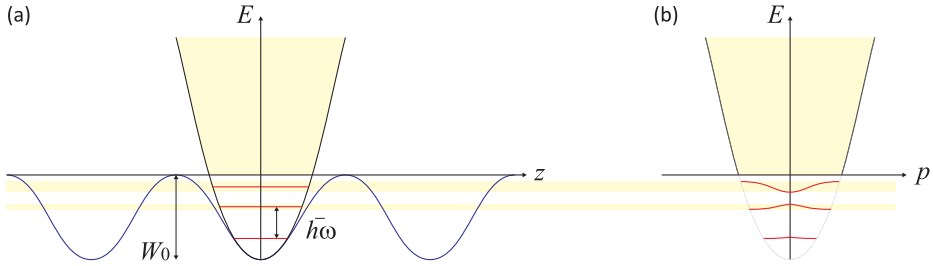


Figure 5.2: (a) Approximation of a periodic potential by a potential harmonic. (b) Dispersion relation in momentum space.

For shallow potentials,  $V_0 \ll \hbar^2 K^2/2m$ , we can neglect the coefficients  $V_0$  in the Eq. (5.39) and we find,

$$\varepsilon \simeq \hbar^2 q^2/2m, \quad (5.41)$$

which corresponds to the dispersion relation for free particles. On the other hand, looking at the bottom of deep potentials,  $V_0 \gg \hbar^2 K^2/2m$ , we can harmonically approximate the cosine potential by  $V(z) \approx -2V_0 + \frac{m}{2}\omega^2 z^2$  with  $\omega = K\sqrt{V_0}/m = \hbar^{-1}\sqrt{2V_0 E_{rec}}$ . For this case we expect,

$$\varepsilon \simeq -2V_0 + \hbar\omega \left(n + \frac{1}{2}\right). \quad (5.42)$$

The exact spectrum of eigenvalues  $\varepsilon$  can be calculated by numerically determining the eigenvalues of the matrix (5.40) for the first Brillouin zone,  $k \in [-K/2, K/2]$ , and the above limits are confirmed.

To estimate the width of the forbidden band, we cut out a  $2 \times 2$  matrix within the matrix  $\hat{H}$  and neglect its coupling with the others submatrices,

$$\hat{H}_s = \begin{pmatrix} \frac{\hbar^2}{2m}(k-K)^2 - V_0 & -\frac{1}{2}V_0 \\ -\frac{1}{2}V_0 & \frac{\hbar^2}{2m}k^2 - V_0 \end{pmatrix}. \quad (5.43)$$

At the edges of the Brillouin zone,  $k = \frac{1}{2}K$ , we get the eigenvalues  $\varepsilon = \frac{\hbar^2 K^2}{m} - V_0 \pm \frac{V_0}{2}$ , that is, the band gap is  $\Delta\varepsilon = V_0$ . Bloch's theorem says that Schrödinger's equation can be solved for any *Bloch states*. These are superpositions of plane wave momentum states [24],

$$\psi_k(z) = e^{ikz} u_k(z), \quad (5.44)$$

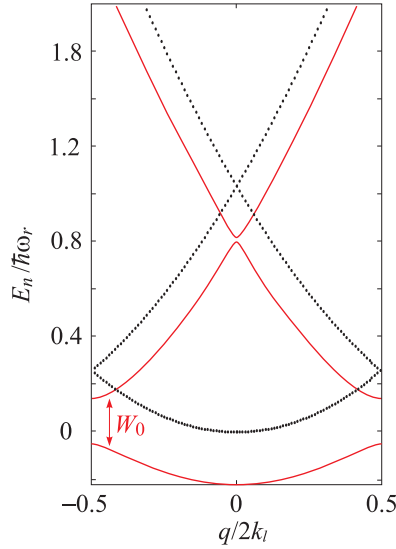


Figure 5.3: (code) Bloch bands with coupling potential (continuous red line) and without potential,  $V_0 = 0$  (dotted black line). The parameters are  $\omega_r = (2\pi) 20$  kHz,  $\omega_{ho} = (2\pi) 12$  kHz,  $\lambda_L = 689$  nm, and  $V_0 = 0.2\hbar\omega_r$ .

with  $u_k(z) = u_k(z + a)$ .

The requirement that  $\psi(z)$  satisfies the Schrödinger equation is equivalent to the condition that  $\mathbf{c}$  satisfies an eigenvalue equation. Let  $U$  be the matrix of the eigenvectors of  $\hat{H}$  and  $\hat{E}$  the diagonal matrix of eigenvalues:  $\hat{H} = U^{-1}\hat{E}U$  gives  $\hat{E}U\mathbf{c} = \varepsilon U\mathbf{c}$ , such that  $U\mathbf{c}$  can be understood as eigenvectors.

Alternatively, we define  $d_{nK+k} \equiv c_{nK+k+K}/c_{nK+k}$ , consequently Eq. (5.39) becomes,

$$d_{nK+k-K} = \frac{V_0}{\frac{\hbar^2}{m}(nK+k)^2 - 2\varepsilon - V_0(2 + d_{nK+k})}. \quad (5.45)$$

### 5.1.4 Bloch oscillations

A *Bloch oscillation* is a phenomenon in solid state physics. It is the oscillation of a particle (e.g., an electron) confined to a periodic potential (e.g. a crystal), when a constant force (e.g., generated by a continuous electric field) acts on it. This phenomenon is very difficult to observe in solid crystals because, due to electron scattering by defects of the lattice [163, 539], the coherent evolution is limited to a small fraction of the Brillouin zone. However, Bloch oscillations were observed in semiconducting superlattices, in ultrathin *Josephson junctions*, and with cold atoms in optical lattices [309, 459].

Let us first show a simple treatment for electrons subject to a constant electric field  $\mathcal{E}$ . The one-dimensional equation of motion is,

$$\hbar \frac{dk}{dt} = -e\mathcal{E}, \quad (5.46)$$

with the solution,

$$k(t) = k(0) - \frac{e\mathcal{E}}{\hbar}t . \quad (5.47)$$

The velocity  $v$  of the electron is given by,

$$v(k) = \frac{1}{\hbar} \frac{d\mathcal{E}}{dk} , \quad (5.48)$$

where  $\mathcal{E}(k)$  denotes the *dispersion relation* for a given energy band. We now assume that it has the following form (tight-binding limit),

$$\mathcal{E} = A \cos ak , \quad (5.49)$$

where  $a$  is the lattice parameter and  $A$  a constant. Then,  $v(k)$  is given by,

$$v(k) = -\frac{Aa}{\hbar} \sin ak , \quad (5.50)$$

and the position of the electron by,

$$x(t) = \int v(k(t))dt = -\frac{A}{e\mathcal{E}} \cos\left(\frac{ae\mathcal{E}}{\hbar}t\right) . \quad (5.51)$$

This shows, that the electron is oscillating in real space. The oscillation frequency, called *Bloch frequency* is given by,

$$\omega_{blo} = \frac{ae|\mathcal{E}|}{\hbar} . \quad (5.52)$$

## 5.2 Optical lattices

Periodic potentials for quantum particles can be realized artificially. A prominent example are *optical lattices* formed by the interference patterns of intersecting laser beams. Tuned sufficiently far away from atomic resonances the periodically structured light field exerts optical forces on the atoms which can be derived from potentials being proportional to the local light intensity. As these forces are relatively weak, the kinetic energy of the atoms must be very low (typically  $\mu\text{K}$ ) to allow for their impact to be relevant. In many cases, the depth of the optical lattice only allows for a small number of localized quantum states, so that the quantum nature of the atomic motion becomes highly relevant. Famous examples are the Bloch oscillations and the Mott insulating states.

We are not yet prepared to understand, how these potential arise from the light-atom interaction, as this topic will only be treated in the Secs. 18.2 and in Chp. 22.6.1. However, this is not necessary to understand many of the features of the atomic dynamics in optical lattices. We will thus simply impose a known periodic potential to a cold atomic cloud and study its energetic band structure and the atomic motion.

Various three-dimensional crystalline geometries have been realized and studied [371, 294, 79]. In the following, we will mainly focus on one-dimensional lattices, leaving a discussion of phenomena specific to three-dimensional lattices to future sections.

### 5.2.1 Atoms in 1D optical lattices

As already pointed out, a periodic optical potential can be generated by two counter-propagating plane wave laser beams,  $e^{\pm ik_l z}$ , with wavevectors  $k_l$  and  $-k_l$  and tuned to the red side of an atomic transition. In this situation the atoms are attracted to the maxima of the light intensity, the antinodes,

$$V(z) = \frac{V_0}{4} |e^{ik_l z} + e^{-ik_l z}|^2 = \frac{V_0}{2} [1 + \cos(2k_l z)] . \quad (5.53)$$

Applying the procedure unfolded in Sec. 5.1.3 to the optical lattice, we expand the motional atomic wavefunction into plane (Bloch) waves,

$$\psi(z) = \sum_{n=-\infty}^{\infty} c_n e^{2iqz} e^{2in k_l z} , \quad (5.54)$$

where  $|c_n(t)|^2$  are the population of momentum states separated by  $2k_l$  in momentum space. Inserting this expansion and the potential (5.53), after removing the constant energy  $V_0/2$ , into the stationary Schrödinger equation,

$$E\psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial z^2} + \frac{V_0}{2} \cos(2k_l z) \psi , \quad (5.55)$$

we obtain, collecting terms oscillating with the same exponential  $e^{2in k_l z}$ ,

$$\boxed{E_n c_n = 4\hbar\omega_{rec} \left(n + \frac{q}{k_l}\right)^2 c_n + \frac{V_0}{4} (c_{n+1} + c_{n-1})} , \quad (5.56)$$

where we defined an abbreviation,

$$\omega_{rec} = \frac{\hbar k_l^2}{2m} \quad (5.57)$$

called *recoil frequency*<sup>2</sup>. The eigenvalue problem (5.56) can be solved numerically for any value of  $q$ , yielding the dispersion relation already exhibited in Fig. 5.3.

To reproduce the dynamics of the matter wave, we start from the time-dependent Schrödinger equation with the same periodic potential. We again expand the time-dependent wavefunction into plane waves via,

$$\psi(z, t) = \sum_{n=-\infty}^{\infty} c_n(t) e^{2in k_l z} , \quad (5.58)$$

and insert this ansatz into the Schrödinger equation,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial z^2} + \frac{V_0}{4} \cos(2k_l x) \psi , \quad (5.59)$$

obtaining a set of equations of motion for the expansion coefficients  $c_n$ ,

$$\boxed{\dot{c}_n = -4i\omega_{rec} n^2 c_n + \frac{V_0}{4i\hbar} (c_{n+1} + c_{n-1})} . \quad (5.60)$$

The temporal evolution of the coefficients  $c_n(t)$  can be simulated numerically.

<sup>2</sup>The reason of the terminology, which will become clear after a study of Sec. 18.2, is that the  $\hbar\omega_{rec}$  is the kinetic energy of an atom having received two units of photonic momenta.

### 5.2.2 Bloch oscillations of atoms in 1D optical lattices

Neutral atoms in a vertical optical lattice are accelerated by gravity, and this accelerated motion leads to Bloch oscillations [163, 539]. To treat this case, we could simply replace the electric force  $-e\vec{\mathcal{E}}$  in the expression (5.52) by the gravitational force  $mg$  and obtain the result,

$$\omega_{blo} = \frac{mg\lambda_l}{2\hbar} , \quad (5.61)$$

with the wavelength  $\lambda_l = 2a$  of the counterpropagating lasers generating the standing wave.

For didactic reasons, however, let us formulate the problem in the language introduced in the previous section extending the Hamiltonian by the gravitational potential<sup>3</sup> (see also Exc. 2.4.7.4),

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \frac{V_0}{2} \cos 2k\hat{z} + mg\hat{z} . \quad (5.62)$$

We define the transformation  $U \equiv e^{-img\hat{z}t/\hbar}$  and find with (2.153) and (2.190) the Hamiltonian in the accelerated frame,

$$\tilde{H} = U^\dagger \hat{H} U + i\hbar \dot{U}^\dagger U = \frac{\tilde{p}^2}{2m} + \frac{V_0}{4} (e^{2ik\hat{z}} + e^{-2ik\hat{z}}) . \quad (5.63)$$

with

$$\tilde{p} \equiv \hat{p} - mgt = U^\dagger \hat{p} U . \quad (5.64)$$

Now, we expand the operators using the rules (??) and (??),

$$\begin{aligned} \tilde{p} &= \int p|p\rangle\langle p|dp = \sum_n (p + 2n\hbar k)|p + 2n\hbar k\rangle\langle p + 2n\hbar k| \\ e^{2ik\hat{z}} &= \int |p + 2\hbar k\rangle\langle p|dp = \sum_n |p + 2(n+1)\hbar k\rangle\langle p + 2n\hbar k| , \end{aligned} \quad (5.65)$$

based on the assumption that every atom can only exist in a superposition of discrete momentum states separated by  $2\hbar k$ , but can have an 'offset' momentum  $p = mv$ , e.g. due to thermal motion. Disregarding thermal motion, we may set in the accelerated frame  $p = 0$ . Then,

$$\tilde{p} = \sum_n 2n\hbar k|2n\hbar k\rangle\langle 2n\hbar k| \quad \text{and} \quad e^{2ik\hat{z}} = \sum_n |2n\hbar k + 2\hbar k\rangle\langle 2n\hbar k| , \quad (5.66)$$

such that,

$$\tilde{H} = \sum_n 4n^2\hbar\omega_{rec}|2n\hbar k\rangle\langle 2n\hbar k| + \frac{V_0}{4} \sum_n (|2n\hbar k + 2\hbar k\rangle\langle 2n\hbar k| + |2n\hbar k\rangle\langle 2n\hbar k + 2\hbar k|) . \quad (5.67)$$

---

<sup>3</sup>For Bose-Einstein condensates, the procedure should be generalized taking into account the energy of the mean field.



With the expansion of the wavefunction  $|\tilde{\psi}\rangle = \sum_n c_n |2n\hbar k\rangle$  the Schrödinger equation becomes [601, 602],

$$\begin{aligned} i\hbar \frac{d}{dt} |\tilde{\psi}\rangle &= i\hbar \sum_n \dot{c}_n |2n\hbar k\rangle \\ &= \sum_n \left( 4n^2 \hbar \omega_{rec} c_n + \frac{V_0}{4} (c_{n-1} + c_{n+1}) \right) |2n\hbar k\rangle = \tilde{H} |\tilde{\psi}\rangle, \end{aligned} \quad (5.68)$$

that is,

$$\dot{c}_n = -4in^2 \omega_{rec} c_n + \frac{V_0}{4i\hbar} (c_{n-1} + c_{n+1}). \quad (5.69)$$

In the lab frame the wavefunction reads,

$$\begin{aligned} |\psi\rangle &= U |\tilde{\psi}\rangle = e^{-img\hat{z}t/\hbar} \sum_n c_n |2n\hbar k\rangle \\ &= \sum_n c_n |2n\hbar k - mgt\rangle = \sum_n c_n |2\hbar k(n - \nu_{blo}t)\rangle, \end{aligned} \quad (5.70)$$

where we introduced the *Bloch frequency*,

$$\boxed{\nu_{blo} = \frac{mg}{2\hbar k}}. \quad (5.71)$$

Finally,

$$\boxed{\dot{c}_n = -4i(n - \nu_{blo}t)^2 \omega_{rec} c_n + \frac{V_0}{4i\hbar} (c_{n-1} + c_{n+1})}. \quad (5.72)$$

The center-of-the mass momentum of the atomic matter wave is,

$$\frac{\langle p \rangle_{lab}}{\hbar k_l} = \sum_n n |c_n(t)|^2 + \nu_{blo}t. \quad (5.73)$$

The Bloch oscillations can be understood in various pictures. The first one, illustrated in 5.4(a), is based on *Bragg reflection*: A resting atom has infinite de Broglie wavelength. Being constantly accelerated by gravity, the matter wave reduces its de Broglie wavelength from  $\infty$  to a value, where it becomes commensurate with the periodicity of the standing light wave potential. At this moment Bragg scattering comes into play, reflecting the atomic motion back into upward direction, and the process starts over again. The atoms evolve like jumping on a trampoline with a frequency given by  $\nu_{blo}$ .

To understand the second picture, we need to address a question we have left aside so far, as this requires a notion of optical forces. It is the question in which way the matter wave interacts with the standing light wave. For the present discussion, it is sufficient to know that the atom must have an internal transition capable of scattering photons from the light beams. As any absorption and emission process transfers a recoil momentum of  $\hbar k_l$  to the atom, we can understand the Bragg scattering process as a so-called *Raman scattering* process: a photon of the laser beam generating the optical lattice coming from the left is absorbed and re-emitted to the left. This is best illustrated in the momentum domain sketched in Fig. 5.4(b). This Raman scattering transfers twice the photonic recoil to the atom. The requirement for commensurability

of the Broglie wavelength and wavelength of the standing light wave is equivalent to saying that the matter wave momentum is equal to the recoil of a single photon. In other words, the matter wave always Bragg-reflected at the edge of a Brillouin zone.

Finally, in the *Bloch state picture*, the dispersion relation of a free particle is distorted due to the periodicity of the potential generated by the standing light wave such as to open a forbidden band. As a consequence, instead of being accelerated without limits, the atom enters the second Brillouin zone, which is to say that it is reflected to the other side of the first Brillouin zone.

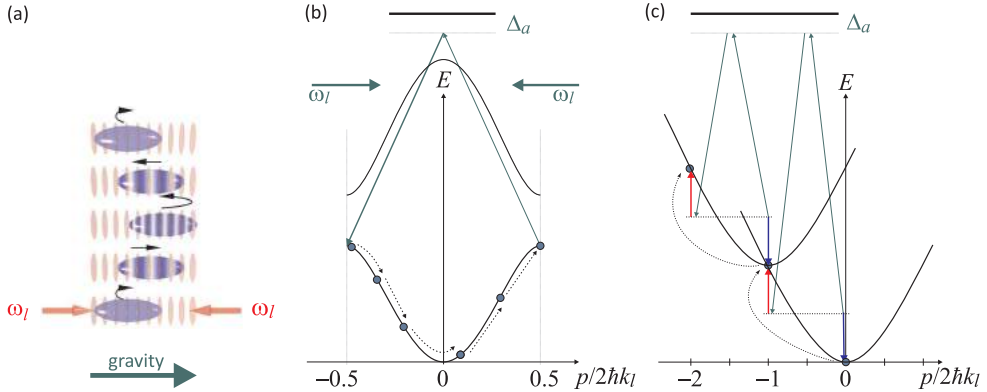


Figure 5.4: Illustration of Bloch oscillations (a) in real space, (b) in momentum space, and (c) in the moving frame. You may also run a movie of Bloch oscillations clicking on ([watch movie](#))!

The additional term, which contains the frequency of the Bloch oscillation  $\nu_{blo}$ , increases linearly over time. As time goes by, a resonance is crossed when  $t = -n\tau_{blo}$ , and the crossing is periodically repeated at every  $n = -1, -2, 0, \dots$  Tracing the matter wave evolution in the laboratory system, we see that whenever the resonance is crossed, the momentum undergoes a change of sign corresponding to a reflection of its motion. We expand the population of the momentum states into plane (Bloch) waves with  $|c_n(t)|^2$ .

Of course there are some conditions that need to be met to observe Bloch oscillations. The transfer of momentum is efficient only in the rapid adiabatic passage (ARP) regime characterized by the conditions  $2(\nu_{blo}/\omega_{rec}) \ll (W_0/4\omega_{rec})^2 \ll 16$ . The first condition requires that the force that drives the atoms to perform the Bloch oscillations must be weak enough to avoid transitions between Bloch bands, which guarantees the adiabaticity of the process. The other condition requires that the optical lattice be weak enough so that the dynamics involves only two adjacent momentum states at the same time and the transfer between the two is successful. A talk on this subject can be watched at ([watch talk](#)). Do the Exc. 5.2.3.1.

We will come back to the topic of optical lattices holding matter waves in Sec. 27.4.2 in the context of Mott insulating states of Bose-Einstein condensates.

**Example 33 (Dicke model of Bloch oscillations in the two-mode approximation):** In the limit where Bloch oscillations can be modeled by a two-level system [602] we may try a representation within the Dicke model and

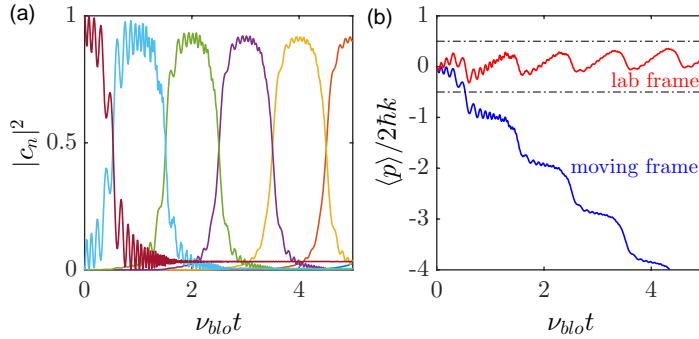


Figure 5.5: (code) Dynamics of Bloch's oscillations calculated from Eq. (5.57). (a) The colored curves show successively populated momentum states. (b) Center-of-mass motion of the wave packet in the lab frame (red) and in the moving frame (blue). The used parameters are  $\omega_{rec} = (2\pi) 4.8$  kHz,  $\nu_{blo} = 0.05\omega_{rec}$ , and  $W_0 = -0.7\omega_{rec}$ .

illustrate the dynamics on a Bloch sphere [598]. The gravitational acceleration corresponds to a modification of kinetic energy without modification of the momentum state populations and without excitation of quantum coherences between them. Since the kinetic energy is represented by the vertical axis of the Bloch sphere, we may visualize acceleration via a rotation of the Bloch sphere, e.g. about the  $y$ -axis. The interpretation of the rotated Bloch sphere remains the same: the  $xy$ -plane shows the coherences and the  $z$ -axis the populations. Once this works, we can treat the thermal atomic cloud as a coherent spin state, e.g. squeeze it [397] or simulate trajectory of individual atoms inhomogeneously [181]<sup>4,5</sup>.

Assuming that, at any time, at most two discrete momentum states  $n$  and  $n+1$  are coupled, the Hamiltonian (5.70) becomes,

$$\begin{aligned} \tilde{H} &= 4\hbar\omega_{rec}n^2|2n\hbar k\rangle\langle 2n\hbar k| + 4\hbar\omega_{rec}(n+1)^2|2(n+1)\hbar k\rangle\langle 2(n+1)\hbar k| \\ &+ \frac{V_0}{4}(|2(n+1)\hbar k\rangle\langle 2n\hbar k| + |2n\hbar k\rangle\langle 2(n+1)\hbar k|) . \end{aligned}$$

Introducing spin operators for every single motional two-level atom,

$$\begin{aligned} \hat{\sigma}^+ &\equiv |p+2\hbar k\rangle\langle p| \quad , \quad \hat{\sigma}^x \equiv \hat{\sigma}^+ + \hat{\sigma}^- \quad , \quad \hat{\sigma}^z \equiv [\hat{\sigma}^-, \hat{\sigma}^+]_- \\ \hat{\sigma}^+ \hat{\sigma}^- &= |p+2\hbar k\rangle\langle p+2\hbar k| = [\hat{\sigma}^-, \hat{\sigma}^+]_+ - [\hat{\sigma}^-, \hat{\sigma}^+]_- = 2 - \hat{\sigma}^z \\ \hat{\sigma}^- \hat{\sigma}^+ &= |p\rangle\langle p| = [\hat{\sigma}^-, \hat{\sigma}^+]_+ + [\hat{\sigma}^-, \hat{\sigma}^+]_- = 2 + \hat{\sigma}^z \quad , \end{aligned}$$

we get,

$$\begin{aligned} \tilde{H} &= 4\hbar\omega_{rec}n^2\hat{\sigma}^-\hat{\sigma}^+ + 4\hbar\omega_{rec}(n+1)^2\hat{\sigma}^+\hat{\sigma}^- + \frac{V_0}{4}(\hat{\sigma}^+ + \hat{\sigma}^-) \\ &= -4\hbar\omega_{rec}(2n+1)\hat{\sigma}^z + 8\hbar\omega_{rec}(2n^2+2n+1) + \frac{V_0}{4}\hat{\sigma}^x . \end{aligned}$$

Finally, we go to the collective Dicke Hamiltonian,

$$\hat{H} = \sum_j \hat{H}_j \quad \text{with} \quad \hat{H}_j = -4\hbar\omega_{rec}(2n+1)\hat{S}_j^z + 8\hbar\omega_{rec}(2n^2+2n+1) + \frac{V_0}{4}\hat{S}_j^x .$$

<sup>4</sup>Note that, In order to simulate a series of Bloch oscillations, we must change the basis by hand after each Bragg reflection.

<sup>5</sup>An interesting question is, whether the Dicke picture can be extended to CARL (see Sec. 22.3.4).

### 5.2.3 Exercises

#### 5.2.3.1 Ex: Purification of Bloch oscillations

Simulations of Bloch oscillations of atoms in an optical lattice for  $W_0 = 0.4\omega_{rec}$  and  $0.8\omega_{rec}$  produce the dynamics exhibited in Fig. 5.6. Interpret the different behaviors.

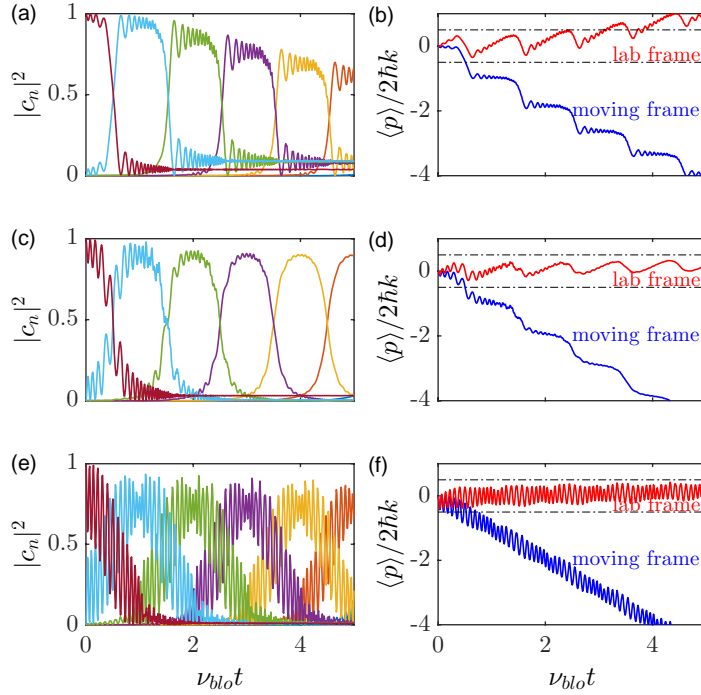


Figure 5.6: (code) Dynamics of Bloch oscillations (a-b) for  $W_0 = 0.4\omega_{rec}$ , (c-d) for  $W_0 = 0.8\omega_{rec}$ , and (e-f) for  $W_0 = 1.6\omega_{rec}$ . Furthermore,  $\omega_{rec} = (2\pi) 4.8$  kHz and  $\nu_{blo} = 0.05\omega_{rec}$ .

#### 5.2.3.2 Ex: Gaussian approximation for Wannier function

Consider a standing light wave producing a dipolar potential of the shape  $V(x) = W_0 \sin^2 kx = \frac{W_0}{2} - \frac{W_0}{2} \cos 2kx$  with  $W_0 \gg E_{rec} = (\hbar k)^2 / 2m$ .

a. Approximate the potential of a single lattice site around  $x = 0$  by a harmonic potential. Calculate for which depth of the dipolar potential the approximated potential supports at least one bound state. What is the spacing of the levels and the characteristic size of the harmonic oscillator  $a_{ho}$ . Write down the normalized ground state wavefunction of the harmonic oscillator.

b. Now, let us consider a 3D cubic lattice made of three identical orthogonal standing light waves. Approximate the ground state Wannier function of a lattice site by appropriately normalized ground state wavefunctions of a harmonic oscillator. Derive

the formula  $U^{3d} = \frac{8}{\pi} k a_d \left( \frac{W_0}{E_{rec}} \right)^{3/4}$  starting from,

$$U^{3D} = g^{3D} \int \omega_{(0,0)}^4(x, y, z) d^3r$$

with  $g^{3D} = \frac{4\pi\hbar a_d}{m}$ .

### 5.2.3.3 Ex: Perturbative treatment of a weak lattice

A weak lattice potential with  $V_0 < E_{rec}$  can be treated in perturbation theory to motivate the resulting opening of a gap in the refolded energy parabola. The unperturbed Hamiltonian  $\hat{H}_0 = p^2/2m$  contains only the kinetic energy and the perturbation is  $V(x) = V_0 \sin^2(kx) = \frac{1}{2}V_0 - \frac{1}{4}V_0(e^{2ikx} + e^{-2ikx})$ .

a. Calculate  $\hat{V}(x)\phi_p(x)$  and show that  $\langle \phi_{p \pm \hbar k} | \hat{V} | \phi_p \rangle$  are the only non-zero matrix elements of the perturbation  $V(x)$  between the eigenstates of  $\hat{H}_0$  (which are the orthonormal plane waves  $\phi_p = e^{ipx/\hbar}$ ). Neglect the constant term of the potential, which only yields a global energy shift.

b. This coupling is relevant around those momenta  $p$ , where  $\phi_p$  has the same energy  $\phi_{p+\hbar k}$  or  $\phi_{p-\hbar k}$ . Show that these momenta are  $p = \mp \hbar k$ .

c. Consider the perturbed system restricted to the basis  $\{|p = -\hbar k\rangle, |p = +\hbar k\rangle\}$  and give the Hamiltonian as  $2 \times 2$  matrix.

d. Diagonalize the matrix and consider the difference of the eigenenergies. Use them to estimate the size of the gap, that the lattice opens between the two lowest bands.

e. Calculate the eigenstates and interpret them by comparing the probability density to the lattice potential.

## 5.3 The Kronig-Penney model

The *Kronig-Penney model* describes the band structure of a lattice. Let us assume a periodic potential of rectangular wells with valleys of widths  $a$  and peaks of widths  $b$ ,

$$V(x) = U_0 \theta_{\text{mod}(x, a+b) \in [a, a+b]} \cdot \quad (5.74)$$

Inserting into the Schrödinger equation the plane wave ansatz  $\psi = Ae^{iKx} + Be^{-iKx}$  for the wavefunction in the valley,  $0 < x < a$ , and  $\psi = Ce^{Qx} + De^{-Qx}$  in the peak,  $-b < x < 0$ , we obtain  $\varepsilon = \hbar^2 K^2/2m$  and  $U_0 - \varepsilon = \hbar^2 Q^2/2m$ . Choosing the constants  $A, B, C, D$  such that  $\psi$  and  $\psi'$  are continuous in  $x = 0, a$ , we derive, using the periodicity of the Bloch wave  $\psi(a < x < a+b) = \psi(-b < x < 0)e^{ik(a+b)}$ ,

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ iK & -iK & -Q & Q \\ e^{iKa} & e^{-iKa} & -e^{-Qb+ik(a+b)} & -e^{Qb+ik(a+b)} \\ iKe^{iKa} & -iKe^{-iKa} & -Qe^{-Qb+ik(a+b)} & Qe^{Qb+ik(a+b)} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 0. \quad (5.75)$$

The determinant of the matrix must be zero, or,

$$\frac{Q^2 - K^2}{2QK} \sinh Qb \sin Ka + \cosh Qb \cos Ka = \cos k(a+b). \quad (5.76)$$

For  $\delta$ -shaped peaks, we let  $b = 0$  and  $U_0 = \infty$  such that  $Q^2ba/2 = P$ , this simplifies to,

$$\frac{P}{Ka} \sin Ka + \cos Ka = \cos ka . \quad (5.77)$$

The dispersion relation for light is different. According to [468],

$$-\frac{\sqrt{\varepsilon} + \sqrt{\varepsilon}^{-1}}{2} \sin(\sqrt{\varepsilon}\omega a/c) \sin(\omega a/c) + \cos(\sqrt{\varepsilon}\omega a/c) \cos(\omega a/c) = \cos ka . \quad (5.78)$$

For  $\varepsilon = 1$  the equation simplifies to  $ka = 2\omega a/c$ .

### 5.3.1 Photonic density of states

The *photonic density of states* in free space in three dimensions is evaluated from [693],

$$dN = 2 \left( \frac{L}{2\pi} \right)^3 \int d^3k = 2 \left( \frac{L}{2\pi} \right)^3 k^2 dk \int d\phi d \cos \theta = \frac{L^3 \omega^2}{\pi^2 c^3} d\omega \equiv D(\omega) d\omega . \quad (5.79)$$

In one dimension,

$$dN = 2 \frac{L}{2\pi} dk = \frac{L}{\pi c} d\omega . \quad (5.80)$$

The density is normalized  $\int_0^{\pi c/L} D(\omega) d\omega = 1$  and the total energy, if all states are populated, is  $E \equiv \int_0^{\pi c/L} \omega D(\omega) d\omega = \pi c/L$ . However, this applies only if  $\omega = ck$ . If the dispersion relation is more complicated, for example, inside a cavity or a forbidden photonic band,  $\omega = \omega(k)$ , we must generalize,

$$D(\omega) = \frac{L}{\pi} \frac{dk}{d\omega} . \quad (5.81)$$

Assuming that the dispersion relation is given by the Kronig-Penney model, we obtain gaps in the density-of-states for those values of  $\omega$  which do not belong to any  $k$ .

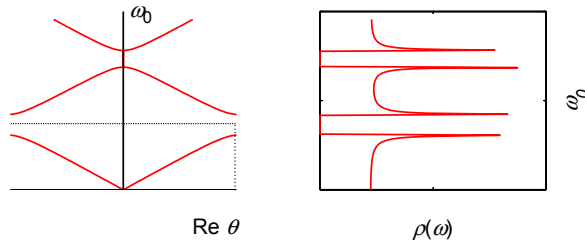


Figure 5.7: Dispersion ratio and state density for a one-dimensional optical lattice.

## 5.3.2 Exercises

### 5.3.2.1 Ex: Mass of photons in a lattice

The effective mass of particles in a lattice is defined as,

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2 E(k)}{dk^2}.$$

Calculate the effective mass of a rubidium atom in a far-detuned optical standing wave.

## 5.4 Further reading

B. Pelle et al., *State-labeling Wannier-Stark atomic interferometers* [\[DOI\]](#)

Min-Kang Zhou et al., *Atomic multiwave interferometer in an optical lattice* [\[DOI\]](#)

T. Hartmann et al., *Dynamics of Bloch oscillations* [\[DOI\]](#)

N. Marzari et al., *Maximally localized Wannier functions: Theory and applications* [\[DOI\]](#)

L. Guidoni et al., *Optical Lattices: Cold Atoms Ordered by Light* [\[DOI\]](#)

N. Marzari et al., *Nonlinear Landau-Zener tunneling* [\[DOI\]](#)

# Chapter 6

## Approximation methods

Virtually every problem going beyond the potential well, the harmonic oscillator, or the hydrogen atom without spin and external fields is impossible to solve analytically. In this chapter we will talk about techniques to solve approximately problems in more realistic situations. There are a number of methods of which we will discuss the only following: 1. The stationary or time-dependent perturbation method is useful for evaluating small perturbations of the system, for example, caused by external electric or magnetic fields; 2. the variational method, which serves to find and improve trial wavefunctions, the initial shapes of which are generally motivated by the symmetries of the system; 3. the semi-classical WKB method; 4. and finally the method of self-consistent fields, which is an iterative method of solving the Schrödinger equation.

### 6.1 Stationary perturbations

#### 6.1.1 Time-independent perturbation theory

We first introduce *time-independent perturbation theory* (TIPT) for multilevel systems. We separate the Hamiltonian into an unperturbed part,

$$\hat{H}^{(0)}|\psi^{(0)}\rangle = E^{(0)}|\psi^{(0)}\rangle, \quad (6.1)$$

and perturbations, which are proportional to a small parameters  $\lambda$ ,

$$\hat{H} = \hat{H}^{(0)} + \lambda\hat{H}^{(1)} + \lambda^2\hat{H}^{(2)} + \dots \quad (6.2)$$

The perturbed wavefunctions are,

$$|\psi\rangle = |\psi^{(0)}\rangle + \lambda|\psi^{(1)}\rangle + \lambda^2|\psi^{(2)}\rangle + \dots, \quad (6.3)$$

and the energies

$$E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \dots \quad (6.4)$$

The contributions  $\propto \lambda^n$  are the *corrections* of order  $n$ . The equation we need to solve now is,

$$\hat{H}|\psi\rangle = E|\psi\rangle. \quad (6.5)$$



By inserting all the expansions above and segregating all orders of  $\lambda^k$ , we find the following system of equations,

$$\begin{aligned}\hat{H}^{(0)}|\psi^{(0)}\rangle &= E^{(0)}|\psi^{(0)}\rangle \\ (\hat{H}^{(0)} - E^{(0)})|\psi^{(1)}\rangle &= (E^{(1)} - \hat{H}^{(1)})|\psi^{(0)}\rangle \\ (\hat{H}^{(0)} - E^{(0)})|\psi^{(2)}\rangle &= (E^{(2)} - \hat{H}^{(2)})|\psi^{(0)}\rangle + (E^{(1)} - \hat{H}^{(1)})|\psi^{(1)}\rangle \\ &\dots\end{aligned}\tag{6.6}$$

### 6.1.1.1 First order energy correction

We now consider eigenstates  $|\psi_n^{(1)}\rangle$  of the perturbed system and expand the first-order correction of the wavefunction in a linear combination of unperturbed eigenvectors  $|\psi_n^{(0)}\rangle \equiv |n\rangle$ ,

$$|\psi_n^{(1)}\rangle = \sum_m |m\rangle \langle m|\psi_n^{(1)}\rangle.\tag{6.7}$$

We insert this expansion into the second equation (6.6) and multiply with  $\langle n|$ ,

$$\langle n|(\hat{H}^{(0)} - E_n^{(0)})\sum_m |m\rangle \langle m|\psi_n^{(1)}\rangle = 0 = \langle n|E_n^{(1)} - \hat{H}^{(1)}|n\rangle.\tag{6.8}$$

We obtain for the first order correction of the energy of unperturbed states,

$$\boxed{E_n^{(1)} = \langle n|\hat{H}^{(1)}|n\rangle}.\tag{6.9}$$

As a first example we will calculate in Exc. 6.1.3.1 the first order correction for the energy of a slightly deformed one-dimensional box potential.

### 6.1.1.2 First order correction for the wavefunction

Now let us have a look at the first-order correction for the wavefunction again considering the second equation (6.6),

$$\langle m|\hat{H}^{(0)} - E_n^{(0)}|\psi_n^{(1)}\rangle = \langle m|E_n^{(1)} - \hat{H}^{(1)}|n\rangle.\tag{6.10}$$

When  $n = m$ , the left side of this equation disappears. Therefore,  $E_n^{(1)} - \langle n|\hat{H}^{(1)}|n\rangle = 0$ , and we can restrict to the terms  $n \neq m$  discarding the terms in  $E_n^{(1)}$ ,

$$\langle m|\psi_n^{(1)}\rangle = \frac{E_n^{(1)}\delta_{mn} - \langle m|\hat{H}^{(1)}|n\rangle}{\hat{E}_m^{(0)} - E_n^{(0)}} = \frac{\langle m|\hat{H}^{(1)}|n\rangle}{E_n^{(0)} - E_m^{(0)}}.\tag{6.11}$$

We obtain for the first-order correction for the energy of the states,

$$\boxed{|\psi_n^{(1)}\rangle = \sum_m |m\rangle \langle m|\psi_n^{(1)}\rangle = \sum_{m \neq n} |m\rangle \frac{\langle m|\hat{H}^{(1)}|n\rangle}{\hat{E}_n^{(0)} - E_m^{(0)}}}.\tag{6.12}$$

This procedure simulates the distortion of the state by blending it with other states. The perturbation induces virtual transitions to other states. The perturbation is large when the blended levels are close.

See Exc. 6.1.3.2. In Exc. 6.1.3.3 we calculate the first order correction due to the finite extension of the hydrogen nucleus. In Exc. 6.1.3.4 we treat the coupling of the energy levels of a two-level system as a first order perturbation, and compare the result with the exact solution. The Stark effect for an electron confined in a box can be discussed (see Exc. 6.1.3.5) in first order TIPT.

### 6.1.1.3 Second order correction for the energy

To calculate the second order correction for the energy we expand the second order correction,

$$|\psi_n^{(2)}\rangle = \sum_m |m\rangle \langle m|\psi_n^{(2)}\rangle, \quad (6.13)$$

import it into the third equation (6.6) and multiply with  $\langle n|$ ,

$$\langle n|(\hat{H}^{(0)} - E_n^{(0)}) \sum_m |m\rangle \langle m|\psi_n^{(2)}\rangle = \langle n|(E_n^{(2)} - \hat{H}^{(2)})|n\rangle + \langle n|(E_n^{(1)} - \hat{H}^{(1)}) \sum_m |m\rangle \langle m|\psi_n^{(1)}\rangle. \quad (6.14)$$

Now,

$$\sum_m \langle m|\psi_n^{(2)}\rangle (E_n^{(0)} - E_m^{(0)}) \delta_{nm} = 0 = E_n^{(2)} - \langle n|\hat{H}^{(2)}|n\rangle + \sum_m \langle m|\psi_n^{(1)}\rangle \left( E_n^{(1)} \delta_{nm} - \langle n|\hat{H}^{(1)}|m\rangle \right). \quad (6.15)$$

The left-hand side of this equation disappears. Also, on the right-hand side, for  $n \neq m$ , the term  $E_n^{(1)} \delta_{nm}$  disappears, and for  $n = m$  the whole parenthesis disappears. Therefore, we can discard the term  $E_n^{(1)}$  and restrict the sum to terms with  $n \neq m$ . Inserting the coefficients  $\langle m|\psi_n^{(1)}\rangle$  calculated in (6.11), we finally obtain,

$$E_n^{(2)} = \langle n|\hat{H}^{(2)}|n\rangle + \sum_{m \neq n} \frac{\langle n|\hat{H}^{(1)}|m\rangle \langle m|\hat{H}^{(1)}|n\rangle}{E_n^{(0)} - E_m^{(0)}}. \quad (6.16)$$

The first term is similar to the first order correction; the eigenvalue of the second order perturbation calculated in the base of the unperturbed states. The second term describes the shift of the energies through possible temporary transitions to other states.

In Exc. 6.1.3.6 we treat a system of three coupled levels up to the second perturbative order. The Stark effect discussed in Exc. 6.1.3.7 needs the TIPT calculation up to the second order.

## 6.1.2 TIPT with degenerate states

Exact calculations show that the effect of a perturbation is larger – but finite – for degenerate states. On the other hand, from the above expressions for the corrections of both energies and wavefunctions, we would infer that these corrections can become very large for small perturbations or even diverge.

Fortunately, the fact that every linear combination of degenerate wavefunctions is an eigenfunction of the Hamiltonian as well gives us the freedom to choose the combination, which is most similar to the final form of the perturbed wavefunctions.

For example, considering a perturbation by a magnetic field it may be advantageous to expand the spherical functions  $Y_{lm}$  on a basis of cylindrical coordinates<sup>1</sup>. We will see in the following that we can solve both problems, the selection of the initial combination and the prevention of divergent denominators at once, without explicitly specifying the expansion.

We consider eigenstates  $|n, \nu\rangle$  with the energy  $E_n^{(0)}$  being  $r$  times degenerate with respect to the quantum number  $\nu$ , where  $\nu = 1, \dots, r$ . All states satisfy

$$\hat{H}^{(0)}|n, \nu\rangle = E_n^{(0)}|n, \nu\rangle. \quad (6.17)$$

We construct linear combinations that most resemble the perturbed states

$$|\psi_{n\mu}^{(0)}\rangle = \sum_{\nu=1}^r c_{\mu\nu}|n, \nu\rangle. \quad (6.18)$$

When the perturbation  $\hat{H}^{(1)}$  is applied, we assume that the state  $|\psi_{n\mu}^{(0)}\rangle$  is distorted towards the similar state  $|\psi_{n\mu}\rangle$ , and the energy changes from  $E_n^{(0)}$  to  $E_{n\mu}$ . We now need the index  $\mu$  to label the energy, since the degeneracy can be removed by the perturbation. As before, we write now,

$$\begin{aligned} \hat{H} &= \hat{H}^{(0)} + \lambda\hat{H}^{(1)} + \dots \\ |\psi_{n\mu}\rangle &= |\psi_{n\mu}^{(0)}\rangle + \lambda|\psi_{n\mu}^{(1)}\rangle + \dots \\ E_{n\mu} &= E_n^{(0)} + \lambda E_{n\mu}^{(1)} + \dots \end{aligned} \quad (6.19)$$

The replacement of these expansions in  $\hat{H}|\psi_{n\mu}\rangle = E_{n\mu}|\psi_{n\mu}\rangle$ , and a collection of the terms in  $\lambda$  up to first order gives,

$$\begin{aligned} \hat{H}^{(0)}|\psi_{n\mu}^{(0)}\rangle &= E_n^{(0)}|\psi_{n\mu}^{(0)}\rangle \\ (E_n^{(0)} - \hat{H}^{(0)})|\psi_{n\mu}^{(1)}\rangle &= (E_{n\mu}^{(1)} - \hat{H}^{(1)})|\psi_{n\mu}^{(0)}\rangle. \end{aligned} \quad (6.20)$$

As before, we try to express the first-order corrections for the wavefunctions through degenerate unperturbed wavefunctions  $|\psi_{n\mu}^{(0)}\rangle$  and non-degenerate wavefunctions<sup>2</sup>  $|\psi_m^{(0)}\rangle$ :

$$|\psi_{n\mu}^{(1)}\rangle = \sum_{\nu} b_{\mu\nu}|\psi_{n\nu}^{(0)}\rangle + \sum_m a_{nm}|\psi_m^{(0)}\rangle. \quad (6.21)$$

Inserting this into the first-order equation (6.20), we obtain,

$$\sum_{\nu} b_{\mu\nu}(E_n^{(0)} - E_n^{(0)})|\psi_{n\nu}^{(0)}\rangle + \sum_m a_{nm}(E_m^{(0)} - E_n^{(0)})|\psi_m^{(0)}\rangle = (E_{n\mu}^{(1)} - \hat{H}^{(1)})|\psi_{n\mu}^{(0)}\rangle. \quad (6.22)$$

The first term disappears. Inserting the expansion (6.18),

$$\sum_m a_{nm}(E_m^{(0)} - E_n^{(0)})|\psi_m^{(0)}\rangle = (E_{n\mu}^{(1)} - \hat{H}^{(1)}) \sum_{\nu} c_{\mu\nu}|n, \nu\rangle, \quad (6.23)$$

<sup>1</sup>Another example would be the preference for the coupled base  $|l, s, j, m_j\rangle$  in comparison to the decoupled base  $|l, m_l, s, m_s\rangle$  knowing that the degeneracy in  $j$  is lifted, when there is an energy associated with interacting angular momenta and the degeneracy in  $m_j$  is lifted, when we apply a magnetic field.

<sup>2</sup>Note that we label all states *which are not degenerate with the state under investigation*  $|\psi_{n\mu}^{(1)}\rangle$  with the index  $m$ , even if there are degeneracies between them.

and multiplying the two sides with  $\langle n, \mu |$ , we get zero on the left-hand side, since we can choose the non-degenerate states to be orthogonal  $\langle n, \nu | m \rangle = \delta_{m,n}$ . Hence,

$$\boxed{\sum_{\nu} c_{\mu\nu} \left[ E_{n\mu}^{(1)} \langle n, \mu | n, \nu \rangle - \langle n, \mu | \hat{H}^{(1)} | n, \nu \rangle \right] = 0} . \quad (6.24)$$

This *secular equation* (one for each  $\mu$ ) represents, in fact, a set of  $r$  linear equations for the coefficients  $c_{\mu\nu}$ . The condition for having non-trivial solutions is,

$$\det \left( \langle n, \nu | \hat{H}^{(1)} | n, \mu \rangle - E_{n\mu}^{(1)} \delta_{\mu,\nu} \right)_{\mu,\nu} = 0 . \quad (6.25)$$

The solution of this *secular determinant* yields the solicited energies  $E_{\mu}^{(1)}$ . Now, the solution of the secular equation (6.24) for each energy value produces those coefficients, which represent the best linear combinations adapted to the perturbation. Unlike in previous calculations with degenerate states, here we consider linear combinations of vectors of the degenerate subspace prior to switching on the perturbation.

In practice, we apply perturbation theory only to the lowest relevant order. That is, we only calculate the second order correction if first order corrections vanish. One famous example is the *quadratic Stark effect* discussed in Sec. 9.3. In the case of eigenvalues, which are degenerate in the absence of perturbation, the first order will always produce a remarkable correction, as in the example of the *linear Stark effect*, also discussed in Sec. 9.3. For this reason, we need not discuss higher perturbation orders in the case of degenerate eigenvalues.

**Example 34 (Perturbation in a system with two degenerate states):** As an example, we consider the following Hamiltonian,

$$\hat{H} = \begin{pmatrix} \Delta & \Omega \\ \Omega & \Delta \end{pmatrix} .$$

The exact solution gives the eigenvalues and eigenvectors,

$$E_1 = \Delta + \Omega \quad , \quad E_2 = \Delta - \Omega \quad , \quad |\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad , \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} .$$

Now we divide the Hamiltonian into an unperturbed part and a perturbation,

$$\hat{H} \equiv \hat{H}^{(0)} + \hat{H}^{(1)} = \begin{pmatrix} \Delta & 0 \\ 0 & \Delta \end{pmatrix} + \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix} .$$

We get in zero order,

$$E_1^{(0)} = \Delta = E_2^{(0)} \quad , \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} ,$$

The application of non-degenerate perturbation theory in first order would give,

$$\langle 1 | \hat{H}^{(1)} | 1 \rangle = 0 = \langle 2 | \hat{H}^{(1)} | 2 \rangle \quad , \quad |\psi_1^{(1)}\rangle = |1\rangle \frac{\langle 1 | \hat{H}^{(1)} | 2 \rangle}{E_1^{(0)} - E_2^{(0)}} \rightarrow \infty \leftarrow -|\psi_2^{(1)}\rangle .$$

That is, the correction of the energy vanishes in first order, while the correction of the wavefunction diverges. Obviously, the  $|\nu\rangle$  obtained by the diagonalization of the matrix  $\hat{H}^{(0)}$  is not adapted to the calculation of the matrix elements  $\hat{H}^{(1)}$ . Now, applying degenerate perturbation theory, we obtain by the secular determinant,

$$0 = \det \left[ \langle \nu | \hat{H}^{(1)} | \mu \rangle - E_{\mu}^{(1)} \delta_{\mu,\nu} \right] = \det \begin{pmatrix} -E_{\mu}^{(1)} & \Omega \\ \Omega & -E_{\mu}^{(1)} \end{pmatrix} = (E_{\mu}^{(1)})^2 - \Omega^2 ,$$

eigenvalues are  $E_1^{(1)} = \Omega$  and  $E_2^{(1)} = -\Omega$  allowing the establishment of the secular equation,

$$\begin{aligned} c_{11} \left[ E_1^{(1)} - \langle 1 | \hat{H}^{(1)} | 1 \rangle \right] - c_{12} \langle 1 | \hat{H}^{(1)} | 2 \rangle &= c_{11}[\Omega - 0] - c_{12}\Omega = 0 \\ -c_{21} \langle 2 | \hat{H}^{(1)} | 1 \rangle + c_{22} \left[ E_2^{(1)} - \langle 2 | \hat{H}^{(1)} | 2 \rangle \right] &= -c_{21}\Omega + c_{22}[-\Omega - 0] = 0 . \end{aligned}$$

We obtain  $c_{11} = c_{12}$  and  $c_{21} = -c_{22}$  and with this,

$$|\psi_1^{(0)}\rangle = \sum_{\nu} c_{1\nu} |\nu\rangle = c_{11}|1\rangle + c_{12}|2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} , \quad |\psi_2^{(0)}\rangle = c_{21}|1\rangle + c_{22}|2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} .$$

Thus, we can verify that the corrections for the eigenenergies,

$$E_1 = E_1^{(0)} + \langle \psi_1^{(0)} | \hat{H}^{(1)} | \psi_1^{(0)} \rangle = \Delta + \Omega \quad , \quad E_2 = E_2^{(0)} + \langle \psi_2^{(0)} | \hat{H}^{(1)} | \psi_2^{(0)} \rangle = \Delta - \Omega ,$$

coincides with the exact calculation made at the beginning. The eigenfunctions  $|\psi_1^{(0)}\rangle$  should be already corrected in zeroth order, which we verify by calculating,

$$|\psi_1^{(1)}\rangle = |\psi_1^{(0)}\rangle \frac{\langle \psi_1^{(0)} | \hat{H}^{(1)} | \psi_2^{(0)} \rangle}{E_1 - E_2} = 0 = |\psi_2^{(1)}\rangle .$$

In Exc. 6.1.3.8 we study a partially degenerate three-level system and the breakdown of the degeneracy due to a perturbation. And in Exc. 6.1.3.9 we will treat a perturbation in a box potential with degenerate energy levels.

## 6.1.3 Exercises

### 6.1.3.1 Ex: One-dimensional well with a deformation in the centre

Consider a one-dimensional potential well between  $-L/2$  and  $L/2$  with infinitely high walls. In the center of the well is a small deformation,

$$H^{(1)} = \begin{cases} \varepsilon & \text{for } -\frac{a}{2} \leq x \leq \frac{a}{2} \\ 0 & \text{outside that region .} \end{cases}$$

Calculate the correction for the eigenenergies in first order and discuss the limits  $a \ll L$  and  $a \rightarrow L$ .

**6.1.3.2 Ex: Perturbation**

Show that the scalar product  $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle$  (from the first-order correction to the state of the 'perturbed' system with the  $n$ -th state of the free Hamiltonian), cancels out when we impose that the 'perturbed' state  $|\psi(\lambda)\rangle$  be normalized and the the product  $\langle \psi_n^{(0)} | \psi(\lambda) \rangle$  be real.<sup>3</sup>

**6.1.3.3 Ex: Extended nucleus**

The expression  $V(r) = -e^2/4\pi\epsilon_0 r$  for the potential energy of an electron in the hydrogen atom implies that the nucleus (the proton) is treated as a point particle. Now suppose that, on the contrary, the charge of the proton  $+e$  is evenly distributed over a sphere of radius  $R = 10^{-13}$  cm.

- Derive the modified potential  $V_m$ , which corresponds to this distribution of the nuclear charge.
- Assume that the wavefunction of the hydrogen atom does not change much due to the modified potential. Calculate in lowest order in  $R/a_B$  the average energetic displacement  $\langle \Delta V \rangle$  for the state  $(n = 1, \ell = 0, m = 0)$ . How will the energy displacement be in comparison to the states  $(n = 2, \ell = 0, m = 0)$  and  $(n = 2, \ell = 1, m = 0)$ ?
- Calculate in the same way  $\langle \Delta V \rangle$  for muonic hydrogen in the ground state.

**6.1.3.4 Ex: Perturbation of a 2-level system**

We consider a two-level system. Without perturbation the system would have the Hamiltonian  $H^{(0)}$ , the eigenenergies  $E_{1,2}^{(0)}$  and the eigenfunctions  $\psi_{1,2}^{(0)}$ . Now we switch on a stationary perturbation of the form  $H^{(1)} = \epsilon(|1\rangle\langle 2| + |2\rangle\langle 1|)$ .

- Calculate the eigenenergies directly solving the perturbed Schrödinger equation.
- Calculate the perturbed energies using TIPT and compare to the exact calculation of the eigenenergies.
- Calculate the eigenstates directly solving the perturbed Schrödinger equation.
- Calculate the perturbed states using TPIT and compare to the exact calculation of the eigenfunctions.

**6.1.3.5 Ex: Stark effect for an electron in a box**

Consider an electron in a one-dimensional box, that is, in a well inside the interval  $x \in [0, a]$  delimited by infinite walls. When a uniform electric field  $\mathcal{E}$  is applied, also in  $x$ -direction, the electron experiences a force equal to  $-e\mathcal{E}$ , being  $-e$  the electron charge, so that the potential energy inside the box becomes  $e\mathcal{E}x$ .

- What is the energy of the ground state of the electron (in first order approximation)? We can assume that  $e\mathcal{E}a$  is much smaller than the ground state energy the electron would have in the absence of electric fields.
- Use first-order TIPT to get an approximation for the ground state wavefunction by calculating the first term of the correction.

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<sup>3</sup>See [141], Cap XI, A-2.

**6.1.3.6 Ex: Perturbed 3-level system until second order TIPT**

Consider the following perturbed Hamiltonian:

$$H = H_0 + H_\lambda = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} + \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & \lambda \\ 0 & \lambda & 0 \end{pmatrix}.$$

- Determine the perturbed eigenvalues and eigenfunctions in first order TIPT.
- Determine the eigenvalues in second order TIPT.

**6.1.3.7 Ex: Stark effect for a charge in a harmonic oscillator**

Consider a charged harmonic oscillator, immersed in a uniform electric field  $\mathcal{E}$ , described by the Hamiltonian  $\hat{H}^{(1)} = \hat{H} + e\mathcal{E}\hat{x}$ , being  $\hat{H} = \hat{p}^2/2m + m\omega^2\hat{x}^2/2$  the Hamiltonian of the free one-dimensional oscillator, and  $e$  the charge of the oscillator.

- Obtain, through TIPT, the eigenenergies (first and second order corrections). Compare the results obtained by TIPT with the analytical ones <sup>4</sup>.
- Same thing for a perturbation of the form  $\rho m\omega^2\hat{x}^2/2$ .
- Same thing for a perturbation  $\sigma\hbar\omega\hat{x}^3$ .

**6.1.3.8 Ex: Three-level system with degeneracy**

Consider the following Hamiltonian  $\hat{H}^{(0)}$  and its perturbation  $\hat{H}^{(1)}$

$$\hat{H}^{(0)} + \hat{H}^{(1)} = \begin{pmatrix} \Delta & 0 & 0 \\ 0 & \Delta & 0 \\ 0 & 0 & \Delta' \end{pmatrix} + \begin{pmatrix} 0 & \Omega & 0 \\ \Omega & 0 & \Omega \\ 0 & \Omega & 0 \end{pmatrix}.$$

Calculate the corrections for the eigenvalues and eigenfunctions up to first order.

**6.1.3.9 Ex: Perturbation in a 3D well with degeneracy**

Consider a particle confined to a three-dimensional, infinite cubic well described by the potential energy  $V(x, y, z) = 0$  for  $0 < x < a$ ,  $0 < y < a$  and  $0 < z < a$  and  $V(x, y, z) = \infty$  outside this region. We know that the particle's stationary states are  $\Psi_{n_x, n_y, n_z}^{(0)}(x, y, z) = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_x\pi}{a}x\right) \sin\left(\frac{n_y\pi}{a}y\right) \sin\left(\frac{n_z\pi}{a}z\right)$ , being  $n_x, n_y, n_z$  positive integers. The associated energies are  $E_{n_x, n_y, n_z}^{(0)} = \frac{\pi^2\hbar^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)$ . Note that the ground state is not degenerate while the first excited state is three times degenerate. Consider that the particle in this box is subject to a perturbation of the shape  $H^{(1)} = V_0$  for  $0 < x < a/2$  and  $0 < y < a/2$  and  $H^{(1)} = 0$  outside this region.

- Obtain the first-order correction for the ground state energy.
- Obtain the first-order correction for the (degenerate) energy of the first excited state, in addition to the *optimal base* (which follows from the linear combinations of degenerate states) which most closely approximates the perturbed states.

<sup>4</sup>See [141], Complement A\_XI.

**6.1.3.10 Ex: Vanishing perturbation orders**

Show that it is impossible to design a perturbation Hamiltonian of the form,

$$\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} + \begin{pmatrix} 0 & \Omega_{12} & \Omega_{13} \\ \Omega_{12}^* & 0 & \Omega_{23} \\ \Omega_{13}^* & \Omega_{23}^* & 0 \end{pmatrix}$$

such that the first and second order corrections vanish.

**6.2 Variational method****6.2.1 The Rayleigh fraction**

Let us assume that we want to calculate the ground state energy  $E_g$  of a system described by a Hamiltonian  $\hat{H}$ , but we do not know the wavefunction, and we do not know how to solve the Schrödinger equation. If at least we had a good idea of the generic form of the solution (Gaussian, sinusoidal, ..), we could choose a trial function with a free parameter and optimize this parameter minimizing the energy, which ought to be minimal for the ground state. This is precisely the idea of the *variational method*. Note that the variational method only works for the ground state.

For any function  $\psi$  we know that the *Rayleigh fraction*  $\mathcal{E}$  satisfies,

$$E_g \leq \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \equiv \mathcal{E} , \quad (6.26)$$

not only when  $\psi$  is the wavefunction of an excited state, but even when it represents a (imperfect) trial to the ground state. Assuming normalized wavefunctions we can discard the denominator  $\langle \psi | \psi \rangle = 1$ . To verify the theorem, we expand the function  $\psi$  into orthonormal (unknown) eigenfunctions,  $|\psi\rangle = \sum_n c_n |\psi_n\rangle$ . Since  $\psi$  is normalized,

$$1 = \langle \psi | \psi \rangle = \sum_{m,n} \langle \psi_m | c_m^* c_n | \psi_n \rangle = \sum_n |c_n|^2 . \quad (6.27)$$

In the same way,

$$\langle \psi | \hat{H} | \psi \rangle = \sum_{m,n} \langle \psi_m | c_m^* \hat{H} c_n | \psi_n \rangle = \sum_n E_n |c_n|^2 . \quad (6.28)$$

As the ground state is that of the lowest energy,  $E_g \leq E_n$ , we have demonstrated the relationship (6.26)

$$E_g = E_g \sum_n |c_n|^2 \leq \sum_n E_n |c_n|^2 = \langle \hat{H} \rangle . \quad (6.29)$$

In practice, the ansatz  $\psi_\alpha$  for the ground state allows us to calculate an energy that must be minimized via

$$\boxed{\frac{\partial \langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle}{\partial \alpha} = 0} . \quad (6.30)$$



In the Excs. 6.2.3.1 and 6.2.3.2 we will approach the fundamental state of a quartic potential and a harmonic oscillator, respectively, by trying several trial wavefunctions and optimizing their free parameters.

## 6.2.2 Rayleigh-Ritz method

A modification of the variational method is the *Rayleigh-Ritz method*. Here, instead of using a trial function, we use a linear combination of eigenfunctions with variable coefficients:  $|\psi\rangle = \sum_k c_k |k\rangle$ . These variables are then optimized to minimize the Rayleigh fraction,

$$E_g \leq \frac{\sum_{k,m} c_k^* c_m \langle k | \hat{H} | m \rangle}{\sum_{k,m} c_k^* c_m \langle k | m \rangle} = \mathcal{E}, \quad (6.31)$$

where we assume real coefficients and eigenfunctions. For this, the derivatives with respect to all coefficients must vanish:

$$\begin{aligned} 0 &\equiv \frac{\partial \mathcal{E}}{\partial c_q} = \frac{\sum_{k,m} \frac{\partial}{\partial c_q} c_k^* c_m \langle k | \hat{H} | m \rangle}{\sum_{k,m} c_k^* c_m \langle k | m \rangle} - \frac{\sum_{k,m} c_k^* c_m \langle k | \hat{H} | m \rangle \sum_{k,m} \frac{\partial}{\partial c_q} c_k^* c_m \langle k | m \rangle}{\left( \sum_{k,m} c_k^* c_m \langle k | m \rangle \right)^2} \\ &= \frac{\sum_{k,m} c_k^* \delta_{qm} \langle k | \hat{H} | m \rangle}{\sum_{k,m} c_k^* c_m \delta_{km}} - \mathcal{E} \frac{\sum_{k,m} c_k^* \delta_{qm} \delta_{km}}{\sum_{k,m} c_k^* c_m \delta_{km}} = \sum_k c_k^* \langle k | \hat{H} | q \rangle - \mathcal{E} c_q^*, \end{aligned} \quad (6.32)$$

using the definition of  $\mathcal{E}$  (6.31). For the expression  $\partial \mathcal{E} / \partial c_q^*$  we get analogous results. Hence,

$$0 = \sum_m c_m (\langle q | \hat{H} | m \rangle - \mathcal{E} \langle q | m \rangle). \quad (6.33)$$

The condition for the existence of solutions is that the secular determinant disappears,

$$0 = \det(\langle q | \hat{H} | m \rangle - \mathcal{E} \langle q | m \rangle). \quad (6.34)$$

The solution of this equation leads to a set of values  $\mathcal{E}$ , and the lowest value,  $\mathcal{E}_{min}$ , is the best approximation for the ground state energy. The coefficients of the wavefunction are obtained by solving the eigenvalue equation (6.33) with  $\mathcal{E}_{min}$ .

In Exc. 6.2.3.3 we will use the Rayleigh-Ritz method to estimate the effect of a finite nuclear mass of the hydrogen atom on the energy levels. In Exc. 6.2.3.4 we will use the Rayleigh-Ritz method to find the maximum number of atoms allowing for a stable Bose-Einstein condensate made of atoms subject to an attractive interatomic force.

## 6.2.3 Exercises

### 6.2.3.1 Ex: Variational method applied to a quartic potential

Determine the ground state energy of the quartic potential  $V(x) = bx^4$  making the variational ansatz  $\psi_\alpha(x) = (\alpha/\pi)^{1/4} e^{-\alpha x^2/2}$ . **Formulae:**

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} \quad , \quad \int_{-\infty}^{\infty} x^2 e^{-x^2} dx = \frac{1}{2} \sqrt{\pi} \quad , \quad \int_{-\infty}^{\infty} x^4 e^{-x^2} dx = \frac{3}{4} \sqrt{\pi}$$

**6.2.3.2 Ex: Variational method applied to the harmonic oscillator**

Obtain, through the variational method, the ground state energy of the one-dimensional harmonic oscillator described by the Hamiltonian  $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$ , and the corresponding wavefunction from the test functions

- $\psi(x) = Ae^{-\alpha x^2}$  being  $\alpha$  a constant;
- $\psi(x) = A/(x^2 + \beta^2)$  being  $\beta$  a constant;
- $\psi(x) = A \cos(\pi x/a)$  between the limits  $\pm a/2$  being  $a$  a constant.

**6.2.3.3 Ex: Effect of finite nuclear mass on hydrogen via Rayleigh-Ritz**

Use the Rayleigh-Ritz method to estimate the impact of the finite mass of the nucleus of the hydrogen atom. To do this, calculate the ground state energy using the exact Hamiltonian, but a basis of wavefunctions assuming an infinitely heavy nucleus. Only take into account the states  $\psi_{100}$  and  $\psi_{200}$ . **Help:** Express the exact Hamiltonian in terms of the infinite-mass Hamiltonian approximating for small corrections of the reduced mass:  $m \equiv m_e/(1 + \gamma) \simeq (1 - \gamma)m_e$ , where  $\gamma \equiv m_e/m_p$ .

**6.2.3.4 Ex: Collapse of a condensate with attractive interactions**

A Bose-Einstein condensate of  ${}^7\text{Li}$  may become unstable due to attractive interatomic force, the scattering length being  $a_s = -27.3a_B$ . Consider the radial Gross-Pitaevskii Hamiltonian derived in Exc. 4.1.5.2 with an external harmonic potential with the oscillation frequency  $\omega_{trp}/(2\pi) = 50$  Hz. Using the variational method to determine the maximum number of atoms allowing for a stable condensate. (Note that the derived minimization condition must be evaluated numerically.)

**6.3 WKB approximation**

The *WKB approximation* (from Wentzel-Kramers-Brillouin) [106, 414, 719] is a method to find approximate solutions for linear differential equations with spatially variable coefficients. It is typically used for calculations in quantum mechanics where the wavefunction is reformulated as an exponential semi-classically expanded function, and then the amplitude or phase is slowly changed. In the following, we present the WKB approximation applied to the Schrödinger equation and exemplify it in some canonical systems.

**6.3.1 WKB approximation applied to the Schrödinger equation**

Starting from the time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x), \quad (6.35)$$

and rewrite it as follows,

$$\frac{d^2 \psi}{dx^2} = k(x)\psi(x). \quad (6.36)$$

with  $k(x) = \sqrt{2m[E - V(x)]/\hbar^2}$ . For now, we will restrict ourselves to energies  $E > V(x)$ . In this scheme, the wavefunctions are usually complex functions, so that we can write them in polar coordinates, containing an amplitude  $A(x)$  and a phase  $\phi(x)$ , which are both real numbers:

$$\psi(x) = A(x)e^{i\phi(x)} . \quad (6.37)$$

Substituting this function into the Schrödinger equation we obtain a system of coupled equations in terms of  $A(x)$  and  $\phi(x)$ ,

$$A'' = A[(\phi')^2 - k^2] \quad \text{and} \quad (A^2\phi')' = 0 . \quad (6.38)$$

The equations (6.39) and (6.37) are completely equivalent to the Schrödinger equation. The second Eq. (6.38) is easy to solve,

$$A = \frac{C}{\sqrt{\phi'}} , \quad (6.39)$$

being  $C$  a real constant. We can not say the same thing about the solution of the first Eq. (6.38). In order to solve it we are going to use the WKB approach, assuming that  $A$  varies slowly, so the term  $A'' \rightarrow 0$ . By doing this approximation we can rewrite Eq. (6.39) in this way:

$$(\phi')^2 = k^2 . \quad (6.40)$$

Solving this last expression we obtain two linearly independent solutions,  $\phi' = \pm k$ . So we get the expression for the phase:

$$\phi(x) = \pm \int k(x)dx . \quad (6.41)$$

We write this indefinite integral, because the constant term can be absorbed by the constant  $C$ . Finally, we obtain the expression for the wavefunction in the WKB approximation:

$$\boxed{\psi(x) = \frac{C}{\sqrt{|k(x)|}} e^{\pm \int |k(x)|dx}} . \quad (6.42)$$

Here, taking the absolute value of the wavevector, we have already generalized for the case that the energy  $E$  of the particle is lower than the potential  $V(x)$  (classically forbidden region).

**Example 35 (WKB approximation):** The WKB approach is a semiclassical method for the solution of the Schrödinger equation that does not require the potential to be a perturbation of a soluble problem. Instead, it only assumes that certain classical quantities having the dimension of an action (energy per time) are much larger than Planck's constant. Inserting the ansatz

$$\psi(x) = Ae^{iS(x)/\hbar} ,$$

into the one-dimensional time-independent Schrödinger equation, we find,

$$-\frac{i\hbar}{2m}S''(x) + \frac{1}{2m}S'(x)^2 + V(x) - E = 0 .$$

Now we expand the exponent in orders of  $\hbar$ ,

$$S(x) = S_0(x) + \hbar S_1(x) + \frac{\hbar^2}{2} S_2(x) + \dots ,$$

and insert it in the above equation. Collecting the orders in  $\hbar$ , we find in the first orders,

$$\begin{aligned} \left[ \frac{1}{2m} S_0'(x)^2 + V(x) - E \right] \hbar^0 &= 0 \\ \left[ -\frac{i\hbar}{2m} S_0''(x) + \frac{1}{m} S_0'(x) S_1'(x) \right] \hbar^1 &= 0 \\ \left[ \frac{1}{2m} S_1'(x)^2 - \frac{i}{2m} S_1''(x) \right] \hbar^2 &= 0 . \end{aligned}$$

The solution of the zeroth order equation,  $S_0(x) = \pm \int^x \sqrt{2m[E - V(x')] dx'}$ , gives

$$\psi(x) = A e^{\pm \frac{i}{\hbar} \int^x \sqrt{2m[E - V(x')] dx'}$$

The WKB approximation can be used to describe continuous potentials (or barriers) by stepwise constant potentials. The transmission  $|T|^2$  through these parts can be obtained by multiplying the individual tunneling probabilities,

$$\ln |T|^2 \simeq -2 \int_{\text{barrier}} \kappa(x) dx ,$$

with  $\kappa(x) = \frac{1}{\hbar} \sqrt{2m[V(x) - E]}$ .

### 6.3.2 Connection formulas

Now let us derive the connection formulas that interconnect solutions with  $E$  above and below  $V(x)$  at the turning points, precisely those regions where WKB fails. We will apply the derivation to a generic confining potential shown in Fig. 6.1.

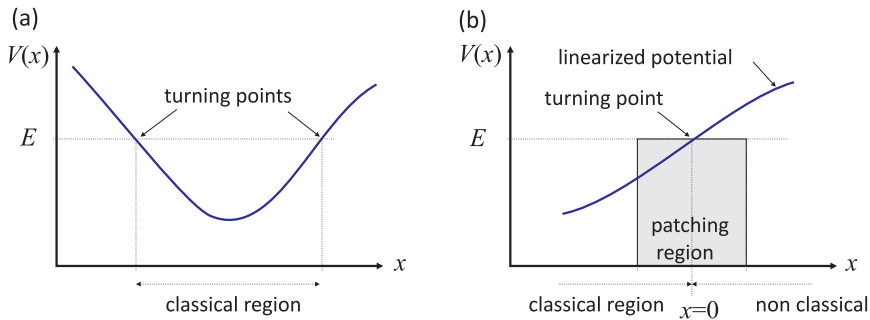


Figure 6.1: (a) Potential for which we want to obtain the connection formula. (b) Turning point.

Let us start with the right turning point Fig. 6.1(a)]. First, we shift the coordinate system so that the turning point coincides with zero, as shown in Fig. 6.1(b). As seen above, the WKB solutions will be given by the following equations:

$$\psi(x) \approx \begin{cases} \frac{1}{\sqrt{k(x)}} \left[ B e^{i \int_x^0 k(x') dx'} + C e^{-i \int_x^0 k(x') dx'} \right] & \text{if } x \leq 0 \\ \frac{1}{\sqrt{k(x)}} D e^{-\int_0^x |k(x')| dx'} & \text{if } x \geq 0 \end{cases} . \quad (6.43)$$

In the vicinity of the turning point we approximate the potential by a straight line (Taylor series expansion up to first order) with the following functional dependence,

$$V(x) \approx E + V'(0)x . \quad (6.44)$$

The Schrödinger equation for this potential acquires the following format,

$$\frac{d^2\psi_t}{dx^2} = \alpha^3 x \psi_t , \quad (6.45)$$

with  $\alpha = [\frac{2m}{\hbar^2}V'(0)]^{1/3}$ . Through a change of variables,  $z = \alpha x$ , we fall back on Airy's equation,

$$\frac{d^2\psi_t}{dz^2} = z \psi_t , \quad (6.46)$$

having as solution a linear combination of the two solutions of the Airy equation,

$$\psi_t(x) = a\text{Ai}(\alpha x) + b\text{Bi}(\alpha x) . \quad (6.47)$$

Now let's have a look at the WKB solutions in the two regions in the vicinity of the turning point. In the classically forbidden region we have  $k(x) = \alpha^{3/2}\sqrt{-x}$ , thus being  $\int_0^x |k(x')|dx' = \frac{2}{3}(\alpha x)^{3/2}$ . Thus, the WKB solution in the classically forbidden region near the turning point will be given by:

$$\psi(x) \approx \frac{D}{\sqrt{\hbar}\alpha^{3/4}x^{1/4}} e^{-\frac{2}{3}(\alpha x)^{3/2}} . \quad (6.48)$$

Using the asymptotic forms of Airy functions in the solution (6.47) we obtain the following expression for  $\psi_t(x)$ ,

$$\psi_p(x) \approx \frac{a}{2\sqrt{\pi}(\alpha x)^{1/4}} e^{-\frac{2}{3}(\alpha x)^{3/2}} + \frac{b}{\sqrt{\pi}(\alpha x)^{1/4}} e^{\frac{2}{3}(\alpha x)^{3/2}} , \quad (6.49)$$

which when compared to equation (6.48) shows us that  $a = \sqrt{\frac{4\pi}{\alpha\hbar}}D$  and  $b = 0$ . Repeating the previous steps in the negative region we see that the WKB solution in the asymptotic forms of the Airy solutions for approximately linear potentials takes the following format (with  $b = 0$ ):

$$\psi(x) \approx \frac{1}{\sqrt{\hbar}\alpha^{3/4}(-x)^{1/4}} \left[ B e^{i\frac{2}{3}(-\alpha x)^{3/2}} + C e^{-i\frac{2}{3}(-\alpha x)^{3/2}} \right] , \quad (6.50)$$

and

$$\psi_p(x) \approx \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}} \frac{1}{2i} \left[ e^{i\pi/4} e^{i\frac{2}{3}(-\alpha x)^{3/2}} - e^{-i\pi/4} e^{-i\frac{2}{3}(-\alpha x)^{3/2}} \right] . \quad (6.51)$$

When compared,  $\frac{a}{2i\sqrt{\pi}}e^{i\pi/4} = \frac{B}{\sqrt{\hbar}\alpha}$  and  $-\frac{a}{2i\sqrt{\pi}}e^{-i\pi/4} = \frac{C}{\sqrt{\hbar}\alpha}$ . Having all this information we can rewrite the WKB solutions for all positions in the potential, including the turning points <sup>5</sup>:

$$\psi(x) \approx \begin{cases} \frac{2D}{\sqrt{k(x)}} \sin \left[ \int_x^{x_2} k(x')dx' + \frac{\pi}{4} \right] , & \text{if } x \leq x_2 \\ \frac{D}{\sqrt{k(x)}} e^{-\int_{x_2}^x |k(x')|dx'} , & \text{if } x \geq x_2 \end{cases} . \quad (6.52)$$

<sup>5</sup>Note that we shifted the turning point to an arbitrary position  $x_2$ .

Repeating the process for a decreasing turning point [left turning point of the potential of Fig. 6.1(a)], we obtain the following expression:

$$\psi(x) \approx \begin{cases} \frac{D'}{\sqrt{k(x)}} e^{-\int_{x_1}^{x_1} |k(x')| dx'} , & \text{if } x \leq x_1 \\ \frac{2D'}{\sqrt{k(x)}} \sin \left[ \int_{x_1}^x k(x') dx' + \frac{\pi}{4} \right] , & \text{if } x \geq x_1 \end{cases} . \quad (6.53)$$

**Example 36 (Harmonic oscillator):** Now we apply the WKB method to a well-known system: the harmonic oscillator. We will calculate its energy levels and the respective eigenfunctions.

**Eigenenergies:** First, note that for a confining potential, and more specifically in the region where  $E \geq V(x)$ , we have the solutions obtained for the left and right turning point, these two solutions must match each other, that is,

$$\frac{2D}{\sqrt{k(x)}} \sin \left[ \int_x^{x_2} k(x') dx' + \frac{\pi}{4} \right] \simeq \frac{2D'}{\sqrt{k(x)}} \sin \left[ \int_{x_1}^x k(x') dx' + \frac{\pi}{4} \right] ,$$

and hence the zeros of these functions, so the arguments of those sines must be equal (except for a multiple of  $\pi$ ),

$$\begin{aligned} \int_x^{x_2} k dx' + \frac{\pi}{4} &= - \int_{x_1}^x k dx' - \frac{\pi}{4} + n\pi \\ \left( \int_{x_1}^x + \int_x^{x_2} \right) k dx' &= \left( n - \frac{1}{2} \right) \pi \\ \int_{x_1}^{x_2} k dx' &= \left( n - \frac{1}{2} \right) \pi , \end{aligned} \quad (6.54)$$

with  $n = 1, 2, \dots$ <sup>6</sup>. With this information we take a harmonic potential of the type  $V(x) = \frac{1}{2} \kappa x^2$ . In this case, the turning points for a given energy  $E$  will be at  $-\sqrt{\frac{2E}{\kappa}}$  and  $\sqrt{\frac{2E}{\kappa}}$ . For this potential we will have that  $k(x) = \sqrt{\frac{2m}{\hbar^2} (E - \frac{1}{2} \kappa x^2)}$ . Calculating the integral of  $k(x)$  between these two turning points we get,

$$\int_{x_1}^{x_2} k(x) dx = \frac{2m}{\hbar} \int_{-\sqrt{2E/\kappa}}^{\sqrt{2E/\kappa}} \sqrt{E - \frac{1}{2} \kappa x^2} dx = \pi E \frac{m}{\kappa} = \left( n - \frac{1}{2} \right) \pi \hbar ,$$

isolating  $E$  and taking  $\omega = \sqrt{\kappa/m}$  we have,

$$E = \left( n - \frac{1}{2} \right) \hbar \omega ,$$

with  $n = 1, 2, \dots$ , the exact spectrum of the harmonic oscillator, but this is just a coincidence.

**Eigenstates:** Now we will calculate the eigenstates of the harmonic oscillator. The eigenfunctions were calculated on a computer. The first graph (Fig. 6.2) compares the first exact excited state with that obtained using the WKB method.

Note that the WKB approach is very good when  $x \rightarrow 0$  and  $x \rightarrow \infty$ , regions where the difference between the oscillator energy and the potential are large ( $E \gg V(x \rightarrow 0)$  and  $E \ll V(x \rightarrow \infty)$ ), because in these regions the wavelength  $\lambda(x)$  acquires the lowest values, since it is proportional to  $|1/\sqrt{E - V(x)}|$ .

<sup>6</sup>Note that  $n \neq 0$ , because the integral (6.54) has to be greater than zero.

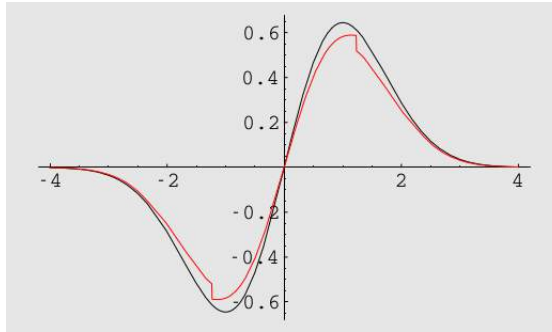


Figure 6.2: First excited state calculated accurately and through the WKB approximation.

Hence, the spatial region in which the potential needs to be practically constant is smaller, which explains why the approximation is closer to the exact solution. In the intermediate regions the difference between  $E$  and  $V(x)$  begins to decrease, and the WKB approximation delivers its worst results.

As we increase the energy of the harmonic oscillator, the approximation becomes better (for the same reason as discussed in the previous paragraph). The following graph illustrates this effect for  $n = 10$ .

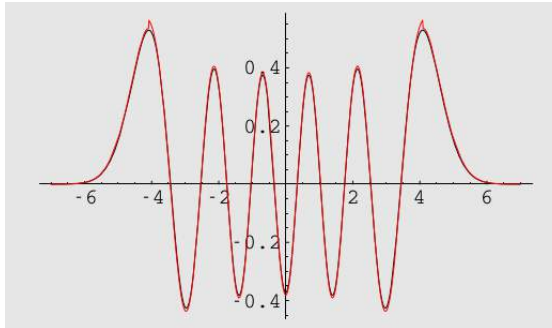


Figure 6.3: Wavefunction of the vibrational state  $n = 10$  calculated exactly and using the WKB approximation.

**Example 37 (Hydrogen atom): Eigenenergies:** For the hydrogen atom the effective potential is given by,

$$V(x) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r} + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}.$$

Note that the WKB method for this case obeys the relation (6.54), hence we get,

$$\begin{aligned} \int_{r_1}^{r_2} p(r) dr &= \sqrt{2m} \int_{r_1}^{r_2} \sqrt{E + \frac{e^2}{4\pi\epsilon_0} \frac{1}{r} - \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}} dr \\ &= \sqrt{-2mE} \int_{r_1}^{r_2} \frac{1}{r} \sqrt{-r^2 - \frac{e^2}{4\pi\epsilon_0 E} r + \frac{\hbar^2}{2mE} l(l+1)} dr. \end{aligned}$$

Notice that  $E < 0$ . Let us make the following substitution to facilitate algebraic manipulations,

$$B = -\frac{e^2}{4\pi\epsilon_0 E} \quad \text{and} \quad C = -\frac{\hbar^2}{2mE} l(l+1) .$$

The turning points  $r_1$  and  $r_2$  are given by the following expressions,

$$r_1 = \frac{B - \sqrt{B^2 - 4C}}{2} \quad \text{and} \quad r_2 = \frac{B + \sqrt{B^2 - 4C}}{2} .$$

Thus, returning to the integral we will have the following:

$$\begin{aligned} \int_{r_1}^{r_2} p(r) dr &= \sqrt{-2mE} \int_{r_1}^{r_2} \frac{1}{r} \sqrt{(r-r_1)(r_2-r)} dr = \sqrt{-2mE} \frac{\pi}{2} (\sqrt{r_2} - \sqrt{r_1})^2 \\ &= \sqrt{-2mE} \frac{\pi}{2} (r_1 + r_2 - 2r_1 r_2) = \sqrt{-2mE} \frac{\pi}{2} (B - 2\sqrt{C}) \\ &= \frac{\pi}{2} \left( -\frac{e^2 \sqrt{2m}}{4\pi\epsilon_0 \sqrt{-E}} - 2\hbar \sqrt{l(l+1)} \right) = \left( n - \frac{1}{2} \right) \pi \hbar . \end{aligned}$$

Isolating  $E$  we obtain the energy spectrum of the hydrogen atom in the WKB approximation:

$$E = -\frac{m}{2\hbar} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{1}{\left[ n - 1/2 + l(l+1) \right]^2} = -\frac{13.6}{\left[ n - 1/2 + l(l+1) \right]^2} eV .$$

For high energies ( $n \gg l$ ), we recover Bohr's expression.

### 6.3.3 Exercises

#### 6.3.3.1 Ex: Energy levels of hydrogen via WKB

Use the WKB approach to calculate the energy levels of the hydrogen atom.

## 6.4 Time-dependent perturbations

Temporal perturbations typically occur when we suddenly switch on an external field that influences the motion or spin of the particles, or when the field varies over time, for example, an electromagnetic field. Let us first study a two-level system subject to a temporal perturbation.

### 6.4.1 Two-level systems

We write the perturbation as

$$\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}(t) . \quad (6.55)$$

As in the case of a stationary perturbation, we write the eigenenergies and -functions of the unperturbed system as

$$\hat{H}^{(0)} |n\rangle = E_n |n\rangle . \quad (6.56)$$



Recalling that this stationary Schrödinger equation was obtained from the time-dependent Schrödinger equation via a separation ansatz (2.56), the temporal evolution of these eigenfunctions is given by,

$$|\psi_n^{(0)}(t)\rangle = |n\rangle e^{-iE_n t/\hbar} . \quad (6.57)$$

For small perturbations we can expect that the ansatz,

$$|\psi^{(1)}(t)\rangle = a_1(t)|\psi_1^{(0)}(t)\rangle + a_2(t)|\psi_2^{(0)}(t)\rangle , \quad (6.58)$$

be good. Note that not only do eigenfunctions oscillate, but the coefficients also depend on time, because the composition of the states can change. The instantaneous probability of finding the system in state  $n$  is  $|a_n(t)|^2$ . Importing the above linear combination into the Schrödinger equation,

$$\left[ \hat{H}^{(0)} + \hat{H}^{(1)}(t) \right] |\psi^{(1)}(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi^{(1)}(t)\rangle , \quad (6.59)$$

we find,

$$\begin{aligned} & a_1 \hat{H}^{(0)} |\psi_1^{(0)}\rangle + a_2 \hat{H}^{(0)} |\psi_2^{(0)}\rangle + a_1 \hat{H}^{(1)} |\psi_1^{(0)}\rangle + a_2 \hat{H}^{(1)} |\psi_2^{(0)}\rangle \\ &= i\hbar \left[ \frac{\partial a_1}{\partial t} |\psi_1^{(0)}\rangle + \frac{\partial a_2}{\partial t} |\psi_2^{(0)}\rangle + a_1 \frac{\partial |\psi_1^{(0)}\rangle}{\partial t} + a_2 \frac{\partial |\psi_2^{(0)}\rangle}{\partial t} \right] \\ \implies & a_1 \hat{H}^{(1)} |\psi_1^{(0)}\rangle + a_2 \hat{H}^{(1)} |\psi_2^{(0)}\rangle = i\hbar \dot{a}_1 |\psi_1^{(0)}\rangle + i\hbar \dot{a}_2 |\psi_2^{(0)}\rangle , \end{aligned} \quad (6.60)$$

because the other terms satisfy the Schrödinger equation of zero order. Replacing the stationary eigenfunctions,

$$a_1 e^{-iE_1 t/\hbar} \hat{H}^{(1)} |1\rangle + a_2 e^{-iE_2 t/\hbar} \hat{H}^{(1)} |2\rangle = i\hbar \dot{a}_1 e^{-iE_1 t/\hbar} |1\rangle + i\hbar \dot{a}_2 e^{-iE_2 t/\hbar} |2\rangle , \quad (6.61)$$

and multiplying this equation with  $\langle 1| \times$  and  $\langle 2| \times$ , we find with the abbreviation  $\hbar\omega_0 \equiv E_2 - E_1$ ,

$$\begin{aligned} i\hbar \dot{a}_1 &= a_1 \langle 1| \hat{H}^{(1)} |1\rangle + a_2 e^{-i\omega_0 t} \langle 1| \hat{H}^{(1)} |2\rangle \\ \text{and } i\hbar \dot{a}_2 &= a_1 e^{i\omega_0 t} \langle 2| \hat{H}^{(1)} |1\rangle + a_2 \langle 2| \hat{H}^{(1)} |2\rangle . \end{aligned} \quad (6.62)$$

Frequently, the perturbation induces only a coupling, but does not directly influence the energies very much,  $\langle n| \hat{H}^{(1)} |n\rangle \simeq 0$ ,

$$\boxed{\dot{a}_1 = a_2 \frac{e^{-i\omega_0 t}}{i\hbar} \langle 1| \hat{H}^{(1)} |2\rangle \quad \text{and} \quad \dot{a}_2 = a_1 \frac{e^{i\omega_0 t}}{i\hbar} \langle 2| \hat{H}^{(1)} |1\rangle} . \quad (6.63)$$

Without perturbation,  $\langle m| \hat{H}^{(1)} |n\rangle = 0$ , no dynamics develops; the eigenfunctions evolve independently.

## 6.4.2 The time-dependent perturbation method

Now, let us turn our attention to systems with many levels.

In *time-dependent perturbation theory* (TDPT) we separate the Hamiltonian into a stationary part and a time-dependent part <sup>7,8</sup>,

$$\hat{H}(t) = \hat{H}^{(0)} + \lambda \hat{H}^{(1)}(t) . \quad (6.64)$$

As usual, this Hamiltonian satisfies the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle . \quad (6.65)$$

Now, we do a unitary transformation into the *interaction picture* with  $S(t) = e^{-i\hat{H}^{(0)}t/\hbar}$  substituting  $|\psi(t)\rangle \equiv S(t)|\psi_I(t)\rangle$  and  $\hat{H}^{(1)}(t) \equiv S(t)\hat{W}(t)S^{-1}(t)$  in the Schrödinger equation. This procedure removes the stationary part, as shown in Sec. 2.4.4,

$$i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = \lambda \hat{W}(t) |\psi_I(t)\rangle . \quad (6.66)$$

If  $\hat{W}(t)$  were also independent of time, the solution would simply be  $|\psi_I(t)\rangle = e^{-i\hat{W}t/\hbar} |\psi_I(0)\rangle$ . Otherwise, we integrate the equation,

$$|\psi_I(t)\rangle = |\psi_I(0)\rangle + \frac{\lambda}{i\hbar} \int_0^t \hat{W}(\tau) |\psi_I(\tau)\rangle d\tau . \quad (6.67)$$

Substituting  $|\psi_I(\tau)\rangle$  by  $|\psi_I(t)\rangle$  we iterate this equation,

$$\begin{aligned} |\psi_I(t)\rangle &= |\psi_I(0)\rangle + \frac{\lambda}{i\hbar} \int_0^t \hat{W}(\tau_1) \left( |\psi_I(0)\rangle + \frac{\lambda}{i\hbar} \int_0^{\tau_1} \hat{W}(\tau_2) |\psi_I(\tau_2)\rangle d\tau_2 \right) d\tau_1 \\ &= |\psi_I(0)\rangle + \frac{\lambda}{i\hbar} \int_0^t \hat{W}(\tau_1) d\tau_1 |\psi_I(0)\rangle + \left( \frac{\lambda}{i\hbar} \right)^2 \int_0^t \hat{W}(\tau_1) \int_0^{\tau_1} \hat{W}(\tau_2) |\psi_I(\tau_2)\rangle d\tau_2 d\tau_1 \\ &= \left[ \sum_{n=1}^N \left( \frac{\lambda}{i\hbar} \right)^n \int_0^t \hat{W}(\tau_1) \int_0^{\tau_1} \hat{W}(\tau_2) \dots \int_0^{\tau_{n-1}} \hat{W}(\tau_n) d\tau_1 d\tau_2 \dots d\tau_n \right] |\psi_I(0)\rangle + o(\lambda^{N+1}) . \end{aligned} \quad (6.68)$$

This is called the *Dyson series*. For  $N = 1$ , we get the first order of the perturbation series <sup>9</sup>,

$$|\psi_I(t)\rangle = \left( 1 + \frac{\lambda}{i\hbar} \int_0^t \hat{W}(\tau) d\tau \right) |\psi_I(0)\rangle . \quad (6.69)$$

The stationary states of the unperturbed Hamiltonian are given by  $\hat{H}^{(0)}|f\rangle = E_f|f\rangle$ . Now, the perturbed states are expanded on this basis,  $|\psi_I(t)\rangle = \sum_f |f\rangle a_f(t)$ .

<sup>7</sup>See Becker-Sauter II, p.118ff and [678], p.104ff. An alternative treatment is found in [440], p.191ff or in Blochinzew, p.332ff.

<sup>8</sup>Note that by substituting  $\hat{W}$  by  $\hat{H}^{(1)}$ , the equation (6.66),  $i\hbar \partial_t |\psi_I(t)\rangle = \hat{H}^{(1)}(t) |\psi_I(t)\rangle$ , corresponds to a first-order perturbative approximation, i.e., the perturbation eigenvalues  $\hat{H}^{(1)}$  are calculated with the eigenvectors of the unperturbed system. Thus, in first order TDPT we can substitute  $\hat{W}$  for  $\hat{H}^{(1)}$ .

<sup>9</sup>For higher orders,

$$|\psi_I(t)\rangle \approx \left[ \sum_{n=1}^N \left( \frac{\lambda}{i\hbar} \right)^n \left( \int_0^t \hat{W}(\tau) d\tau \right)^n \right] |\psi_I(0)\rangle = T \left[ \exp \left( \frac{\lambda}{i\hbar} \int_0^t \hat{W}(\tau) d\tau \right) \right] |\psi_I(0)\rangle .$$

The expansion coefficients are <sup>10</sup>,

$$a_f(t) = \langle f|\psi_I(t)\rangle = \langle f|\psi_I(0)\rangle + \frac{\lambda}{i\hbar} \langle f| \int_0^t S^{-1}(\tau) \hat{H}^{(1)}(\tau) S(\tau) |\psi_I(0)\rangle d\tau. \quad (6.70)$$

Now, we assume that the system be initially in the eigenstate  $|\psi_I(0)\rangle = |i\rangle$ . The amplitudes then are,

$$\begin{aligned} a_{i \rightarrow f}(t) &= \langle f|i\rangle + \frac{\lambda}{i\hbar} \int_0^t e^{iE_f\tau/\hbar} \langle f|\hat{H}^{(1)}(\tau)|i\rangle e^{-iE_i\tau/\hbar} d\tau \\ &= \delta_{if} + \frac{\lambda}{i\hbar} \int_0^t \langle f|\hat{H}^{(1)}(\tau)|i\rangle e^{i\omega_{if}\tau} d\tau. \end{aligned} \quad (6.71)$$

The varying potential is considered a perturbation, and a variation of the system's state is observed. As the energy is not conserved,  $[\partial_t, \hat{H}(t)] \neq 0$ , the time-dependence is not separable and the system exchanges energy with the potential. In first-order perturbation theory we only consider weak perturbations, i.e. the initial state is gradually emptied,  $a_{i \rightarrow i}(dt) \simeq a_{i \rightarrow i}(0) = 1$ . For an initially empty state the growth is obviously considerable. For  $i \neq f$  we have,

$$\boxed{da_{i \rightarrow f}(t) = a_{i \rightarrow f}(t + dt) - a_{i \rightarrow f}(t) = \frac{\lambda}{i\hbar} \langle f|\hat{H}^{(1)}(t)|i\rangle e^{i\omega_{if}t} dt}. \quad (6.72)$$

This formula is nothing more than a generalization of the formula (6.63) obtained for a two-level system assuming that the initial state does not deplete considerably. In Exc. 6.4.5.1 we calculate the dynamics of a harmonic oscillator perturbed by a decaying force.

## 6.4.3 Specific perturbations

### 6.4.3.1 Sudden switch-on of a constant perturbation

To begin with, we consider a constant perturbation  $\hat{H}^{(1)}$  suddenly switched on at  $t = 0$ . In Schrödinger's picture we can rewrite Eq. (6.71),

$$a_{i \rightarrow f}(t) = \delta_{if} + \frac{\lambda}{i\hbar} \langle f|\hat{H}^{(1)}|i\rangle \int_0^t e^{i\omega_{if}\tau} d\tau = \delta_{if} + \frac{\lambda}{i\hbar} \langle f|\hat{H}^{(1)}|i\rangle \frac{-1 + e^{i\omega_{if}t}}{\omega_{if}}. \quad (6.73)$$

We obtain for  $i \neq f$ ,

$$\boxed{|a_{i \rightarrow f}(t)|^2 = \frac{\lambda^2}{\hbar^2} |\langle f|\hat{H}^{(1)}|i\rangle|^2 \frac{\sin^2(\omega_{if}t/2)}{(\omega_{if}/2)^2}}. \quad (6.74)$$

For long times we calculate the rate <sup>11</sup>,

$$\frac{d}{dt} |a_{i \rightarrow f}(t)|^2 = \frac{\lambda^2}{\hbar^2} |\langle f|\hat{H}^{(1)}|i\rangle|^2 \frac{\sin \omega_{if}t}{\omega_{if}/2} \xrightarrow{t \rightarrow \infty} \frac{2\pi\lambda^2}{\hbar^2} |\langle f|\hat{H}^{(1)}|i\rangle|^2 \delta(\omega_f - \omega_i), \quad (6.75)$$

<sup>10</sup>We could define the coefficients in Schrödinger's picture,  $a_f \equiv \langle f|\psi\rangle$ , but this would only introduce a phase factor,  $a_{i \rightarrow f} \rightarrow a_{i \rightarrow f} e^{i(E_f - E_i)t/\hbar}$ , which is unimportant for absolute values  $|a_{i \rightarrow f}|^2$ . This corresponds to a transformation to a rotating system, which will be discussed in Sec. 14.2.1.

<sup>11</sup>We use the trigonometric rule  $\sin x = 2 \sin \frac{x}{2} \cos \frac{x}{2}$ .

where we use the representation of the Dirac function,

$$\delta(x) = \lim_{t \rightarrow \infty} \frac{1}{2\pi} \int_{-t}^t e^{ikx} dk = \lim_{t \rightarrow \infty} \frac{t}{\pi} \text{sinc } xt . \quad (6.76)$$

The  $\delta$ -function in (6.75) ensures that, for infinitely sharp steps, transitions are impossible, unless the energy of the final state is the same as the one of the initial state. This points to the fact that infinitely sharp steps are not a realistic physical concept.

In practice, the changes applied to a system are often slow and the observation times are long, because the frequencies of the transitions are high  $\omega_{fi}/2\pi \simeq$  THz. Let us assume that the perturbation be switched on within a time constant  $\gamma^{-1}$ . In Exc. 6.4.5.2 we will study how the rapidity of a perturbation influences the transition rate. We will see via a temporal analysis of  $|a_{i \rightarrow f}(t)|^2$ , that for slow variations,  $\gamma \ll \omega_{fi}$ , the system adiabatically approaches the final situation. For  $\gamma \simeq \omega_{fi}$ , the system receives a shock and exhibits oscillating transients. For  $\gamma > \omega_{fi}$ , we observe violent oscillations with largest amplitudes.

### 6.4.3.2 Periodic perturbations

We now consider the case of an oscillatory perturbation, for example an electromagnetic field. In principle, knowledge of the system's response to periodic perturbations allows us to treat arbitrary perturbations, since we can expand them in Fourier series. We first treat transitions between discrete levels, before considering states embedded in continua,

$$\hat{H}^{(1)}(t) = \begin{cases} 0 & \text{for } t < 0 \\ 2\hbar\hat{\Omega}_0 \cos \omega t & \text{for } t \geq 0 \end{cases} . \quad (6.77)$$

With the abbreviation  $\Omega_{fi} \equiv \langle f | \hat{\Omega}_0 | i \rangle$  the transition rate is,

$$\begin{aligned} a_{i \rightarrow f}(t) &= -i\Omega_{fi} \int_0^t 2e^{i\omega_{fi}\tau} \cos \omega\tau d\tau \\ &= -i\Omega_{fi} \left[ \frac{e^{i(\omega_{fi}+\omega)t} - 1}{i(\omega_{fi}+\omega)} + \frac{e^{i(\omega_{fi}-\omega)t} - 1}{i(\omega_{fi}-\omega)} \right] . \end{aligned} \quad (6.78)$$

The first term being small, we neglect it doing a so-called *rotating wave approximation* (RWA). We obtain,

$$|a_{i \rightarrow f}(t)|^2 = |\Omega_{fi}|^2 \frac{\sin^2 \frac{1}{2}(\omega_{fi} - \omega)t}{\frac{1}{4}(\omega_{fi} - \omega)^2} . \quad (6.79)$$

This result coincides with the formula (6.74), except that the energy difference between the states  $\omega_{fi}$  is shifted by the frequency of the perturbation  $\omega$ . The quantity  $\Delta_{fi} \equiv \omega - \omega_{fi}$  is called a detuning. The transition probability is maximal, when we are at resonance, that is  $\Delta_{fi} = 0$ . In this case,

$$|a_{i \rightarrow f}(t)|^2 \longrightarrow |\Omega_{fi}|^2 t^2 . \quad (6.80)$$

This can be seen by expanding the numerator in a Taylor series for small  $(\omega_{fi} - \omega)t$ .

Note, that the probability exceeds 1 for long times, which can not be. In fact, the restriction to the first order in the Taylor expansion used in the derivation of the last

equation is no longer valid for long times, when  $(\omega_{f_i} - \omega)t > 1$ , and we need to take into account higher orders.

**Example 38 (The Rabi formula):** Let us now consider a periodic perturbation oscillating at frequency  $\omega = \omega_0 + \Delta$ , where  $\Delta$  is called the *detuning* from the resonance  $\omega_0$ ,

$$H^{(1)} = -e\mathbf{E}(\mathbf{r}, t) \cdot \mathbf{r} = -eE_0\hat{\varepsilon} \cos(kz - \omega t) \cdot \mathbf{r} . \quad (6.81)$$

Then,

$$\langle 2|H^{(1)}|1\rangle = -eE_0 \cos(kz - \omega t)\langle 2|r|1\rangle = \hbar\Omega \cos(kz - \omega t) , \quad (6.82)$$

where we call

$$\Omega \equiv \frac{-eE_0\langle 2|r|1\rangle}{\hbar} \quad (6.83)$$

the *Rabi frequency*. With this abbreviation the Eqs. (6.63) become,

$$\dot{a}_1 = -i\Omega a_2 e^{-i\omega_0 t} \cos(kz - \omega t) \quad \text{and} \quad \dot{a}_2 = -i\Omega^* a_1 e^{i\omega_0 t} \cos(kz - \omega t) . \quad (6.84)$$

Neglecting fast-rotating terms doing the so-called *rotating wave approximation* (RWA) and choosing the position of the atom to be  $z = 0$  we derive,

$$\dot{a}_1 \simeq -\frac{i\Omega}{2} a_2 e^{i\Delta t} \quad \text{and} \quad \dot{a}_2 \simeq -\frac{i\Omega^*}{2} a_1 e^{-i\Delta t} . \quad (6.85)$$

With the equations of motion we can, starting from initial values for  $a_1(0)$  and  $a_2(0)$ , calculate the temporal evolution.

We solve this system of differential equations by differentiating one and substituting the other,

$$\ddot{a}_2 = -i\dot{a}_1 \frac{\Omega^*}{2} e^{-i\Delta t} - a_1 \Delta \frac{\Omega^*}{2} e^{-i\Delta t} = -\frac{|\Omega|^2}{4} a_2 - i\Delta \dot{a}_2 . \quad (6.86)$$

We find solutions via the ansatz  $a_2 = e^{-i\Delta t/2}(Ae^{iGt/2} + Be^{-iGt/2})$ . The equation for  $a_2$  yields,

$$\begin{aligned} & \left(\frac{i}{2}G - \frac{i}{2}\Delta\right)^2 Ae^{i(G-\Delta)t/2} + \left(-\frac{i}{2}G - \frac{i}{2}\Delta\right)^2 Be^{i(-G-\Delta)t/2} \\ &= -\frac{|\Omega|^2}{4} (Ae^{i(G-\Delta)t/2} + Be^{i(-G-\Delta)t/2}) \\ & - i\Delta \left[ \left(\frac{i}{2}G - \frac{i}{2}\Delta\right) Ae^{i(G-\Delta)t/2} + \left(-\frac{i}{2}G - \frac{i}{2}\Delta\right) Be^{i(-G-\Delta)t/2} \right] . \end{aligned} \quad (6.87)$$

Separating the parts in  $A$  and in  $B$  we obtain two equations with the same result,

$$G^2 = |\Omega|^2 + \Delta^2 . \quad (6.88)$$

$G$  is called the *generalized Rabi frequency*. Using the initial conditions,  $a_1(0) = 1$  and  $a_2(0) = 0$ , we can fix one of the coefficients  $A$  and  $B$ , since  $a_2(0) = A + B = 0$ ,

$$a_2 = 2iAe^{-i\Delta t/2} \sin \frac{G}{2} t . \quad (6.89)$$

We now import this solution into the differential equation for  $a_1$ ,

$$\dot{a}_1 = -i\frac{\Omega}{2} a_2 e^{i\Delta t} = \Omega A e^{i\Delta t/2} \sin \frac{G}{2} t . \quad (6.90)$$

The integral is,

$$a_1(t) = \int_0^t \Omega A e^{i\Delta t'/2} \sin \frac{G}{2} t' dt' = -\frac{2A}{\Omega^*} e^{i\Delta t/2} \left( G \cos \frac{G}{2} t - i\Delta \sin \frac{G}{2} t \right). \quad (6.91)$$

Using the normalization condition,

$$\begin{aligned} 1 &= |a_1|^2 + |a_2|^2 = \left| -\frac{2A}{\Omega^*} e^{i\Delta t/2} \left( G \cos \frac{G}{2} t - i\Delta \sin \frac{G}{2} t \right) \right|^2 + \left| 2iA e^{-i\Delta t/2} \sin \frac{G}{2} t \right|^2 \\ &= \frac{4A^2}{|\Omega|^2} \left( G^2 \cos^2 \frac{G}{2} t + \Delta^2 \sin^2 \frac{G}{2} t \right) + 4A^2 \sin^2 \frac{G}{2} t = 4A^2 \frac{G^2}{|\Omega|^2}. \end{aligned} \quad (6.92)$$

Hence,  $A = |\Omega|/2G$ . In general, we can choose  $\Omega$  real, and the final solution is,

$$\boxed{a_1(t) = -e^{i\Delta t/2} \left( \cos \frac{G}{2} t + \frac{-i\Delta}{G} \sin \frac{G}{2} t \right) \quad \text{and} \quad a_2(t) = \frac{i\Omega}{G} e^{-i\Delta t/2} \sin \frac{G}{2} t}. \quad (6.93)$$

This results has already been obtained in Exc. 2.4.7.1 using a different approach. When the energies  $E_n$  are degenerate, under the influence of the perturbation, the populations of the system oscillate with the Rabi frequency  $\Omega$ . When the energies are different, the oscillation frequency  $G$  is higher, but the amplitude decreases as well. The initially empty state never reaches unitary population. In Exc. 6.4.5.3 we calculate the time required to allow the perturbation to invert the population of a two-level system, in Exc. 6.4.5.4 we study the maximum achievable inversion as a function of detuning, and in Exc. 6.4.5.5 we analyze the dynamics of a system subject to sequences of pulses.

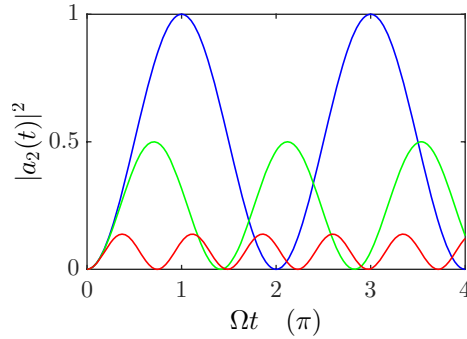


Figure 6.4: (code) Probability  $|a_2(t)|^2$  for the atom to be in the excited state for  $\Omega = \Gamma$  and  $\Delta = 0$  (blue),  $\Delta = \Gamma$  (green), and  $\Delta = 2.5\Gamma$  (red). Time is in units of  $1/\Gamma$ .

Note, that the *Rabi formula* (6.93) can be derived exactly without perturbative calculus. In Exc. 6.4.5.6 we show a derivation using the Laplace transformation method.

### 6.4.3.3 Transitions to continuous levels

When there are several final states,  $f \in F$ , the formula (6.79) must be generalized. The total transition probability,

$$P_{i \rightarrow F}(t) = \sum_{f \in F} |a_{i \rightarrow f}(t)|^2, \quad (6.94)$$

corresponds to the probability of the initial state  $|i\rangle$  to be depleted. When the final state lies within a continuum, the sum in (6.94) must be replaced by an integral. With the *density of states* written in the form  $\rho(E)$ , where  $\rho(E)dE$  is the number of states found in the energy range between  $E$  and  $E + dE$ , the transition probability is <sup>12</sup>,

$$P_{i \rightarrow F}(t) = \int_{E_{min}}^{E_{max}} |a_{i \rightarrow f}(t)|^2 \rho(E_f) dE_f, \quad (6.95)$$

where  $E \in [E_{min}, E_{max}]$  is the regime of energies within reach of the periodic perturbation. Now, plugging in the expressions (6.79),

$$P_{i \rightarrow F}(t) = \int_{E_{min}}^{E_{max}} |\Omega_{fi}|^2 \frac{\sin^2 \frac{1}{2\hbar}(E_{fi} - E)t}{\frac{1}{4\hbar^2}(E_{fi} - E)^2} \rho(E_f) dE_f. \quad (6.96)$$

Using the representation of the Dirac function,

$$\delta(x) = \lim_{t \rightarrow \infty} \frac{t}{\pi} \text{sinc}^2 xt, \quad (6.97)$$

with the substitution  $x \equiv (E_{fi} - E)/2\hbar$ , we obtain after sufficiently long times <sup>13</sup>,

$$P_{i \rightarrow F}(t) = \int_{E_{min}}^{E_{max}} |\Omega_{fi}|^2 t^2 \frac{\pi}{t} \delta\left(\frac{E_{fi} - E}{2\hbar}\right) \rho(E_f) dE_f = 2\pi\hbar t |\Omega_{fi}|^2 \rho(E_i + E). \quad (6.98)$$

The transition rate is,

$$\frac{dP_{i \rightarrow F}(t)}{dt} = \pi |\Omega_{fi}|^2 \rho(E_i + E). \quad (6.99)$$

For narrow distributions we may substitute the density of states  $\rho$  by a  $\delta$ -distribution,

$$\boxed{\frac{dP_{i \rightarrow F}}{dt} = \frac{2\pi}{\hbar} |\langle f | \hat{H}^{(1)} | i \rangle|^2 \delta(E_{fi} - E)}, \quad (6.100)$$

where we went back to the definition of the perturbation Hamiltonian (6.77). This expression is called *Fermi's Golden rule*. In Exc. 6.4.5.7 we will calculate the *photoelectric effect*.

#### 6.4.3.4 Continuous frequency distribution

To derive Eq. (6.79), we considered perturbations with fixed oscillation frequencies. To handle frequency distributions  $\varrho(\omega)$ , we must generalize this equation by calculating the integral,

$$\begin{aligned} |a_{i \rightarrow f}(t)|^2 &= |\Omega_{fi}|^2 \int \varrho(\omega) \frac{\sin^2 \frac{1}{2}(\omega_{fi} - \omega)t}{\frac{1}{4}(\omega_{fi} - \omega)^2} d\omega \\ &\simeq |\Omega_{fi}|^2 t \varrho(\omega_{fi}) \int_{-\infty}^{\infty} \text{sinc}^2 x dx = \pi t |\Omega_{fi}|^2 \varrho(\omega_{fi}), \end{aligned} \quad (6.101)$$

again using the representation (6.97) of the Dirac function. The approximation  $\varrho(\omega) = \varrho(\omega_{fi})$  can be used if the width of the sinc function is much narrower than the frequency distribution, which is the case for sufficiently long times,  $t \gg \pi/2\Delta_{fi}$ .

<sup>12</sup>With  $\rho(E) \equiv \sum_{f \in F} \delta(E_f - E)$  the integral is converted back into a sum.

<sup>13</sup>Remember  $\delta(ax) = \frac{1}{|a|} \delta(x)$ .

### 6.4.4 Transition rates for higher-order perturbations

The evolution from an initial state  $|i\rangle$  that the system occupies at time  $t_0$  to some final state  $|\psi\rangle$ , which may be a superposition, occupied at time  $t$ , is ruled by the solution of the Schrödinger equation,

$$|\psi\rangle = e^{-i\hat{H}(t-t_0)/\hbar}|i\rangle. \quad (6.102)$$

The probability to encounter  $|\psi\rangle$  in a given state  $|f\rangle$  is  $|\langle f|\psi\rangle|^2$ , and the *transition rate* is simply the derivative of this. The transition rate *out of the initial state* into any other final state is, consequently

$$\boxed{\frac{1}{\tau} = \sum_f \frac{d}{dt} |\langle f|e^{-i\hat{H}(t-t_0)/\hbar}|i\rangle|^2}. \quad (6.103)$$

From this formula we can already see, that at short times, when we can expand the exponential to first order, we will recover the results of (6.72).

Let us now consider a time-independent perturbation in the Schrödinger picture,

$$\hat{H}(t) = \hat{H}^{(0)} + \hat{H}^{(1)}, \quad (6.104)$$

where the time dependence is entirely left to the wavefunction. Now, we expand the propagator  $e^{-i\hat{H}(t-t_0)}$  in a perturbative series<sup>14</sup>. Unfortunately, generally  $[\hat{H}^{(0)}, \hat{H}^{(1)}] \neq 0$ , so that  $e^{-i\hat{H}t} \neq e^{-i\hat{H}^{(0)}t}e^{-i\hat{H}^{(1)}t}$ . But we can calculate,

$$i\frac{d}{dt}e^{i\hat{H}^{(0)}t}e^{-i\hat{H}t} = -\hat{H}^{(0)}e^{i\hat{H}^{(0)}t}e^{-i\hat{H}t} + e^{i\hat{H}^{(0)}t}\hat{H}e^{-i\hat{H}t} = e^{i\hat{H}^{(0)}t}\hat{H}^{(1)}e^{-i\hat{H}t}. \quad (6.105)$$

Integrating both sides and resolving for  $e^{-i\hat{H}t}$ ,

$$e^{-i\hat{H}t} = e^{-i\hat{H}^{(0)}t} \left\{ e^{i\hat{H}^{(0)}t_0}e^{-i\hat{H}t_0} - i \int_{t_0}^t e^{i\hat{H}^{(0)}t_1}\hat{H}^{(1)}e^{-i\hat{H}t_1} dt_1 \right\}. \quad (6.106)$$

We want to analyze a steady-state situation, that is, we assume that the interaction as gradually built up in an infinitely remote past. Hence, we can set  $\hat{H} = \hat{H}^{(0)}$  for  $t_0 \rightarrow -\infty$ ,

$$e^{-i\hat{H}t} = e^{-i\hat{H}^{(0)}t} \left\{ 1 - i \int_{-\infty}^t e^{i\hat{H}^{(0)}t_1}\hat{H}^{(1)}e^{\varepsilon t_1}e^{-i\hat{H}t_1} dt_1 \right\}, \quad (6.107)$$

where the term  $e^{\varepsilon t_1}$ , with  $\varepsilon \rightarrow 0$ , is inserted to guarantee a smooth switch-on. We iterate,

$$\boxed{\begin{aligned} e^{-i\hat{H}t} &= e^{-i\hat{H}^{(0)}t} \left\{ 1 - i \int_{-\infty}^t e^{i\hat{H}^{(0)}t_1}\hat{H}^{(1)}e^{\varepsilon t_1} \times \right. \\ &\quad \left. \times e^{-i\hat{H}^{(0)}t} \left[ 1 - i \int_{-\infty}^{t_1} e^{i\hat{H}^{(0)}t_2}\hat{H}^{(1)}e^{\varepsilon t_2}e^{-i\hat{H}t_2} dt_2 \right] dt_1 \right\}. \end{aligned}} \quad (6.108)$$

<sup>14</sup>We drop the  $\hbar = 1$  for the following calculation to simplify the notation.



We calculate the matrix elements up to second order substituting  $\hat{H}$  with  $\hat{H}^{(0)}$  in the last integral,

$$\begin{aligned}
& \langle f | e^{-i\hat{H}t} | i \rangle \tag{6.109} \\
& \simeq \langle f | e^{-i\hat{H}^{(0)}t} \left\{ 1 - \imath \int_{-\infty}^t e^{i\hat{H}^{(0)}t_1} \hat{H}^{(1)} e^{\varepsilon t_1} e^{-i\hat{H}^{(0)}t_1} \left[ 1 - \imath \int_{-\infty}^{t_1} e^{i\hat{H}^{(0)}t_2} \hat{H}^{(1)} e^{\varepsilon t_2} e^{-i\hat{H}^{(0)}t_2} dt_2 \right] dt_1 \right\} | i \rangle \\
& = e^{-i\omega_f t} \langle f | i \rangle - \imath e^{-i\omega_f t} \int_{-\infty}^t e^{i\omega_f t_1} \langle f | \hat{H}^{(1)} | i \rangle e^{\varepsilon t_1} e^{-i\omega_i t_1} dt_1 \\
& \quad - e^{-i\omega_f t} \int_{-\infty}^t e^{i\omega_f t_1} \langle f | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i \rangle e^{\varepsilon t_1} e^{-i\omega_i t_1} \sum_m | m \rangle \langle m | \int_{-\infty}^{t_1} e^{i\hat{H}^{(0)}t_2} \hat{H}^{(1)} | i \rangle e^{\varepsilon t_2} e^{-i\omega_i t_2} dt_2 dt_1 .
\end{aligned}$$

where we separated the perturbation orders and inserted  $\sum_m | m \rangle \langle m | = 1$  using the closure relation. Using the time-independence of  $\hat{H}^{(1)}$ ,

$$\begin{aligned}
& \langle f | e^{-i\hat{H}t} | i \rangle \simeq e^{-i\omega_f t} \delta_{fi} - \imath e^{-i\omega_f t} \langle f | \hat{H}^{(1)} | i \rangle \int_{-\infty}^t e^{(i\omega_f - i\omega_i + \varepsilon)t_1} dt_1 \tag{6.110} \\
& \quad - e^{-i\omega_f t} \sum_m \langle f | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i \rangle \int_{-\infty}^t e^{(i\omega_f - i\omega_i + \varepsilon)t_1} \int_{-\infty}^{t_1} e^{(i\omega_m - i\omega_i + \varepsilon)t_2} dt_2 dt_1 \\
& = e^{-i\omega_f t} \delta_{fi} - \imath e^{-i\omega_f t} \langle f | \hat{H}^{(1)} | i \rangle \frac{e^{(i\omega_f - i\omega_i + \varepsilon)t}}{i(\omega_f - \omega_i) + \varepsilon} \\
& \quad - e^{-i\omega_f t} \sum_m \langle f | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i \rangle \int_{-\infty}^t e^{(i\omega_f - i\omega_m + \varepsilon)t_1} \frac{e^{(i\omega_m - i\omega_i + \varepsilon)t_1}}{i(\omega_m - \omega_i) + \varepsilon} dt_1 \\
& = e^{-i\omega_f t} \delta_{fi} - \imath \langle f | \hat{H}^{(1)} | i \rangle \frac{e^{(-i\omega_i + \varepsilon)t}}{i(\omega_f - \omega_i) + \varepsilon} \\
& \quad - e^{-i\omega_f t} \sum_m \frac{\langle f | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i \rangle}{i(\omega_m - \omega_i) + \varepsilon} \int_{-\infty}^t e^{(i\omega_f - i\omega_i + 2\varepsilon)t_1} dt_1 \\
& = e^{-i\omega_f t} \delta_{fi} - \imath \langle f | \hat{H}^{(1)} | i \rangle \frac{e^{(-i\omega_i + \varepsilon)t}}{i(\omega_f - \omega_i) + \varepsilon} - \sum_m \frac{\langle f | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i \rangle}{i(\omega_m - \omega_i) + \varepsilon} \frac{e^{(-i\omega_i + 2\varepsilon)t}}{i(\omega_f - \omega_i) + 2\varepsilon} .
\end{aligned}$$

These three terms represent the zeroth, first, and second perturbation orders of the propagation operator (6.102). They are also called *Feynman propagators*. Now, we can calculate the transition rate up to second order,

$$\begin{aligned}
\frac{1}{\tau} &= \frac{d}{dt} \sum_f \left| \langle f | e^{-i\hat{H}t} | i \rangle \right|^2 \tag{6.111} \\
&= \lim_{\varepsilon \rightarrow 0} \sum_f \left| \langle f | \hat{H}^{(1)} | i \rangle - \sum_m \frac{\langle f | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i \rangle}{-i(\omega_m - \omega_i) - i\varepsilon} \right|^2 \frac{d}{dt} \left| \frac{e^{(-i\omega_i + \varepsilon)t}}{i(\omega_f - \omega_i) + \varepsilon} \right|^2 \\
&= \sum_f \left| \langle f | \hat{H}^{(1)} | i \rangle - \sum_m \frac{\langle f | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i \rangle}{(\omega_m - \omega_i)} \right|^2 \lim_{\varepsilon \rightarrow 0} \frac{2\varepsilon e^{2\varepsilon t}}{(\omega_f - \omega_i)^2 + \varepsilon^2} .
\end{aligned}$$

The last fraction is a representation of the  $\delta$ -function. Reintroducing  $\hbar$ , we finally obtain,

$$\boxed{\frac{1}{\tau} = \frac{2\pi}{\hbar^2} \sum_f \left| \langle f | \hat{H}^{(1)} | i \rangle + \frac{1}{\hbar} \sum_m \frac{\langle f | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i \rangle}{\omega_i - \omega_m} \right|^2 \delta(\omega_f - \omega_i)} . \tag{6.112}$$

The first term is *Fermi's Golden rule*, the second order corresponds to the *Kramers-Heisenberg formula*, which serves to describe Thomson, Rayleigh and Raman scattering. The generalization of this transition rate to all perturbation orders can be written,

$$\frac{1}{\tau} = \frac{2\pi}{\hbar^2} \sum_f \left| \langle f | \left( \hat{H}^{(1)} + \frac{1}{\hbar} \sum_m \frac{\hat{H}^{(1)} |m\rangle \langle m| \hat{H}^{(1)}}{\omega_i - \omega_m} + \dots \right. \right. \quad (6.113)$$

$$\left. \left. + \frac{1}{\hbar^{n-1}} \sum_{m_1, \dots, m_{n-1}} \frac{\hat{H}^{(1)} |m_1\rangle \langle m_1| \dots |m_{n-1}\rangle \langle m_{n-1}| \hat{H}^{(1)}}{(\omega_i - \omega_{m_1}) \dots (\omega_i - \omega_{m_{n-1}})} \right) |i\rangle \right|^2 \delta(\omega_{fi}) .$$

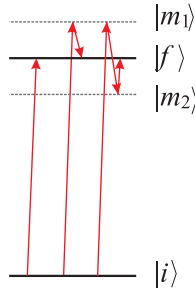


Figure 6.5: Graphical illustration of the various transitions orders. From left to right: absorption, Raman transition via an intermediate virtual state  $|m_1\rangle$ , three-photon process via two intermediate virtual states  $|m_1\rangle$  and  $|m_2\rangle$ .

## 6.4.5 Exercises

### 6.4.5.1 Ex: Perturbed harmonic oscillator

Consider a one-dimensional harmonic oscillator (HO) initially prepared ( $t = -\infty$ ) in the ground state  $|0\rangle$  of the unperturbed Hamiltonian  $H^{(0)} = \hbar\omega\hat{a}^\dagger\hat{a}$ , such that  $H^{(0)}|n\rangle = E_n|n\rangle$  with  $E_n = n\hbar\omega$ .

a. Through the expression,  $a_f(t) \approx \frac{1}{i\hbar} \int_{t_i}^{t_f} W_{fi} e^{i\omega_{fi}t} dt$ , and the perturbative Hamiltonian  $W(t) = -e\mathcal{E}x e^{-t^2/\tau^2}$  ( $x$  is the position operator of the HO), applied between  $t = -\infty$  and  $t = +\infty$ , calculate the probability of the system to be in the excited state  $|n\rangle$ , specifying  $n$ , at  $t = +\infty$ . Analyze the result.

b. Do the same for a shape-changing perturbation,  $W(t) = \Lambda x^2 e^{-t^2/\tau^2}$ .

### 6.4.5.2 Ex: Impact of the rapidity of a perturbation

Here we consider a slow variation,

$$\hat{W}(t) = \begin{cases} 0 & \text{for } t < 0 \\ W_0(1 - e^{-\gamma t}) & \text{for } t \geq 0 \end{cases} ,$$

with  $\gamma \ll \omega_{fi}$ .

- Calculate the transition rate for long times,  $t \gg \gamma^{-1}$ .
- Analyze the transition rate at a given time as a function of  $\gamma$ .

### 6.4.5.3 Ex: Rabi oscillation

The population of a degenerate two-level system be initially in state  $|1\rangle$ . What should be the duration of a perturbation to transfer the population to state  $|2\rangle$ ?

### 6.4.5.4 Ex: Rabi method

Free atoms be illuminated by light pulses characterized by the Rabi frequency  $\Omega$ , whose pulse area is (i)  $\int_0^t \Omega dt = \pi$  and (ii)  $= 2\pi$ . For which frequency tuning  $\Delta = \omega - \omega_0$  the excited state population is maximum? Draw the spectral profile of the population in the range  $-5 < \Delta/\Omega < 5$ .

### 6.4.5.5 Ex: Ramsey fringes

- Consider a two-level atom illuminated by a  $\frac{\pi}{2}$ -pulse of nearly resonant light,  $G \simeq \Omega$ , and calculate the ground and excited state amplitudes.
- How do the amplitudes evolve after the pulse if the detuning  $\Delta$  is small but non-zero?
- Derive the solution for  $|a_2(t)|^2$  of the equations (6.63) for the resonant case ( $\Delta = 0$ ) assuming the following initial conditions,  $a_2(0) = \frac{e^{i\phi}}{\sqrt{2}}$  and  $a_2(t = \frac{\pi}{2\Omega}) = 0$  if  $\phi = 0$ .
- Discuss the case of two consecutive  $\frac{\pi}{2}$ -pulses separated by a time interval  $T$ .

### 6.4.5.6 Ex: Two-level atom via Laplace transformation

Solve the problem of a two-level atom interacting with a laser using the Laplace transformation method.

### 6.4.5.7 Ex: Photoelectric effect

A hydrogen atom ground state in the ground state  $1s$  is placed in an electric field  $\mathbf{E}(t) = \mathbf{E}_0 \cos \omega t$ , such that  $W(t) = -e\mathbf{r} \cdot \mathbf{E}(t) = W_0 e^{-i\omega t} + W_0^\dagger e^{i\omega t}$  with  $W_0 = e\mathbf{r} \cdot \mathbf{E}_0/2$ . Find, via Fermi's Golden rule,

$$R = \frac{2\pi}{\hbar} |\langle f | W(t) | i \rangle|^2 \rho(E_f - E_i \mp \hbar\omega),$$

using the density of states  $\rho(E_k) dE_k = V/(2\pi)^3 k^2 dk d\Omega$ , the probability per unit of time for the atom to be ionized, by exciting from the ground state  $\psi_{100}(\mathbf{r}) = e^{-r/a_B}/(\pi a_B^3)^{1/2}$  to the state described by the plane wave  $\psi_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k} \cdot \mathbf{r}}/V^{1/2}$ . Simplify the calculation by assuming  $\mathbf{E}_0 = E_0 \hat{\mathbf{e}}_z$  and  $\mathbf{k} = k \hat{\mathbf{e}}_z$ .

**6.4.5.8 Ex: Kicked harmonic oscillator in second order perturbation**

Consider a one-dimensional harmonic oscillator initially in its ground state kicked via the  $\hat{H}^{(1)}(t) = e^{ik\hat{x}}\Theta(t)$ , as discussed in Sec. 3.6.2. Calculate the transition rate (6.103) to the final state  $|f\rangle = |0\rangle$  in first and second order perturbation theory.

**6.4.5.9 Ex: Dynamic Stark shift induced by blackbody radiation**

Calculate the dynamic Stark shift induced by blackbody radiation at  $T = 300$  K on the 1 MHz large strontium intercombination line at 698 nm.

## 6.5 Further reading

et al., [\[DOI\]](#)



# Chapter 7

## Appendices to 'Quantum Mechanics'

This chapter compiles some fundamental functions and polynomials, which are relevant in quantum theory.

### 7.1 Quantities and formulas in quantum mechanics

#### 7.1.1 Atomic units

A system of units commonly used in atomic physics is the one of *atomic units*. This system is based on the system of Gaussian units (CGS) <sup>1</sup> defined by,

$$e_{cgs} = e/\sqrt{4\pi\epsilon_0} \quad , \quad a_B = 1/\alpha \times \hbar/m_e c = \hbar^2/m_e e_{cgs}^2 \quad , \quad \hbar = 1 \quad . \quad (7.1)$$

With this fixing we give the energy in terms of  $e_{cgs}^2/a_B$ , the wavevector in terms of  $1/a_B$ , the distance in terms of  $a_B$  and the mass in terms of  $m_e$ , such that,

$$\begin{aligned} \tilde{E} &= E/(e_{cgs}^2/a_B) \quad , & (7.2) \\ \tilde{k} &= k a_B \quad , \\ \tilde{R} &= R/a_B \quad , \\ \tilde{\mu} &= \mu/m_e \quad . \end{aligned}$$

This notation simplifies formulas in atomic physics. For example:

$$\begin{aligned} k = \sqrt{\frac{2\mu}{\hbar^2}(E - V)} \quad \text{becomes} \quad \tilde{k} = \sqrt{2\tilde{\mu}(\tilde{E} - \tilde{V})} \quad , & (7.3) \\ V = C_6 \frac{e_{cgs}^2 a_B^5}{R^6} \quad \text{becomes} \quad \tilde{V} = \frac{C_6}{\tilde{R}^6} \quad . \end{aligned}$$

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<sup>1</sup>See the script *Eletrodinamics* by the same author [Scripts/EletroMagnetismoScript](#) .

## 7.2 Clebsch-Gordan and Wigner symbols

### 7.2.1 $\{3j\}$ -symbols

*Clebsch-Gordan coefficients* are used to describe spin coupling<sup>2</sup>. The Clebsch-Gordans are related to Wigner's  $\{3j\}$ -symbols,

$$\begin{aligned} \left( \begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array} \right) &= \left( \begin{array}{ccc} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{array} \right) = (-1)^{j_1-j_2+m} \sqrt{\Delta(j_1, j_2, j_3)} \times \\ &\times \sqrt{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j+m)!(j-m)!} \\ &\sum_t \frac{(-1)^t}{t!(m_1-j_2+j+t)!(-j_1-m_2+j+t)!(j_1+j_2-j-t)!(j_1-m_1-t)!(j_2+m_2-t)!} , \end{aligned} \quad (7.4)$$

with the abbreviation,

$$\Delta(j_1, j_2, j_3) \equiv \frac{(j_1+j_2-j_3)!(j_1-j_2+j_3)!(-j_1+j_2+j_3)!}{(j_1+j_2+j_3+1)!} . \quad (7.5)$$

### 7.2.2 $\{6j\}$ -symbols

$\{6j\}$ -symbols describe the recoupling of two spins. They can be evaluated by,

$$\left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ J_1 & J_2 & J_3 \end{array} \right\} = \sqrt{\Delta(j_1, j_2, j_3) \Delta(j_1, J_2, J_3) \Delta(J_1, j_2, J_3) \Delta(J_1, J_2, j_3)} \sum_t \frac{(-)^t (t+1)!}{f(t)} , \quad (7.6)$$

where  $f(t) = (t-j_1-j_2-j_3)!(t-j_1-J_2-J_3)!(t-J_1-j_2-J_3)!(t-J_1-J_2-j_3)!(j_1+j_2+J_1+J_2-t)!(j_2+j_3+J_2+J_3-t)!(j_3+j_1+J_3+J_1-t)!$ .

### 7.2.3 $\{9j\}$ -symbols

$\{3j\}$ -symbols describe the recoupling of three spins. They can be evaluated by,

$$\left\{ \begin{array}{ccc} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{array} \right\} = \sum_g (-)^{2g} (2g+1) \left\{ \begin{array}{ccc} j_1 & j_2 & J_{12} \\ J_{34} & J & g \end{array} \right\} \left\{ \begin{array}{ccc} j_3 & j_4 & J_{34} \\ j_2 & g & J_{24} \end{array} \right\} \left\{ \begin{array}{ccc} J_{13} & J_{24} & J \\ g & j_1 & j_3 \end{array} \right\} . \quad (7.7)$$

$\{9j\}$ -symbols satisfy the following orthogonality relation,

$$\sum_{J_{12}, J_{34}} \hat{J}_{12} \hat{J}_{34} \hat{H}_{13} \hat{H}_{24} \left\{ \begin{array}{ccc} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ H_{13} & H_{24} & J \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{array} \right\} = \delta_{J_{13} H_{13}} \delta_{J_{24} H_{24}} . \quad (7.8)$$

## 7.3 Functions and polynomials

<sup>2</sup>See [28], p.111 or [678], p.119.

### 7.3.1 The Gauss function

Indefinite integrals:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\pi/a} \quad \text{and} \quad \int_0^{\infty} x^n e^{-ax^2} dx = \frac{\Gamma(\frac{n+1}{2})}{2a^{\frac{n+1}{2}}}. \quad (7.9)$$

Higher momenta:

$$\int_{x_0}^{x_1} e^{-ax^2} dx = xe^{-ax^2} \Big|_{x_0}^{x_1} + 2a \int_{x_0}^{x_1} x^2 e^{-ax^2} dx. \quad (7.10)$$

### 7.3.2 Bessel functions

The integral definition of the *Bessel function*, the *von Neumann function*, and the *Hankel function* of the first and second kind are:

$$J_k(x) = \frac{1}{\pi} \int_0^{\pi} \cos(k\tau - x \sin \tau) d\tau = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i(x \sin \tau - k\tau)} d\tau \quad (7.11)$$

$$N_k(x) = \dots$$

$$H_k^{(1,2)} = J_k \pm iN_k.$$

The derivative,

$$2 \frac{dJ_k(x)}{dx} = J_{k-1}(x) - J_{k+1}(x). \quad (7.12)$$

Sum rules (empirically found),

$$\sum_{k=-\infty}^{\infty} J_k(x) = \sum_{k=-\infty}^{\infty} J_k(x)^2 = 1 \neq \sum_{k=-\infty}^{\infty} |J_k(x)|^2. \quad (7.13)$$

The *spherical Bessel function*, the *spherical von Neumann function*, and the *spherical Hankel function* of the first and second kind are defined by:

$$j_k(x) = \sqrt{\frac{\pi}{2x}} J_{k+1/2}(x) \quad (7.14)$$

$$n_k(x) = \sqrt{\frac{\pi}{2x}} N_{k+1/2}(x) = (-1)^{k+1} \sqrt{\frac{\pi}{2x}} J_{-k-1/2}(x)$$

$$h_k^{(1,2)} = j_k \pm in_k.$$

The series,

$$j_k(x) = (-x)^k \left( \frac{1}{x} \frac{d}{dx} \right)^k \frac{\sin x}{x}, \quad n_k(x) = -(-x)^k \left( \frac{1}{x} \frac{d}{dx} \right)^k \frac{\cos x}{x}. \quad (7.15)$$

The derivative,

$$j'_k(x) = \frac{k}{x} j_k(x) - j_{k+1}(x). \quad (7.16)$$



### 7.3.3 Hermite polynomials

The definition of the *Hermite polynomials*:

$$H_n(x) = \left(2x - \frac{d}{dx}\right)^n \cdot 1 = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} = \frac{2^n}{\sqrt{\pi}} \int_{-\infty}^{\infty} (x + it)^n e^{-t^2} dt \quad (7.17)$$

$$He_n(x) \equiv 2^{-n/2} H_n(x) .$$

Orthogonality and normalization:

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = \sqrt{\pi} 2^n n! \delta_{mn} . \quad (7.18)$$

Recursion:

$$\frac{d}{dx} H_n(x) = 2H_{n-1}(x) \quad (7.19)$$

$$\frac{d}{dx} e^{-x^2} H_n(x) = e^{-x^2} H_{n+1}(x)$$

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) .$$

Particular values:

$$H_{2n+1}(0) = 0 \quad (7.20)$$

$$H_{2n+1}(0) = (-1)^n 2^n (2n - 1)!!$$

Series:

$$H_{2n}(x) = \sum_{k=0}^{\infty} \frac{(2n)!}{(2k)!} \frac{(-1)^{n-k}}{(n-k)!} (2x)^{2k} \quad (7.21)$$

$$H_{2n-1}(x) = \sum_{k=0}^{\infty} \frac{(2n+1)!}{(2k+1)!} \frac{(-1)^{n-k}}{(n-k)!} (2x)^{2k+1}$$

$$H_n(x) = n! \sum_{k=0}^{int(n/2)} \frac{1}{k!} \frac{(-1)^k}{(n-2k)!} (2x)^{n-2k} .$$

### 7.3.4 Laguerre polynomials

The definition of the *Laguerre polynomials* is:

$$L_n^{(m)}(x) \equiv \frac{e^x x^{-m}}{m!} \frac{d^n}{dx^n} (e^{-x} x^{n+m}) \quad (7.22)$$

$$L_n \equiv L_n^{(0)}(x) .$$

Series:

$$L_n^{(m)}(x) = \sum_{k=0}^n \binom{n+m}{n-k} \frac{(-x)^k}{k!} . \quad (7.23)$$

Recursion:

$$\frac{d}{dx} L_n^{(m)}(x) = -L_{n-1}^{(m+1)}(x) . \quad (7.24)$$

Related functions:

$$\begin{aligned} u_{mn}(\varepsilon) &\equiv e^{-\varepsilon^2} \cdot (i\varepsilon)^{n-m} \cdot \sqrt{\frac{m!}{n!}} \cdot L_m^{n-m}(\varepsilon^2) \\ u_{mn}(0) &\approx (i\varepsilon)^{n-m} \cdot \sqrt{\frac{n!}{m!(n-m)!^2}} \\ u_{n+1,n}(0) &\approx i\varepsilon \cdot \sqrt{n+1} . \end{aligned} \quad (7.25)$$

Fourier transforms:

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-ax^2} x^{2k} \cos xp \cdot dx &= \frac{(-1)^k \sqrt{\pi}}{2^k \sqrt{a^{2k+1}}} \cdot e^{p^2/4a} \cdot He_{2k}(p/\sqrt{2a}) \\ \int_{-\infty}^{\infty} e^{-x^2/2} x^{2m} L_n^{2m}(x^2) \cos xp \cdot dx &= \frac{(-1)^m \sqrt{\pi}}{\sqrt{2n!}} \cdot e^{-p^2/2} \cdot He_n(p) He_{n+2m}(p) \\ \int_{-\infty}^{\infty} e^{-x^2/2} x^{2m+1} L_n^{2m+1}(x^2) \sin xp \cdot dx &= \frac{(-1)^m \sqrt{\pi}}{\sqrt{2n!}} \cdot e^{-p^2/2} \cdot He_n(p) He_{n+2m+1}(p) \\ \int_{-\infty}^{\infty} e^{-ax-bp} f(|x-p|) \cdot dx dp &= \frac{1}{a+b} \left[ \int_{-\infty}^{\infty} e^{-ax} f(x) dx + \int_{-\infty}^{\infty} e^{-bp} f(p) dp \right] . \end{aligned} \quad (7.26)$$

### 7.3.5 Legendre polynomials

The definition of *Legendre polynomials* is:

$$\begin{aligned} P_n(x) &\equiv \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n \\ P_n^{(-m)}(x) &\equiv (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) . \end{aligned} \quad (7.27)$$

Series:

$$P_n^{(m)}(x) = \frac{(-1)^m (n+m)!}{2^m m! (n-m)!} (1-x^2)^{m/2} \left[ + \frac{1 - \frac{(n-m)!(m+n+1)!}{11(m+1)!} \frac{1-x}{2}}{\frac{(n-m)!(n-m+1)!(m+n+1)!(m+n+2)!}{2!(m+1)!(m+2)!}} \left(\frac{1-x}{2}\right)^2 - \dots \right] . \quad (7.28)$$

### 7.3.6 Spherical harmonics

The definition of *spherical harmonics* is [718]:

$$Y_{\ell m}(\vartheta, \varphi) \equiv \sqrt{\frac{2\ell+1}{4\pi}} \sqrt{\frac{(\ell-|m|)!}{(\ell+|m|)!}} P_{\ell}^{|m|}(\cos(\vartheta)) e^{im\varphi} . \quad (7.29)$$

The lowest *spherical harmonics* are:

$$\begin{aligned} Y_0^{(0)} &= \frac{1}{2} \sqrt{\frac{1}{\pi}} & Y_0^{(1)} &= \frac{1}{2} \sqrt{\frac{3}{\pi}} \cos \theta \\ Y_{\pm 1}^{(1)} &= \mp \frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{\pm i\phi} & Y_0^{(2)} &= \frac{1}{4} \sqrt{\frac{5}{\pi}} (3 \cos^2 \theta - 1) \\ Y_{\pm 1}^{(2)} &= \mp \frac{1}{2} \sqrt{\frac{15}{2\pi}} \sin \theta \cos \theta e^{\pm i\phi} & Y_{\pm 2}^{(2)} &= \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{\pm 2i\phi} \end{aligned} \quad (7.30)$$

### 7.3.7 Vector spherical harmonics

The definition of *vector spherical harmonics* is [718]:

$$\mathbf{Y}_{j\ell m}(\mathbf{r}) \equiv (-1)^{1-\ell-m} \sqrt{2j+1} \sum_q \begin{pmatrix} \ell & 1 & j \\ m-q & q & -m \end{pmatrix} Y_{\ell m-q}(\vartheta, \varphi) \hat{\mathbf{e}}_q. \quad (7.31)$$

#### 7.3.7.1 The Gamma function

The definition of the *Gamma function* is:

$$\Gamma(x+1) = x\Gamma(x) \quad , \quad \Gamma(1/2) = \sqrt{\pi}. \quad (7.32)$$

### 7.3.8 Riemann zeta-function

The definition of the *Riemann zeta-function* is,

$$g_\eta(1) = \zeta(\eta) \quad , \quad (7.33)$$

where,

$$g_\eta(z) = \sum_{t=1}^{\infty} \pm \frac{(\pm z)^t}{t^\eta} = \frac{1}{\Gamma(\eta)} \int_0^{\infty} \frac{x^{\eta-1} dx}{z^{-1}e^x \pm 1}, \quad (7.34)$$

is also called the Bose/Fermi function. The upper sign holds for bosons, the lower for fermions. The *Sommerfeld expansion*,

$$\begin{aligned} \int_0^{\infty} \frac{g(x) dx}{e^{x-y} + 1} &= \int_0^y g(x) dx + \int_0^{\infty} \frac{g(y+x)^{\eta-1} dx}{e^x + 1} - \int_0^x \frac{g(y-x)^{\eta-1} dx}{e^x + 1} \\ &\approx \int_0^y g(x) dx + \frac{\pi^2}{6} g'(x) + \dots \end{aligned} \quad (7.35)$$

holds for  $z \gg 1$  and yields,

$$f_\eta(e^y) \approx \frac{x^\eta}{\Gamma(\eta+1)} \left( 1 + \frac{\pi^2 \eta(\eta-1)}{6x^2} + \frac{7\pi^4 \eta(\eta-1)(\eta-2)(\eta-3)}{360x^4} + \dots \right). \quad (7.36)$$

For small  $z$  both functions converge towards,

$$c_\eta(z) = \frac{1}{\Gamma(\eta)} \int_0^{\infty} \frac{x^{\eta-1} dx}{z^{-1}e^x} = c_{\eta-1}(z) = z. \quad (7.37)$$

The derivative is,

$$\frac{\partial f_\eta(Z)}{\partial Z} = \frac{\partial}{\partial Z} \sum_{t=1}^{\infty} -\frac{(-Z)^t}{t^\eta} = \sum_{t=1}^{\infty} \frac{(-Z)^{t-1}}{t^{\eta-1}} = \frac{1}{Z} \sum_{t=1}^{\infty} -\frac{(-Z)^t}{t^{\eta-1}} = \frac{f_{\eta-1}(Z)}{Z}, \quad (7.38)$$

or,

$$\begin{aligned} \frac{\partial f_\eta(Z)}{\partial Z} &= \frac{1}{\Gamma(\eta)} \frac{\partial}{\partial Z} \int_0^{\infty} \frac{x^{\eta-1} dx}{Z^{-1}e^x + 1} = \frac{1}{\Gamma(\eta)} \int_0^{\infty} \frac{x^{\eta-1} Z^{-2} e^x dx}{(Z^{-1}e^x + 1)^2} \\ &= \frac{1}{Z\Gamma(\eta)} \int_0^{\infty} x^{\eta-1} \frac{d}{dx} \frac{-1}{Z^{-1}e^x + 1} dx = \frac{\eta-1}{Z\Gamma(\eta)} \int_0^{\infty} \frac{x^{\eta-2}}{Z^{-1}e^x + 1} dx = \frac{f_{\eta-1}(Z)}{Z}. \end{aligned} \quad (7.39)$$

## 7.4 Further reading

I.S. Gradshteyn and I.M. Ryzhik, *Table of integrals, series, and products* [\[ISBN\]](#)



Part II

Atomic and Molecular  
Physics



# Chapter 8

## Electron spin and the atomic fine structure

The energy structure of hydrogen calculated by Bohr's model from the non-relativistic Hamiltonian agrees very well with the experimental measurements. However, in high-resolution experiments, small deviations were observed as energy shifts and splittings of spectral lines. These deviations, called *fine structure*, were not predicted by theory, which suggests that there are weak additional effects that do not strongly affect the position of the spectral lines but remove the energy degeneracy of the orbital quantum number  $\ell$ :  $E = E_{n,\ell}$ .

As a possible explanation we have the fact that the electrons present relativistic mass and momentum. In order to estimate the relevance of relativistic corrections let us estimate the electron velocity in the fundamental hydrogen states given by  $E_1 = -\hbar^2/2m_e a_B^2$ . Using the definitions of the Bohr radius,  $a_B = 4\pi\epsilon_0\hbar^2/(m_e e^2)$ , and the *fine structure constant*

$$\alpha \equiv \frac{e^2}{4\pi\epsilon_0\hbar c} \simeq \frac{1}{137}, \quad (8.1)$$

we obtain,

$$v = \sqrt{\frac{2E_1}{m_e}} = \frac{\hbar}{m_e a_B} = \frac{e^2}{4\pi\epsilon_0\hbar} = \alpha c, \quad (8.2)$$

which shows that the electron velocity is very high and that relativistic effects may indeed be *not negligible*.

### 8.1 The Dirac equation

#### 8.1.1 The Klein-Gordon equation for bosons

The Schrödinger equation for a free particle is based on the non-relativistic energy-momentum dispersion relation,

$$E = \frac{p^2}{2m_e}. \quad (8.3)$$

and the definitions of the quantum operators for energy and momentum,

$$E = i\hbar \frac{\partial}{\partial t} \quad \text{and} \quad \mathbf{p} = -i\hbar \nabla. \quad (8.4)$$



As already discussed in Sec. 2.1.2 we can, in order to find a relativistic wave equation, try the approach of inserting the quantum operators into the relativistic energy-momentum relation <sup>1</sup>.

$$E^2 = c^2 p^2 + m_e^2 c^4 . \quad (8.5)$$

We obtain,

$$\left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \left( \frac{m_e c}{\hbar} \right)^2 \right] \psi = 0 . \quad (8.6)$$

This is the *Klein-Gordon equation*. The stationary solution of this equation is a spherical wave,

$$\psi = \psi_0 \frac{1}{r} e^{-2\pi r / \lambda_C} , \quad (8.7)$$

where  $\lambda_C = h/m_e c$  is the *Compton wavelength*. We show this in Exc. 8.1.5.1. For example, in the case of heavy bosonic particles, such as a field of  $\pi$ -mesons,  $\psi$  is the *Yukawa potential*.

In the framework of the *standard model*, it is believed that matter is composed of two fundamental types of particles, bosons and fermions. Bosons are exchanged between fermions conveying the interaction between them. A typical example is the one of two electrons whose Coulomb interaction is mediated by the exchange of photons. Bosons obey the Klein-Gordon equation, fermions the Dirac equation derived in the following section.

## 8.1.2 The Dirac equation for fermions

In 1928 Paul Dirac, at the age of 26, developed an approach to a relativistic wave equation which differed from the Klein-Gordon equation. Motivated by the observation that the photon, being the relativistic particle *par excellence*, obeys a linear energy-momentum relation of the form  $\omega = ck$ , he attempted to derive a linear dispersion relation in  $E$  and  $p$  for heavy particles via the following ansatz:

$$E = \alpha_0 m_e c^2 + \alpha_1 c p_x + \alpha_2 c p_y + \alpha_3 c p_z . \quad (8.8)$$

Replacing energy and momentum with their respective operators <sup>2</sup>,

$$i\hbar \frac{\partial}{\partial t} \phi = \alpha_0 m_e c^2 \phi - i c \hbar \left( \alpha_1 \frac{\partial}{\partial x} + \alpha_2 \frac{\partial}{\partial y} + \alpha_3 \frac{\partial}{\partial z} \right) \phi . \quad (8.9)$$

We must now ensure that the relativistic energy-momentum condition (8.5) be satisfied.

**Example 39 (Derivation of the Dirac equation):** Taking the square on the right-hand side of the equation (8.9),

$$\begin{aligned} & [\alpha_0 m_e c^2 - i c \hbar (\alpha_1 \partial_x + \alpha_2 \partial_y + \alpha_3 \partial_z)] [\alpha_0 m_e c^2 - i c \hbar (\alpha_1 \partial_x + \alpha_2 \partial_y + \alpha_3 \partial_z)] \\ &= m_e^2 c^4 \alpha_0^2 - i c \hbar m_e c^2 [(\alpha_0 \alpha_1 + \alpha_1 \alpha_0) \partial_x + (\alpha_0 \alpha_2 + \alpha_2 \alpha_0) \partial_y + (\alpha_0 \alpha_3 + \alpha_3 \alpha_0) \partial_z] \\ &\quad - c^2 \hbar^2 [\alpha_1^2 \partial_x^2 + \alpha_2^2 \partial_y^2 + \alpha_3^2 \partial_z^2] \\ &\quad - c^2 \hbar^2 [(\alpha_1 \alpha_2 \partial_x \partial_y + \alpha_2 \alpha_1 \partial_y \partial_x) + (\alpha_2 \alpha_3 \partial_y \partial_z + \alpha_3 \alpha_2 \partial_z \partial_y) + (\alpha_3 \alpha_1 \partial_z \partial_x + \alpha_1 \alpha_3 \partial_x \partial_z)] . \end{aligned}$$

<sup>1</sup>Using the covariant notation with  $p_\mu \equiv (E/c, \mathbf{p})$ :  $p_\mu p^\mu = E^2/c^2 - p^2 = m_e^2 c^2$  is a Lorentz invariant.

<sup>2</sup>We introduce the abbreviation  $\partial_k \equiv \frac{\partial}{\partial x_k}$

For this expression to be identical to the relativistic energy-momentum condition (8.5),

$$m_e^2 c^4 - c^2 \hbar^2 [\partial_x^2 + \partial_y^2 + \partial_z^2],$$

we need to postulate for all  $i = 0, \dots, 4$ , that  $\alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij}$ .

Obviously, the condition

$$[\alpha_i, \alpha_j]_+ = 2\delta_{ij} \quad (8.10)$$

can not be satisfied if the  $\alpha_i$  are numbers. The idea of Dirac was to interpret the variables  $\alpha_i$  as matrices. These matrices act as operators on appropriate states, which are no longer scalar wavefunctions but vectors. Each component of the vector is a wavefunction in the usual sense. The Hilbert space is extended to be the product space of the usual spatial wavefunctions and a finite-dimensional vector space.

**Example 40 (Calculation with matrices of operator):** To give an idea of how the algebra works we consider a general situation. As the operator we choose the product,

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\partial}{\partial x}$$

and as the wavefunction vector we choose,

$$\begin{pmatrix} e^{ik_1 x} \\ e^{ik_2 x} \end{pmatrix}.$$

Applying the operator on the state vector we get,

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\partial}{\partial x} \begin{pmatrix} e^{ik_1 x} \\ e^{ik_2 x} \end{pmatrix} = \begin{pmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{pmatrix} \begin{pmatrix} e^{ik_1 x} \\ e^{ik_2 x} \end{pmatrix} = \begin{pmatrix} 0 + \frac{\partial}{\partial x} e^{ik_2 x} \\ \frac{\partial}{\partial x} e^{ik_1 x} + 0 \end{pmatrix} = \begin{pmatrix} ik_2 e^{ik_2 x} \\ ik_1 e^{ik_1 x} \end{pmatrix}.$$

The matrices  $\alpha_i$  must satisfy the condition (8.10). It is possible to show that this requires at least four-dimensional matrices of the following form:

$$\alpha_0 = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix} \quad \text{and} \quad \alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \quad (8.11)$$

where  $j = x, y, z = 1, 2, 3$ . In this notation the components of the matrices are also matrices:

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (8.12)$$

called *Pauli spin matrices*. The state vector must also have four dimensions,

$$\vec{\vec{\Phi}}(\mathbf{r}, t) = \begin{pmatrix} \vec{\phi}(\mathbf{r}, t) \\ \vec{\chi}(\mathbf{r}, t) \end{pmatrix} \quad \text{with} \quad \vec{\phi}(\mathbf{r}, t) = \begin{pmatrix} \phi_1(\mathbf{r}, t) \\ \phi_2(\mathbf{r}, t) \end{pmatrix} \quad \text{and} \quad \vec{\chi}(\mathbf{r}, t) = \begin{pmatrix} \chi_1(\mathbf{r}, t) \\ \chi_2(\mathbf{r}, t) \end{pmatrix}. \quad (8.13)$$

$\phi_j$  are called *large components*,  $\chi_j$  are called *small components*. This designation is explained later. Combining the matrices  $\alpha_j$  to a three-dimensional vector  $\vec{\alpha}$ , we can now write the Dirac equation (8.9) like,

$$\boxed{i\hbar \partial_t \vec{\vec{\Phi}}(\mathbf{r}, t) = (m_e c^2 \alpha_0 + c \vec{\alpha} \cdot \mathbf{p}) \vec{\vec{\Phi}}(\mathbf{r}, t)}. \quad (8.14)$$

Or, using the notation (8.11) and combining the Pauli matrices  $\sigma_j$  to a three-dimensional vector  $\vec{\sigma}$ , we can write the Dirac equation as:

$$\boxed{i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \vec{\phi} \\ \vec{\chi} \end{pmatrix} = \left[ m_e c^2 \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix} + c \begin{pmatrix} 0 & \vec{\sigma} \cdot \mathbf{p} \\ \vec{\sigma} \cdot \mathbf{p} & 0 \end{pmatrix} \right] \begin{pmatrix} \vec{\phi} \\ \vec{\chi} \end{pmatrix}}. \quad (8.15)$$

The non-diagonal matrix,

$$\begin{pmatrix} 0 & \vec{\sigma} \cdot \mathbf{p} \\ \vec{\sigma} \cdot \mathbf{p} & 0 \end{pmatrix} \quad (8.16)$$

couples large and small components.

**Example 41 (Covariant and relativistically invariant form of Dirac's equation):** To demonstrate its relativistic invariance it is useful to rewrite the Dirac equation in a way in which time and space appear on equal footings. For this we introduce new matrices,

$$\gamma^0 \equiv \alpha_0 \quad \text{and} \quad \gamma^k = \gamma^0 \alpha_k. \quad (8.17)$$

We obtain,

$$\gamma^0 = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix} \quad \text{and} \quad \gamma^k = \begin{pmatrix} 0 & \sigma_k \\ -\sigma_k & 0 \end{pmatrix}. \quad (8.18)$$

We also define another important matrix by,

$$\gamma_5 \equiv \nu \gamma_0 \gamma_1 \gamma_2 \gamma_3 = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}. \quad (8.19)$$

With this, using Einstein's notation <sup>3</sup>, the Dirac equation (8.13) adopts the form,

$$i\hbar \gamma^\mu \partial_\mu \psi - mc\psi = 0. \quad (8.20)$$

The complete system is summarized in the Minkowski metrics of time-space in the form,

$$[\gamma^\mu, \gamma^\nu]_+ = 2\eta^{\mu\nu}, \quad (8.21)$$

for  $\mu, \nu = 0, \dots, 5$ , that is, all matrices  $\gamma_k$  anticommute.

The Dirac equation can now be interpreted as an eigenvalue equation, where the rest mass is proportional to the eigenvalue of a momentum quadrivector, the proportionality constant being the speed of light:

$$P_{\text{op}} \psi = mc\psi, \quad (8.22)$$

Using  $\not{\partial}$  in the Feynman slash notation, which includes the  $\gamma$ -matrices, as well as a summation over the components of the spinor in the derivative, the Dirac equation becomes:

$$i\hbar \not{\partial} \psi - mc\psi = 0. \quad (8.23)$$

A fundamental theorem states that, if two distinct sets of matrices are given, which both satisfy Clifford's relations, then they are connected to each other by a similarity transformation:

$$\gamma'^\mu = S^{-1} \gamma^\mu S. \quad (8.24)$$

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<sup>3</sup> $\partial_0 \equiv \frac{1}{c} \partial_t$

If, in addition, the matrices are all unitary, as is the case of Dirac's set, then  $S$  is unitary,

$$\gamma'^{\mu} = U^{\dagger} \gamma^{\mu} U . \quad (8.25)$$

### 8.1.2.1 Anti-particles

Disregarding for a moment the non-diagonal matrix, the Dirac equation separates into two independent equations,

$$i\hbar \frac{\partial \vec{\phi}}{\partial t} = m_e c^2 \vec{\phi} \quad \text{and} \quad i\hbar \frac{\partial \vec{\chi}}{\partial t} = -m_e c^2 \vec{\chi} . \quad (8.26)$$

These are eigenenergy equations with the eigenvalues  $m_e c^2$  and  $-m_e c^2$ . The state with negative energy is interpreted as *anti-particle*. Therefore, the non-diagonal matrix mixes particles and anti-particles. We will study in Exc. 8.1.5.2 the so-called *Zitterbewegung* as a solution of the Dirac equation.

### 8.1.2.2 Particles and anti-particles in the non-relativistic limit

To reduce the Dirac equation to the non-relativistic Schrödinger equation, we first need to get rid of the rest energy. To do so, we separate a fast oscillation, whose frequency corresponds to the rest mass of the electron via the following ansatz, where  $\mathbf{u}$  and  $\mathbf{v}$  vary slowly in time:

$$\vec{\Phi}(\mathbf{r}, t) = e^{-i\omega_0 t} \begin{pmatrix} \mathbf{u}(\mathbf{r}, t) \\ \mathbf{v}(\mathbf{r}, t) \end{pmatrix} , \quad \hbar\omega_0 = m_e c^2 , \quad (8.27)$$

with the temporal derivative,

$$i\hbar \dot{\vec{\Phi}} = \left[ m_e c^2 \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} + i\hbar \begin{pmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{v}} \end{pmatrix} \right] e^{-i\omega_0 t} . \quad (8.28)$$

We insert this into the Dirac equation,

$$\left[ m_e c^2 \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} + i\hbar \begin{pmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{v}} \end{pmatrix} \right] e^{-i\omega_0 t} = \left[ m_e c^2 \begin{pmatrix} \mathbf{u} \\ -\mathbf{v} \end{pmatrix} + c\vec{\sigma} \cdot \mathbf{p} \begin{pmatrix} \mathbf{v} \\ \mathbf{u} \end{pmatrix} \right] e^{-i\omega_0 t} \quad (8.29)$$

finally obtaining,

$$i\hbar \dot{\mathbf{u}} = c(\vec{\sigma} \cdot \mathbf{p})\mathbf{v} \quad , \quad i\hbar \dot{\mathbf{v}} = c(\vec{\sigma} \cdot \mathbf{p})\mathbf{u} - 2m_e c^2 \mathbf{v} . \quad (8.30)$$

Since  $\mathbf{u}$  and  $\mathbf{v}$  only vary slowly in time, the derivatives on the left-hand side are small quantities. However, the condition that both derivatives must zero is too strong, because it leads to the trivial solution  $\mathbf{u} = 0$  and  $\mathbf{v} = 0$ . We find the first non-trivial solution by the condition  $\dot{\mathbf{v}} = 0$ . The second equation then becomes,

$$\mathbf{v} = \frac{1}{2m_e c} (\vec{\sigma} \cdot \mathbf{p})\mathbf{u} . \quad (8.31)$$

Inserted into the first equation,

$$i\hbar\dot{\mathbf{u}} = c \frac{(\vec{\sigma} \cdot \mathbf{p})^2}{2m_e c} \mathbf{u} . \quad (8.32)$$

We need, therefore, to evaluate the expression  $(\vec{\sigma} \cdot \mathbf{p})^2$ ,

$$\vec{\sigma} \cdot \mathbf{p} = \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & -p_z \end{pmatrix} \quad \text{and} \quad (\vec{\sigma} \cdot \mathbf{p})^2 = \mathbf{p}^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \quad (8.33)$$

Inserted into the differential equation (8.32) for  $\mathbf{u}$  we obtain precisely the Schrödinger equation for a free particle,

$$\boxed{i\hbar\dot{\mathbf{u}} = \frac{\mathbf{p}^2}{2m_e} \mathbf{u}} . \quad (8.34)$$

Let us return to the question, why we call  $\mathbf{u}$  the *strong* component. We have from the equation (8.31),

$$\mathbf{v}^\dagger \mathbf{v} = \frac{1}{(2m_e c)^2} (\vec{\sigma} \cdot \mathbf{p})^2 \mathbf{u}^\dagger \mathbf{u} = \frac{1}{2m_e c^2} \frac{\mathbf{p}^2}{2m_e} \mathbf{u}^\dagger \mathbf{u} , \quad (8.35)$$

and since  $\frac{\mathbf{p}^2}{2m_e} \ll m_e c^2$  follows immediately  $\mathbf{v}^\dagger \mathbf{v} \ll \mathbf{u}^\dagger \mathbf{u}$ .

In this non-relativistic approximation the components  $\mathbf{u}$  are much larger than the components  $\mathbf{v}$ . The mixture between particles and antiparticles only matters when  $\frac{\mathbf{p}^2}{2m_e} \simeq m_e c^2$ , resp.,  $\frac{1}{2} m_e v^2 \simeq m_e c^2$  or  $|v| \simeq c$ . The electron only receives small positronic contributions as it approaches the speed of light. In the ground state of the hydrogen atom the electron has a velocity of  $v = \alpha c \simeq c/137$ . That is, the contribution of the weak components is small, but present.

**Example 42 (Vanishing rest mass):** Let us note that for the case of vanishing rest mass,  $m_e = 0$ , the Dirac equation (8.15) dramatically simplifies. Taking the time derivative of the upper equation (8.15) and inserting the lower equation (8.15), we find,

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \vec{\phi} = \frac{1}{c^2} \frac{c\vec{\sigma} \cdot \mathbf{p}}{i\hbar} \frac{\partial}{\partial t} \vec{\chi} = -\frac{(\vec{\sigma} \cdot \mathbf{p})^2}{\hbar^2} \vec{\phi} = -\frac{\mathbf{p}^2}{\hbar^2} \vec{\phi} = \nabla^2 \vec{\phi} . \quad (8.36)$$

I.e. we recover a Helmholtz type wave equation.

### 8.1.2.3 The spin

We consider the operator defined by [199, 200],

$$\hat{\mathbf{s}} \equiv \frac{\hbar}{2} \vec{\sigma} , \quad (8.37)$$

and we calculate the commutation relations between its components. From the definitions (8.12) we obtain the rule,

$$[\hat{s}_x, \hat{s}_y] = \frac{\hbar^2}{4} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \frac{\hbar^2}{4} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = i\hbar \hat{s}_z . \quad (8.38)$$

In general terms the following holds true:  $[s_i, s_j] = \epsilon_{ijk} \hbar s_k$ . It is interesting to compare this with the commutation relation for the orbital angular momentum  $[\hat{l}_i, \hat{l}_j] = \epsilon_{ijk} \hbar \hat{l}_k$ . The coincidence suggests a generalization of the concept of angular momentum: We now call *angular momentum operator* every three-dimensional vector operator satisfying this commutation relation<sup>4</sup>. We consider the eigenvalue equation for  $\hat{s}_z$ , which is incorporated in the Dirac equation,

$$\hat{s}_z \vec{\phi} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = m_s \hbar \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \quad (8.39)$$

The eigenvalues are obviously  $m_s = \pm \frac{1}{2}$ . The angular momentum related to the matrices  $\mathbf{S}$  is obviously half-integer. We are dealing here with a new type of angular momentum, which is not included in the usual definition of *orbital* angular momentum  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ . The new angular momentum is called *intrinsic* angular momentum or *spin* of the particle. The spin represents a new structure or dimension additional to space comparable to the polarization of light. The photons of a circularly polarized light beam also contribute to an intrinsic angular momentum, which however in this case is integer.

In Exc. 8.1.5.3 we will see that neither  $\hat{l}_z$  nor  $\hat{s}_z$  are constants of motion of the Hamiltonian (8.15), but the sum  $\hat{j}_z \equiv \hat{l}_z + \hat{s}_z$ ,

$$[\hat{j}_z, \hat{H}] = 0. \quad (8.40)$$

#### 8.1.2.4 The stationary Dirac equation

By a similar treatment as in the Schrödinger equation one can deduce a stationary Dirac equation (8.14) via a separation of the time variable. Making for the time an exponential ansatz,

$$\vec{\phi}(\mathbf{r}, t) = \vec{\phi}(\mathbf{r}) e^{-iEt/\hbar} \quad \text{and} \quad \vec{\chi}(\mathbf{r}, t) = \vec{\chi}(\mathbf{r}) e^{-iEt/\hbar}, \quad (8.41)$$

we obtain coupled stationary equations for the large and small components,

$$(E - m_e c^2) \vec{\phi}(\mathbf{r}) = c \boldsymbol{\sigma} \cdot \mathbf{p} \vec{\chi}(\mathbf{r}) \quad \text{and} \quad (E + m_e c^2) \vec{\chi}(\mathbf{r}) = c \boldsymbol{\sigma} \cdot \mathbf{p} \vec{\phi}(\mathbf{r}). \quad (8.42)$$

### 8.1.3 The relativistic electron in a central Coulomb field

#### 8.1.3.1 Minimal coupling

In atomic physics we are mainly interested in electrons bound to a potential (e.g., generated by an atomic nucleus), that is, we must introduce electromagnetic forces into the Dirac equation. Therefore, we now consider the interaction of a charged particle with an electromagnetic field given by the vector potential  $\mathbf{A}$  and by the electrostatic potential  $U$ , such that the electric and magnetic fields,

$$\vec{\mathcal{E}} = -\nabla U - \frac{\partial \mathbf{A}}{\partial t} \quad \text{and} \quad \vec{\mathcal{B}} = \nabla \times \mathbf{A}, \quad (8.43)$$

<sup>4</sup>This concept can be derived from the requirement of symmetry under rotation of space as discussed in Sec. 2.5.

allow to calculate the Coulomb-Lorentz force. In the Hamiltonian formulation of electrodynamics the interaction can be described simply by the transition <sup>5</sup>,

$$\boxed{\hat{\mathbf{p}} \longrightarrow \hat{\mathbf{p}} - q\mathbf{A} \equiv \vec{\pi} \quad \text{and} \quad \hat{H} \longrightarrow \hat{H} + qU} . \quad (8.44)$$

called the *minimal coupling*. We briefly mentioned this already in Sec. 2.5.3, and the rules will be derived in Sec. 9.1. In addition to the substitution of the momentum, we must add the scalar potential  $qU$ , and we obtain the Dirac equation for a particle inside an applied electromagnetic field,

$$i\hbar\vec{\partial} \vec{\Phi} = (m_e c^2 \alpha_0 + c\vec{\alpha} \cdot \vec{\pi} + qU) \vec{\Phi} , \quad (8.45)$$

in generalization of Eq. (8.14).

### 8.1.3.2 Solving the stationary Dirac equation

Let us, for now, disregard external magnetic fields,  $\mathbf{A} = 0$ . Then, the stationary Dirac equation (8.42) becomes,

$$[E - qU(\mathbf{r}) - m_e c^2] \vec{\phi}(\mathbf{r}) = c\sigma \cdot \mathbf{p} \vec{\chi}(\mathbf{r}) \quad (8.46)$$

$$[E - qU(\mathbf{r}) + m_e c^2] \vec{\chi}(\mathbf{r}) = c\sigma \cdot \mathbf{p} \vec{\phi}(\mathbf{r}) .$$

For the Coulomb potential,

$$qU(r) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad (8.47)$$

the Dirac equation can be solved algebraically [201, 283, 288, 251] <sup>6</sup>. The calculation is more complicated than the resolution of the Schrödinger equation for hydrogen derived in Secs. 4.1.4 and 4.2.1 and will be sketched in the following.

**Example 43 (Dirac equation in spherical coordinates):** The goal of the following calculation is to express the Dirac equation for an electron in a central Coulomb field in spherical coordinates, i.e.  $r$  and  $p_r = -i\hbar\partial_r$  instead of  $\mathbf{p}$ . The starting point is the Dirac equation (8.15),

$$i\hbar\partial_t \vec{\Phi}(\mathbf{r}, t) = \hat{H} \vec{\Phi}(\mathbf{r}, t) , \quad (8.48)$$

with the Hamiltonian in the minimal coupling (8.44),

$$\hat{H} \equiv m_e c^2 \alpha_0 + c\vec{\alpha} \cdot [\mathbf{p} - q\mathbf{A}(\mathbf{r})] + qU(\mathbf{r}) \quad (8.49)$$

$$\text{with } \mathbf{A} = 0 \quad \text{and} \quad U(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0 r} .$$

We adopt the standard procedure from non-relativistic physics, which consists in rewriting the Hamiltonian in terms of observables, which commute with the Hamiltonian <sup>7</sup>.

<sup>5</sup>In quadrivectorial notation:  $\pi_\mu = p_\mu - qA_\mu$  with  $p_\mu = \begin{pmatrix} E/c \\ \mathbf{p} \end{pmatrix}$  and  $A_\mu = \begin{pmatrix} U/c \\ \mathbf{A} \end{pmatrix}$ .

<sup>6</sup>See also [http://einstein.drexel.edu/~bob/Term\\_Reports/Whitehead.3.pdf](http://einstein.drexel.edu/~bob/Term_Reports/Whitehead.3.pdf)

<sup>7</sup>Typical examples are the Hamiltonian of the harmonic oscillator (3.76) written in terms of  $\hat{n} \equiv \hat{a}^\dagger \hat{a}$  or the Hamiltonian of the hydrogen atom (4.34) written in terms of  $\mathbf{L}^2$ .

The goal is to calculate the quantity  $\vec{\alpha} \cdot \mathbf{p}$  appearing in the above Hamiltonian. As a first steps we define the following quantities,

$$\begin{array}{l} \mathbf{L} \equiv \mathbf{r} \times \mathbf{p} \quad \text{satisfying} \quad \mathbf{L} \times \mathbf{L} = i\hbar\mathbf{L} \\ \mathbf{S} \equiv \frac{\hbar}{2}\vec{\zeta} \equiv \frac{\hbar}{2}\gamma_5\vec{\alpha} \\ \mathbf{J} \equiv \mathbf{L} + \mathbf{S} \\ \hbar j' \equiv \alpha_0(\gamma_5\vec{\alpha} \cdot \mathbf{L} + \hbar) \\ r\varepsilon \equiv \vec{\alpha} \cdot \mathbf{r} \end{array} . \quad (8.50)$$

remembering that  $\gamma_5 = -i\alpha_1\alpha_2\alpha_3 = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}$  is the transformation exchanging particles and anti-particles. The first important relationship we have to derive is,

$$(\vec{\alpha} \cdot \mathbf{B})(\vec{\alpha} \cdot \mathbf{C}) = (\mathbf{B} \cdot \mathbf{C}) + i\gamma_5\vec{\alpha} \cdot (\mathbf{B} \times \mathbf{C}) . \quad (8.51)$$

It holds for  $[\vec{\alpha}, \mathbf{B}] = 0 = [\vec{\alpha}, \mathbf{C}]$  and will be proven in 8.1.5.4. Exploiting this relationship, we see that the scalar quantity  $\varepsilon$  satisfies,

$$\varepsilon^2 = \frac{1}{r^2}(\vec{\alpha} \cdot \mathbf{r})^2 = \frac{1}{r^2}[\mathbf{r} \cdot \mathbf{r} + i\vec{\alpha} \cdot (\mathbf{r} \times \mathbf{r})] = 1 . \quad (8.52)$$

Furthermore, with the definition of  $j'$  we show,

$$\begin{aligned} r\varepsilon\vec{\alpha} \cdot \mathbf{p} &= (\vec{\alpha} \cdot \mathbf{r})(\vec{\alpha} \cdot \mathbf{p}) = \mathbf{r} \cdot \mathbf{p} + i\gamma_5\vec{\alpha} \cdot (\mathbf{r} \times \mathbf{p}) \\ &= \mathbf{r} \cdot \mathbf{p} + i\gamma_5\vec{\alpha} \cdot \mathbf{L} = rp_r + i\alpha_0\hbar j' - i\hbar , \end{aligned} \quad (8.53)$$

where the relationship  $\mathbf{r} \cdot \mathbf{p} = rp_r$  is verified in Exc. 8.1.5.5(c). Hence,

$$\vec{\alpha} \cdot \mathbf{p} = \varepsilon \left( p_r + \frac{i\hbar(\alpha_0 j' - 1)}{r} \right) , \quad (8.54)$$

The final radial Hamiltonian is,

$$\hat{H} = m_e c^2 \alpha_0 + c\varepsilon \left( p_r - i\frac{\hbar}{r} \right) + \frac{vc\varepsilon\alpha_0\hbar j'}{r} - \frac{e^2}{4\pi\varepsilon_0 r} . \quad (8.55)$$

For now the choice of the quantities  $\varepsilon$  and  $j'$  must seem arbitrary, so we will have to discover their properties. We will see that  $j'$  is a non-zero integer related to the total angular momentum  $j$ . The following properties will be proven in Exc. 8.1.5.5(a) and (b),

$$\begin{aligned} (\hbar j')^2 &= \mathbf{J}^2 + \frac{\hbar^2}{4} \\ [\hbar j', \hat{H}]_- &= [\varepsilon, \hat{H}]_- = [\alpha_0, \hat{H}]_- = 0 . \end{aligned} \quad (8.56)$$

Hence, we got a collection of radial variables being constants of motion of the Dirac Hamiltonian.

**Example 44 (Resolving the spherical Dirac equation):** We will now search a solution to the spherical Dirac equation with the Hamiltonian (8.55). Noticing that the matrix  $\alpha_0$  is diagonal and the matrix  $\varepsilon$  counter-diagonal (just like the Dirac matrices  $\vec{\alpha}$ ), we may break down the stationary radial Dirac equation



into 2 by 2 matrices. Using the fact that  $\varepsilon$  commutes with all other terms and anti-commutes with  $\alpha_0$  and that  $\varepsilon^{-1} = \varepsilon^\dagger$  is a unitary transformation, we may go to a new basis via,

$$\begin{pmatrix} m_e c^2 - \frac{e^2}{4\pi\varepsilon_0 r} & -i c p_r - c \frac{\hbar}{r} - c \frac{\hbar j'}{r} \\ i c p_r + c \frac{\hbar}{r} - c \frac{\hbar j'}{r} & -m_e c^2 - \frac{e^2}{4\pi\varepsilon_0 r} \end{pmatrix} \begin{pmatrix} \vec{\phi} \\ \varepsilon \vec{\chi} \end{pmatrix} = E \begin{pmatrix} \vec{\phi} \\ \varepsilon \vec{\chi} \end{pmatrix}. \quad (8.57)$$

Substituting  $\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c}$  and  $a_\pm \equiv \frac{\hbar}{m_e c \mp E/c}$  (that is,  $\pm m_e c^2 - E \equiv \pm \frac{\hbar c}{a_\pm}$ ), we find,

$$\begin{pmatrix} \frac{1}{a_+} - \frac{\alpha}{r} & -\frac{d}{dr} - \frac{j'+1}{r} \\ \frac{d}{dr} - \frac{j'-1}{r} & -\frac{1}{a_-} - \frac{\alpha}{r} \end{pmatrix} \begin{pmatrix} \vec{\phi} \\ \varepsilon \vec{\chi} \end{pmatrix} = 0. \quad (8.58)$$

Assuming the existence of solutions of the form,

$$\begin{pmatrix} \vec{\phi} \\ \varepsilon \vec{\chi} \end{pmatrix} = \frac{e^{-r/a}}{r} \begin{pmatrix} \vec{f} \\ \vec{g} \end{pmatrix}, \quad (8.59)$$

where  $a \equiv \sqrt{a_+ a_-} = \hbar \left( m_e^2 c^2 - \frac{E^2}{c^2} \right)^{-1/2}$  [that is,  $\frac{d}{dr} \frac{e^{-r/a}}{r} = \frac{e^{-r/a}}{r} \left( -\frac{1}{a} - \frac{1}{r} \right)$ ], we find,

$$\begin{pmatrix} \frac{1}{a_+} - \frac{\alpha}{r} & -\frac{d}{dr} - \frac{1}{a} - \frac{j'}{r} \\ \frac{d}{dr} - \frac{1}{a} - \frac{j'}{r} & -\frac{1}{a_-} - \frac{\alpha}{r} \end{pmatrix} \begin{pmatrix} \vec{f} \\ \vec{g} \end{pmatrix} = 0. \quad (8.60)$$

Next we expand the unknown function  $\vec{f}$  and  $\vec{g}$  as series,

$$\vec{f}(r) = \sum_{s=-\infty}^{\infty} f_s r^s \quad \text{and} \quad \vec{g}(r) = \sum_{s=-\infty}^{\infty} g_s r^s. \quad (8.61)$$

These are then substituted into our system of equations. In order for the equation to go to zero as required, each term in the resulting series must separately go to zero. The coefficient of the  $r_s$  terms are,

$$\begin{aligned} \frac{f_s}{a_+} - \alpha f_{s+1} - (s+1+j')g_{s+1} + \frac{g_s}{a} &= 0 \\ \frac{g_s}{a_-} - \alpha g_{s+1} - (s+1-j')f_{s+1} + \frac{f_s}{a} &= 0. \end{aligned} \quad (8.62)$$

These can be combined by multiplying the first equation (8.62) by  $a$  and the second by  $a_-$  and then subtracting the former from the latter. Exploiting  $\frac{a}{a_+} = \frac{a_-}{a}$ , this gives us an expression directly relating the  $f_s$  coefficients with the  $g_s$  coefficients,

$$[\alpha a - a_+(s-j')]f_s + [\alpha a_- + a(s+j')]g_s = 0. \quad (8.63)$$

To obtain the values of the coefficients we consider the boundary conditions. The functions  $\vec{f}(r)$  and  $\vec{g}(r)$  must go to zero at  $r = 0$ , because the functions  $\vec{\phi}$  and  $\vec{\chi}$  would otherwise diverge there due to the  $r^{-1}$  term. This means that there is some smallest  $s$  below which the series does not continue. We call this  $s_0$ , and it has the property,

$$f_{s_0-1} = g_{s_0-1} = 0. \quad (8.64)$$

Plugging this into the equations (8.62), we find,

$$\begin{aligned}\alpha f_{s_0} + (s_0 + j')g_{s_0} &= 0 \\ \alpha g_{s_0} - (s_0 - j')f_{s_0} &= 0.\end{aligned}\tag{8.65}$$

Combining these equations we can write the value  $s_0$  in a very simple form,

$$s_0 = \sqrt{j'^2 - \alpha^2}.\tag{8.66}$$

This places a lower bound on the series. Note that this bound becomes imaginary if  $\alpha > j'$ . This will be discussed in more detail shortly.

The upper bound of the series is also useful. It can be shown that the series must terminate if the energy eigenvalue is to be less than  $m_e c^2$  [201]. The implication of this result is that if the series terminates at index  $s_1$  such that,

$$f_{s_1+1} = g_{s_1+1} = 0.\tag{8.67}$$

Then, using equations (8.62) and (8.63), we have,

$$\frac{s_1}{a} = \frac{1}{2} \left( \frac{1}{a_-} - \frac{1}{a_+} \right) \alpha = \frac{E}{\hbar c} \alpha,\tag{8.68}$$

where we have used the definitions of the coefficients  $a_{\pm}$  to expand them. Squaring this expression and expanding  $a$  using its definition, we get,

$$s_1^2 \left( m_e c^2 - \frac{E^2}{c^2} \right) = \alpha^2 \frac{E^2}{c^2}.\tag{8.69}$$

This can be solved for the energy eigenvalues,

$$E = \pm m_e c^2 \left( 1 + \frac{\alpha^2}{s_1^2} \right)^{-1/2}.\tag{8.70}$$

Note that the 'negative energy' solution corresponds to positron energy levels. From here forward, we drop the negative root and look only at the electron solution.

The two end points of the series, the indices  $s_0$  and  $s_1$  are separated by an integer number of steps. Calling this integer  $n'$  we can write,

$$s_1 = n' + s_0 = n' + \sqrt{j'^2 - \alpha^2}.\tag{8.71}$$

Plugging this into (8.70) gives a result for the energy eigenvalues in terms of only the two quantum numbers  $n'$  and  $j'$ ,

$$E_{n',j'} = m_e c^2 \left[ 1 + \frac{\alpha^2}{\left( n' + \sqrt{j'^2 - \alpha^2} \right)^2} \right]^{-1/2}.$$

This is the final result quoted for the energy eigenvalues of the hydrogenic atom by Dirac [201]. It turns out that later developments in the field [283, 288] prefer to use an equivalent set of quantum numbers that maps more closely to the familiar ones. The number  $j'$  is closely related to the total angular momentum quantum number  $j$ .  $j'$  has the range 1, 2, 3, while  $j$  has the range  $\frac{1}{2}$ ,  $\frac{3}{2}$ ,  $\frac{5}{2}$ . It is natural, and in fact correct, to make the identifications,

$$j' = j + \frac{1}{2},\tag{8.72}$$

and

$$n' = n - j' = n - j - \frac{1}{2}, \quad (8.73)$$

for the principal quantum number  $n$  [283]. Combining these two adjustments with equation (8.72), we get the *Sommerfeld fine-structure formula*,

$$E_{n,j} = m_e c^2 \left[ 1 + \frac{\alpha^2}{\left( n - j - \frac{1}{2} + \sqrt{\left( j + \frac{1}{2} \right)^2 - \alpha^2} \right)^2} \right]^{-1/2}, \quad (8.74)$$

with  $j = |\ell \pm \frac{1}{2}|$  and  $\ell = 0, 1, \dots$ . The derivation of the form of the actual wave functions  $\vec{\phi}(r)$  and  $\vec{\chi}(r)$  is very tedious [283] and will not be reproduced here.

The energy predicted by the Sommerfeld fine-structure formula (8.74) depends on two quantum numbers. The degeneracy of the orbital angular momentum  $\mathbf{j}$  is lifted, and the new quantum number besides the main quantum number  $n$  is that of the total angular momentum  $j$ . The intransparent expression can be expanded by  $\alpha$ ,

$$E_{n,j} \simeq m_e c^2 \left[ 1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{2n^3} \left( \frac{1}{j + 1/2} - \frac{3}{4n} \right) \right]. \quad (8.75)$$

The second term reproduces the energy of Bohr's model, but there are correction terms proportional to  $\alpha^4$ . We will show in Secs. 8.1.4, that the energy levels, called *fine structure*, result from several relativistic corrections of different origins.

In the expression (8.75) for the electron energy in the Coulomb potential, the last term is positive and proportional to  $1/n^4$ . It describes relaxation of the binding due to the contribution of weak components. The term containing the quantum number  $j$  is called the spin-orbit coupling. To better understand this contribution we must first analyze more deeply the matrices  $\vec{\sigma}$ .

### 8.1.3.3 Dirac's Hamiltonian in the sub-relativistic limit

Defining the energy  $E' = E - m_e c^2$ , the stationary Dirac equation (8.46) for an electron of charge  $q = -e$  in an external electrostatic potential  $U(\mathbf{r})$  can be written,

$$[E' - qU(\mathbf{r})]\vec{\phi} = c\vec{\sigma} \cdot \mathbf{p}\vec{\chi} \quad \text{and} \quad [E' - qU(\mathbf{r}) + 2m_e c^2]\vec{\chi} = c\vec{\sigma} \cdot \mathbf{p}\vec{\phi}. \quad (8.76)$$

resolving the second equation for the wavefunction  $\vec{\chi}$  and substituting it into the first,

$$E'\vec{\phi} = qU(\mathbf{r})\vec{\phi} + \vec{\sigma} \cdot \mathbf{p} \frac{1}{2m_e} \left( 1 + \frac{E' - qU(\mathbf{r})}{2m_e c^2} \right)^{-1} \vec{\sigma} \cdot \mathbf{p}\vec{\phi}. \quad (8.77)$$

In the non-relativistic limit,

$$E' - qU \simeq \frac{\mathbf{p}^2}{2m_e} \ll m_e c^2, \quad (8.78)$$

we get by Taylor expansion of the second term in the bracket,

$$E'\vec{\phi} \simeq qU(\mathbf{r})\vec{\phi} + \vec{\sigma} \cdot \mathbf{p} \frac{1}{2m_e} \left( 1 - \frac{E' - qU(\mathbf{r})}{2m_e c^2} \right) \vec{\sigma} \cdot \mathbf{p}\vec{\phi}. \quad (8.79)$$

Now,  $\vec{\sigma} \cdot \mathbf{p}$  is an operator entity, which acts on the subsequent operators and wavefunctions. We thus have to apply the product rule,  $(\vec{\sigma} \cdot \mathbf{p})V\psi = V(\vec{\sigma} \cdot \mathbf{p})\psi + [(\vec{\sigma} \cdot \mathbf{p})V]\psi$ , to the first occurrence of operator this operator in equation (8.77),

$$E'\vec{\phi} \simeq qU(\mathbf{r})\vec{\phi} + \frac{1}{2m_e} \left(1 - \frac{E' - qU(\mathbf{r})}{2m_e c^2}\right) (\vec{\sigma} \cdot \mathbf{p})^2 \vec{\phi} + \frac{q}{4m_e^2 c^2} [(\vec{\sigma} \cdot \mathbf{p})U(\mathbf{r})](\vec{\sigma} \cdot \mathbf{p})\vec{\phi}. \quad (8.80)$$

In the following we will make use of a general relationship which is similar to (8.51),

$$(\vec{\sigma} \cdot \mathbf{B})(\vec{\sigma} \cdot \mathbf{C}) = (\mathbf{B} \cdot \mathbf{C}) + i\vec{\sigma} \cdot (\mathbf{B} \times \mathbf{C}). \quad (8.81)$$

It holds for  $[\vec{\sigma}, \mathbf{B}] = 0 = [\vec{\sigma}, \mathbf{C}]$  and will be demonstrated in Exc. 8.1.5.4. The relationship yields,

$$(\vec{\sigma} \cdot \mathbf{p})^2 = \mathbf{p}^2 \quad \text{and} \quad [(\vec{\sigma} \cdot \mathbf{p})U(\mathbf{r})](\vec{\sigma} \cdot \mathbf{p}) = \mathbf{p}U(\mathbf{r}) \cdot \mathbf{p} + i\vec{\sigma} \cdot [\mathbf{p}U(\mathbf{r}) \times \mathbf{p}], \quad (8.82)$$

so that expressing the momentum operator by  $\mathbf{p} = -i\hbar\nabla$  wherever it acts on the potential,

$$E'\vec{\phi} \simeq qU(\mathbf{r})\vec{\phi} + \frac{1}{2m_e} \left(1 - \frac{E' - qU(\mathbf{r})}{2m_e c^2}\right) \mathbf{p}^2 \vec{\phi} - \frac{\hbar^2 q}{4m_e^2 c^2} \nabla U(\mathbf{r}) \cdot \nabla \vec{\phi} + \frac{\hbar}{4m_e^2 c^2} \vec{\sigma} \cdot [\nabla U(\mathbf{r}) \times \mathbf{p}]\vec{\phi}. \quad (8.83)$$

Also, with  $U(\mathbf{r}) = U(r)$ ,

$$\nabla U(r) = \frac{\partial U}{\partial r} \nabla r = \frac{\partial U}{\partial r} \frac{\mathbf{r}}{r} \quad \text{and} \quad \nabla U(r) \cdot \nabla = \frac{\partial U}{\partial r} \hat{\mathbf{e}}_r \cdot \nabla = \frac{\partial U}{\partial r} \frac{\partial}{\partial r}. \quad (8.84)$$

We get,

$$\begin{aligned} E'\vec{\phi} &= qU(\mathbf{r})\vec{\phi} + \frac{1}{2m_e} \left(1 - \frac{E' - qU(\mathbf{r})}{2m_e c^2}\right) \mathbf{p}^2 \vec{\phi} - \frac{\hbar^2}{4m_e^2 c^2} \frac{\partial qU}{\partial r} \frac{\partial}{\partial r} \vec{\phi} + \frac{\hbar q}{4m_e^2 c^2} \vec{\sigma} \cdot \left[ \frac{1}{r} \frac{\partial U}{\partial r} \mathbf{r} \times \mathbf{p} \vec{\phi} \right] \\ &\simeq \left( \frac{\mathbf{p}^2}{2m_e} + qU(r) - \frac{\mathbf{p}^4}{8m_e^3 c^2} + \frac{q}{2m_e^2 c^2} \frac{1}{r} \frac{\partial U}{\partial r} \mathbf{s} \cdot \mathbf{l} - \frac{\hbar^2 q}{4m_e^2 c^2} \frac{\partial U}{\partial r} \frac{\partial}{\partial r} \right) \vec{\phi}. \end{aligned} \quad (8.85)$$

where we again applied the non-relativistic approximation (8.78) in the second line and made use of the definitions  $\mathbf{s} = \frac{\hbar}{2}\vec{\sigma}$  and  $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ . The term in the bracket can be used as the Hamiltonian allowing to calculate the fine structure as first-order perturbations to the non-relativistic energy levels obtained from non-relativistic theory,

$$\hat{H} \simeq \frac{\mathbf{p}^2}{2m_e} - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} - \frac{\mathbf{p}^4}{8m_e^3 c^2} - \frac{e}{2m_e^2 c^2} \frac{1}{r} \frac{\partial U}{\partial r} \mathbf{s} \cdot \mathbf{l} - \frac{\hbar^2 e}{4m_e^2 c^2} \frac{\partial U}{\partial r} \frac{\partial}{\partial r}. \quad (8.86)$$

The first two terms are those arising from Bohr's atom model, the third one is a correction due to the relativistic velocity of the electron, the fourth comes from the electron's spin-orbit coupling, and the fifth is called the Darwin term. All contributions represent perturbations to the non-relativistic Schrödinger theory of Bohr's atom and will be discussed extensively in Secs. 8.2. We will show in 8.1.5.6 that  $\hat{\mathbf{I}}^2$ ,  $\hat{\mathbf{s}}^2$ , and  $\hat{\mathbf{j}}^2$  are constants of motion of the above Hamiltonian.

### 8.1.4 The Pauli equation

When we calculated the electron's energy in the Coulomb potential (8.86), we only considered the electrostatic potential of the nucleus, letting the potential vector  $\mathbf{A}$  be zero. As long as we do not apply an external magnetic field this is correct, because the internal magnetism of the atom is already completely enclosed in the Dirac equation. On the other hand, we know that the atom contains moving charges, that is, currents which generate magnetic fields<sup>8</sup>. Furthermore, the spins of the electron and of the proton produce magnetic moments, which ought to interact with the magnetic fields. Hence, the existence of magnetic effects in an atom is to be expected.

These magnetic effects can be discussed in a more transparent way applying a Schrödinger-like equation with minimal coupling to electromagnetic fields (8.44) to a two-component spinor  $\vec{\phi}$ . This Schrödinger-like equation can be obtained from Dirac's equation (8.76) via a stronger non-relativistic approximation, which consists in completely neglecting the weak component  $[E' - qU(\mathbf{r})]\vec{\chi}$ . On the other hand, we allow for the existence of magnetic fields via the substitution  $\mathbf{p} \rightarrow \vec{\pi}$ . The equation for the strong component (8.77) then becomes,

$$E'\vec{\phi} = qU(\mathbf{r})\vec{\phi} + \frac{(\vec{\sigma} \cdot \vec{\pi})^2}{2m_e}\vec{\phi}. \quad (8.87)$$

We can again apply the formula (8.81) to calculate,

$$\begin{aligned} (\vec{\sigma} \cdot \vec{\pi})^2\psi &= \vec{\pi}^2\psi + i\vec{\sigma} \cdot (\vec{\pi} \times \vec{\pi})\psi = \vec{\pi}^2\psi + iq\vec{\sigma} \cdot [-\mathbf{p} \times \mathbf{A}(\mathbf{r}) - \mathbf{A}(\mathbf{r}) \times \mathbf{p}]\psi \\ &= \vec{\pi}^2\psi - \hbar q\vec{\sigma} \cdot \{\nabla \times [\mathbf{A}(\mathbf{r})\psi] + \mathbf{A}(\mathbf{r}) \times \nabla\psi\} \\ &= \vec{\pi}^2\psi - \hbar q\vec{\sigma} \cdot [\nabla \times \mathbf{A}(\mathbf{r})]\psi = [\mathbf{p} - q\mathbf{A}(\mathbf{r})]^2\psi - \hbar q\vec{\sigma} \cdot \vec{\mathcal{B}}(\mathbf{r})\psi. \end{aligned} \quad (8.88)$$

In the case of an electron ( $e = -q$ ) we obtain the so-called *Pauli equation*,

$$E'\vec{\phi} = \left[ \frac{1}{2m_e} (-i\hbar\nabla + e\mathbf{A})^2 + \frac{e\hbar}{2m_e}\vec{\sigma} \cdot \vec{\mathcal{B}} - eU(\mathbf{r}) \right] \vec{\phi}, \quad (8.89)$$

which corresponds to a Schrödinger-like equation for a two-component spinor  $\vec{\phi}$  with the Hamiltonian,

$$\hat{H} \simeq \frac{\mathbf{p}^2}{2m_e} - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} - \frac{i\hbar e}{2m_e} (\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla) + \frac{e}{m_e} \mathbf{s} \cdot \vec{\mathcal{B}}, \quad (8.90)$$

neglecting terms in  $\mathbf{A}^2$ . Note however, that the kinetic energy is calculated with the *momentum projected onto the spin*,  $\vec{\sigma} \cdot \vec{\pi}$ . The third term can be simplified within the Coulomb gauge  $\nabla \cdot \mathbf{A} = 0$  yielding,

$$\hat{H}_{int} = \frac{e}{m_e} (\mathbf{A} \cdot \mathbf{p}). \quad (8.91)$$

The Pauli equation serves for a classical (non-relativistic) approach to the electron's spin-orbit coupling, as we will see below and in the discussion of the fine structure in Sec. 8.2.2.

<sup>8</sup>The spin of the electron does not generate a magnetic field, in contrast to the angular momentum caused by its *orbital motion*. It only interacts with the environment through the requirement of symmetrization for being a fermion.

### 8.1.4.1 Dipole moment of the orbital angular momentum

The rotational motion of a charge,  $-e$ , creates a current  $I$ , corresponding to a current density,

$$\mathbf{j}(\mathbf{r}') = I \hat{\mathbf{e}}_\phi \delta(r - r') \delta(z') = -e \frac{\mathbf{v}}{2\pi r} \delta(r - r') \delta(z'). \quad (8.92)$$

Hence, the dipole moment caused by the circular motion of an electron is,

$$\begin{aligned} \vec{\mu}_\ell &= \frac{1}{2} \int_V \mathbf{r} \times \mathbf{j}(\mathbf{r}') d^3 r' \\ &= \frac{1}{4\pi} \mathbf{r} \times \int_0^{2\pi} d\phi' \int_{-\infty}^{\infty} dz' \int_0^{\infty} r' dr' \frac{-e\mathbf{v}}{r} \delta(r - r') \delta(z') = \frac{-1}{2} e \mathbf{r} \times \mathbf{v} = \frac{-e}{2m_e} \mathbf{l}, \end{aligned} \quad (8.93)$$

with the angular momentum  $\mathbf{l} = \mathbf{r} \times m_e \mathbf{v}$ . The quotient  $\gamma_e \equiv -e/2m_e$  is called *gyromagnetic ratio* of the electron. We often use the *Bohr magneton*,  $\mu_B \equiv \hbar e/2m_e$ , which represents the elementary unit of spin,

$$\boxed{\frac{\vec{\mu}_\ell}{\mu_B} = -g_l \frac{\mathbf{l}}{\hbar}}. \quad (8.94)$$

The *g-factor* of a system having any angular momentum  $\mathbf{l}$  is defined as a proportionality constant between the normalized dipole moment and the normalized angular momentum.  $g_\ell \equiv \frac{\mu_\ell}{\ell \mu_B} = 1$  takes into account possible corrections between our classical derivation and quantum mechanics.

### 8.1.4.2 Pauli's model of spin-orbit coupling

The aim of this section is to demonstrate the relationship between the spin-orbit coupling term in Dirac's Hamiltonian (8.86) and the spin-magnetic field coupling term in Pauli's Hamiltonian (8.90).

A comparison of Pauli's expression with the energy of a magnetic moment in the field  $\vec{\mathcal{B}}$ ,

$$\hat{H}_{\ell s} = -\vec{\mu}_s \cdot \vec{\mathcal{B}}, \quad (8.95)$$

suggests the following connection between the spin and the magnetic moment:

$$-\vec{\mu}_s \cdot \vec{\mathcal{B}} = \frac{e\hbar}{2m_e} \vec{\sigma} \cdot \vec{\mathcal{B}} = \frac{e}{m_e} \mathbf{s} \cdot \vec{\mathcal{B}}. \quad (8.96)$$

We conclude, that the electron carries, besides mass, charge and spin, also a magnetic dipole moment,

$$\boxed{\frac{\vec{\mu}_s}{\mu_B} = -\frac{e}{m_e} \mathbf{s} = -2 \frac{\mathbf{s}}{\hbar}}, \quad (8.97)$$

For the *g-factor* of the electron, we obtain  $g_e = 2$ <sup>9</sup>. Neutron and proton are also fermions with spin  $\frac{1}{2}$ , but they do not obey the Dirac equation! Their *g-factors* are

<sup>9</sup>The exact value is  $g_e \equiv \frac{\mu_s}{s \mu_B} = 2.002319314\dots$ . The deviation  $g_e - 2 \simeq \frac{\alpha}{\pi} - 0.164 \frac{\alpha^2}{\pi^2}$  is due to the coupling of the spin to the fluctuations of the electromagnetic vacuum. We need to use quantum electro-dynamical methods to calculate the corrections.

$g_{proton} = 5.5858$  and  $g_{neutron} = -3.8261$ . The large deviation from  $g = 2$  points to the existence of an internal structure.

The rapid motion of the electron within the electrostatic field  $\vec{\mathcal{E}}$  of the nucleus produces, following the theory of relativity, in the electron's reference frame a magnetic field  $\vec{\mathcal{B}}'$  with which the electronic spin can interact. As we will show in Exc. 8.1.5.7, the field seen by the electron can be approximated in first order in  $v/c$  by,

$$\vec{\mathcal{B}}' \simeq \frac{\mathbf{v}}{c^2} \times \vec{\mathcal{E}}. \quad (8.98)$$

With this the interaction energy (8.95) becomes,

$$\begin{aligned} \hat{H}_{\ell s} &= -\vec{\mu}_s \cdot \vec{\mathcal{B}}' = \frac{e}{m_e c^2} \mathbf{s} \cdot (\mathbf{v} \times \vec{\mathcal{E}}) = -\frac{e}{m_e^2 c^2} \mathbf{s} \cdot (\mathbf{p} \times \nabla U) \\ &= -\frac{e}{m_e^2 c^2} \mathbf{s} \cdot \left( \mathbf{p} \times \frac{\mathbf{r}}{r} \frac{\partial U}{\partial r} \right) = -\frac{1}{m_e^2 c^2 r} \mathbf{s} \cdot \mathbf{l} \frac{\partial V(r)}{\partial r}, \end{aligned} \quad (8.99)$$

with  $V(r) = -eU(r)$ .

The resulting interaction energy coincides, apart from a factor  $\frac{1}{2}$  [679], with the one obtained in the from Dirac's equation (8.86). The deviation, called *Thomas factor*, is due to the necessity to transform back into the inertial system of the nucleus. This transformation, called *Thomas precession*, must be done by a Lorentz transformation, which is not trivial with electron continuously changing its propagation direction on its circular orbit. The transformation introduces the additional factor of  $\frac{1}{2}$ <sup>10</sup>.

## 8.1.5 Exercises

### 8.1.5.1 Ex: Yukawa potential

Show, that Yukawa's potential satisfies the Klein-Gordon equation.

### 8.1.5.2 Ex: Zitterbewegung

Zitterbewegung is a hypothetical rapid motion of elementary particles, in particular electrons, that obey the Dirac equation. The existence of such motion was first proposed by Erwin Schrödinger in 1930 as a result of his analysis of the wave packet solutions of the Dirac equation for relativistic electrons in free space, in which an interference between positive and negative energy states produces what appears to be a fluctuation (at the speed of light) of the position of an electron around the median, with a frequency of  $2m_e c^2/\hbar$ , or approximately  $1.6 \cdot 10^{21}$  rad/s. For the hydrogen atom, the Zitterbewegung produces the Darwin term which plays the role in the fine structure as a small correction of the energy level of the  $s$ -orbitals.

Use the Heisenberg equation to derive, from Dirac's Hamiltonian, equations of motion for the position operator  $\hat{\mathbf{r}}$  and the 'velocity operator'  $\hat{\vec{\alpha}}$ . Solve the equation of motion and identify the Zitterbewegung.

Zitterbewegung of a free relativistic particle has never been observed experimentally. However, it has been simulated twice. First, with a trapped ion, by putting it in

<sup>10</sup>This is a kinematic effect in space-time: the Lorentz transformations for systems moving with non-collinear velocities can not simply be concatenated, but must be rotated, too [251, 361].

an environment such that the non-relativistic Schrödinger equation for the ion has the same mathematical form as the Dirac equation (although the physical situation is different) [263]. Then, in 2013, it was simulated in a setup with Bose-Einstein condensates [426].

### 8.1.5.3 Ex: Constants of motion of Dirac's Hamiltonian 1

Show that  $\hat{L}_z$  with  $\hat{\mathbf{L}} \equiv \mathbf{r} \times \hat{\mathbf{p}}$  and  $\hat{S}_z$  with  $\hat{\mathbf{S}} \equiv \frac{\hbar}{2}\gamma_5\vec{\alpha}$  defining  $\gamma_5 \equiv -i\alpha_1\alpha_2\alpha_3$  are not constants of motions, but  $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ , that is,

$$[\hat{H}, \hat{J}_z] = [\hat{H}, \hat{L}_z + \hat{S}_z] = 0 . \quad (8.100)$$

### 8.1.5.4 Ex: Calculating with Dirac matrices

a. Prove that, if  $[\mathbf{B}, \vec{\sigma}] = 0 = [\mathbf{C}, \vec{\sigma}]$  where  $\vec{\sigma}$  are the Pauli matrices, then,

$$(\vec{\sigma} \cdot \mathbf{B})(\vec{\sigma} \cdot \mathbf{C}) = \mathbf{B} \cdot \mathbf{C} + i\vec{\sigma} \cdot (\mathbf{B} \times \mathbf{C}) . \quad (8.101)$$

b. Prove that, if  $[\mathbf{B}, \vec{\alpha}] = 0 = [\mathbf{C}, \vec{\alpha}]$  where  $\vec{\alpha}$  are the Dirac matrices, then,

$$(\vec{\alpha} \cdot \mathbf{B})(\vec{\alpha} \cdot \mathbf{C}) = \mathbf{B} \cdot \mathbf{C} + i\gamma_5\vec{\alpha} \cdot (\mathbf{B} \times \mathbf{C}) . \quad (8.102)$$

c. Show that the spin defined as,

$$\mathbf{S} = \frac{\hbar}{2}\vec{\zeta} \quad \text{where} \quad \vec{\zeta} \equiv \gamma_5\vec{\alpha} = \mathbb{I} \otimes \vec{\sigma} \quad (8.103)$$

obeys different commutation rules than the Dirac matrices.

d. Conclude that,

$$(\vec{\zeta} \cdot \mathbf{B})(\vec{\zeta} \cdot \mathbf{C}) = \mathbf{B} \cdot \mathbf{C} + i\vec{\zeta} \cdot (\mathbf{B} \times \mathbf{C}) . \quad (8.104)$$

### 8.1.5.5 Ex: Constants of motion of Dirac's Hamiltonian 2

In this exercise we will prove the relationships (8.56):

a. Prove,

$$(\hbar j')^2 = \mathbf{J}^2 + \frac{\hbar^2}{4} . \quad (8.105)$$

b. Prove,

$$[\hbar j', \hat{H}]_- = 0 . \quad (8.106)$$

c. Prove,

$$\mathbf{r} \cdot \mathbf{p} = -i\hbar r \frac{\partial}{\partial r} . \quad (8.107)$$

d. Prove,

$$[\varepsilon, \hat{H}]_- = 0 . \quad (8.108)$$



**8.1.5.6 Ex: Constants of motion in the  $\mathbf{L} \cdot \mathbf{S}$ -coupling**

Consider a particle of mass  $\mu$  described by the Hamiltonian  $\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 + V(r) + \xi(r)\mathbf{L} \cdot \mathbf{S}$ , being  $V(r)$  a central potential,  $\mathbf{L}$  and  $\mathbf{S}$  its orbital angular momentum and spin.

- Obtain the commutation relations  $[\mathbf{L}, \hat{H}]$ ,  $[\mathbf{S}, \hat{H}]$  and  $[\mathbf{L} + \mathbf{S}, \hat{H}]$  for the cases without and with spin-orbit interaction  $\xi(r)\mathbf{L} \cdot \mathbf{S}$  introduced by relativistic corrections.
- Calculate  $[\mathbf{L}^2, \hat{H}]$ ,  $[\mathbf{S}^2, \hat{H}]$  and  $[\mathbf{J}^2, \hat{H}]$ .

**8.1.5.7 Ex: Magnetic field generated by the orbiting proton at the location of the electron**

Calculate the magnetic field generated by the orbiting proton as it is perceived by the electron.

**8.2 Fine structure of hydrogen-like atoms via TIPT**

The wave equation that simultaneously satisfies the requirements of quantum mechanics and special relativity is the *Dirac equation*. In free space including electromagnetic interactions it describes all massive particles of semi-integer spin with parity as a symmetry, such as electrons and quarks. It was the first theory to fully explain special relativity in the context of quantum mechanics. The Dirac equation describes the fine structure of the hydrogen spectrum in a completely rigorous manner. The equation also implied the existence of a new form of matter, antimatter, previously unsuspected and unobserved. The equation also justifies a posteriori the introduction of spinors, that is, of the vector wavefunctions introduced by Pauli in a heuristic way. We have seen in the last section that, in the limit of high but non-relativistic velocities, the Dirac equation adopts the form of a Schrödinger equation with the modified Hamiltonian (8.86),

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{H}_{rl} + \hat{H}_{\ell s} + \hat{H}_{dw} + \hat{H}_{lamb} \\ &= \left( \frac{p^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0 r} \right) - \frac{p^4}{8m_e^3 c^2} + \frac{1}{2m_e^2 c^2} \frac{1}{r} \frac{dV}{dr} \mathbf{l} \cdot \mathbf{s} + \frac{\pi\hbar^2}{2m_e^2 c^2} \frac{Ze^2}{4\pi\epsilon_0} \delta^3(\mathbf{r}) + \hat{H}_{lamb} . \end{aligned} \quad (8.109)$$

We will discuss the various terms in the following sections. Note that the expression for the Darwin term differs from that of (8.86). We will see in Exc. 8.2.6.1, that they are, in fact, equivalent.

**8.2.1 Correction for relativistic velocities**

The first correction in the expression,  $\hat{H}_{rl}$  in Eq. (8.109), comes from the expansion of the relativistic energy for small velocities up to second order,

$$E_{kin} = \sqrt{p^2 c^2 + m_e^2 c^4} \simeq m_e c^2 + \frac{p^2}{2m_e} - \frac{p^4}{8m_e^3 c^2} + \dots \quad (8.110)$$

The correction is of the order of magnitude,

$$\frac{H_{rl}}{H_0} = \frac{\frac{p^4}{8m_e^3c^2}}{\frac{p^2}{2m_e}} = \frac{v^2}{4c^2} \simeq \frac{\alpha^2}{4} \approx 0.01\% . \quad (8.111)$$

Due to the degeneracy of these states, it would be appropriate to use perturbation theory with degenerate states. However, as  $\hat{H}_{rl}$  only depends on spatial coordinates commuting with  $\mathbf{l}$  and  $\mathbf{s}$ , the degeneracy is not very important, since  $\hat{H}_{rl}$  is already diagonal in the base  $|n, \ell, m\rangle$ , that is,  $\langle n, \ell, m | n', \ell', m' \rangle = \delta_{\ell\ell'} \delta_{mm'}$ . Starting from,

$$\begin{aligned} \hat{H}_{rl} &= -\frac{p^4}{8m_e^3c^2} = -\frac{1}{2m_e c^2} \left( \frac{p^2}{2m_e} \right)^2 = -\frac{1}{2m_e c^2} \left( \hat{H}_0 + \frac{Ze^2}{4\pi\epsilon_0 r} \right)^2 \\ &= -\frac{1}{2m_e c^2} \left( \hat{H}_0 - \frac{2E_n n^2}{\tilde{r}} \right)^2 , \end{aligned} \quad (8.112)$$

with  $\tilde{r} \equiv \frac{Zr}{a_B}$  and using as an abbreviation the energies of hydrogen following Bohr's model,

$$E_n = \langle n, \ell | \hat{H}_0 | n, \ell \rangle = -\frac{Z^2 e^2}{4\pi\epsilon_0} \frac{1}{2a_B n^2} = -\frac{m_e c^2}{2} \frac{Z^2 \alpha^2}{n^2} . \quad (8.113)$$

We have

$$\begin{aligned} \Delta E_{rl} &= \langle n, \ell | \hat{H}_{rl} | n, \ell \rangle \\ &= -\frac{1}{2m_e c^2} \left[ \langle n, \ell | \hat{H}_0^2 | n, \ell \rangle - \langle n, \ell | \frac{4E_n n}{\tilde{r}} \hat{H}_0 | n, \ell \rangle + \langle n, \ell | \left( \frac{2E_n n}{\tilde{r}} \right)^2 | n, \ell \rangle \right] \\ &= \frac{Z^2 \alpha^2}{4E_n n^2} \left[ E_n^2 - 4E_n^2 n^2 \frac{1}{n^2} + 4E_n^2 n^4 \frac{1}{n^3(\ell + \frac{1}{2})} \right] , \end{aligned} \quad (8.114)$$

using the eigenvalues calculated in (4.53). Finally, we obtain the following relativistic correction,

$$\Delta E_{rl} = E_n (Z\alpha)^2 \left[ \frac{1}{n(\ell + \frac{1}{2})} - \frac{3}{4n^2} \right] . \quad (8.115)$$

Obviously, the degeneracy with respect to the angular momentum  $\ell$  is lifted by this correction.

### 8.2.2 Correction due to spin-orbit coupling

The second correction,  $\hat{H}_{\ell s}$  in the expression (8.109), called *spin-orbit interaction*, is a relativistic correction due to the fact that the electron moves rapidly within the electrostatic field  $\vec{\mathcal{E}}$  generated by the nucleus. Considering the fundamental orbit and the fact that the angular momenta are of the order of  $\hbar$  we can estimate the importance of this effect,

$$\frac{H_{\ell s}}{H_0} = \frac{\frac{1}{2m_e^2 c^2} \frac{1}{r} \frac{e^2}{4\pi\epsilon_0 r^2} \mathbf{l} \cdot \mathbf{s}}{\frac{p^2}{2m_e}} \simeq \frac{\frac{1}{2m_e^2 c^2} \frac{e^2}{4\pi\epsilon_0} \frac{1}{a_B^3} \hbar^2}{\frac{e^2}{4\pi\epsilon_0 a_B}} = \frac{1}{2m_e^2 c^2} \frac{\hbar^2}{a_B^2} = \frac{\alpha^2}{2} \approx 0.01\% . \quad (8.116)$$

**Example 45 (Classical derivation of the spin-orbit interaction):** In the following, we will derive the expression from classical arguments borrowed from electrodynamic theory. Seen from the rest system of the electron being at position  $\mathbf{x} = 0$ , it is the proton that orbits around the electron. This orbit creates a current,  $-\mathbf{j}(\mathbf{r}')$ , which generates a magnetic field. Following the *Biot-Savart's law* the potential vector and the amplitude of the field are,

$$\mathbf{A}(\mathbf{x}) = \frac{\mu_0}{4\pi} \int_V \frac{-\mathbf{j}(\mathbf{r}') d^3 r'}{|\mathbf{x} - \mathbf{r}'|}, \quad (8.117)$$

respectively,

$$\begin{aligned} \vec{\mathbf{B}}(\mathbf{x}) &= \nabla_x \times \mathbf{A}(\mathbf{x}) = \frac{\mu_0}{4\pi} \int_V \frac{(\mathbf{x} - \mathbf{r}') \times \mathbf{j}(\mathbf{r}')}{|\mathbf{x} - \mathbf{r}'|^3} d^3 r' \\ &= -\frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} dz' \int_0^{\infty} r' dr' \int_0^{2\pi} d\phi \frac{(\mathbf{x} - \mathbf{r}') \times \mathbf{v}}{|\mathbf{x} - \mathbf{r}'|^3} \frac{Ze}{2\pi r} \delta(r - r') \delta(z') \\ &= \frac{Ze\mu_0}{4\pi} \frac{(\mathbf{x} - \mathbf{r}) \times \mathbf{v}}{|\mathbf{x} - \mathbf{r}|^3}, \end{aligned} \quad (8.118)$$

where we replaced the expression for the current density (8.92). With the expression for the *Coulomb potential* between the electron and the proton and its radial derivative,

$$V(r) = \frac{-Ze^2}{4\pi\epsilon_0 r}, \quad \frac{1}{r} \frac{dV(r)}{dr} = \frac{Ze^2}{4\pi\epsilon_0 r^3}, \quad (8.119)$$

we have at the position of the electron,

$$\begin{aligned} \vec{\mathbf{B}}(\mathbf{0}) &= \frac{Ze\mu_0}{4\pi} \frac{-\mathbf{r} \times \mathbf{v}}{r^3} = -\frac{\epsilon_0\mu_0}{e} \frac{\mathbf{r} \times \mathbf{v}}{r} \frac{dV(r)}{dr} \\ &= -\frac{1}{ec^2} \frac{\mathbf{r} \times \mathbf{v}}{r} \frac{dV(r)}{dr} = -\frac{1}{em_e c^2 r} \frac{dV(r)}{dr} \mathbf{l}. \end{aligned} \quad (8.120)$$

The advantage of introducing the potential  $V$  is, that this expression also holds for more complicated atoms with many electrons, where the potential may deviate considerably from the Coulombian potential. Note, that the magnetic field is very strong,  $B \simeq \xi(a_B)\hbar/\mu_B \approx 5$  T. Inserting the magnetic field into Pauli's expression (8.95) together with the magnetic moment of the spin (8.97),

$$\hat{H}_{\ell s} = -\vec{\mu}_s \cdot \vec{\mathbf{B}}(\mathbf{0}) = \frac{1}{m_e^2 c^2} \mathbf{s} \cdot \mathbf{l} \frac{1}{r} \frac{dV(r)}{dr}. \quad (8.121)$$

where we still have to apply the corrective *Thomas factor* of  $\frac{1}{2}$ .

The interaction operator can be written,

$$\hat{H}_{\ell s} = \xi(r) \mathbf{l} \cdot \mathbf{s}, \quad (8.122)$$

with the abbreviation,

$$\xi(r) \equiv \frac{-1}{2m_e^2 c^2 r} \frac{dV}{dr} = -\frac{Ze^2}{8\pi\epsilon_0 m_e^2 c^2} \frac{1}{r^3} = \frac{E_n Z^2 \alpha^2 n^2}{\hbar^2} \frac{1}{\tilde{r}^3}, \quad (8.123)$$

with  $\tilde{r} \equiv Zr/a_B$  and using the formulas (4.53).

After the introduction of the spin, the Hilbert space of the particles' wavefunctions must be extended. The wavefunctions are now products of spatial wavefunctions and spin eigenvectors:

$$|n, \ell, m_\ell, m_s\rangle = R_{n\ell}(r)Y_{\ell m}(\theta, \phi) \begin{pmatrix} s_1 \\ s_2 \end{pmatrix}. \quad (8.124)$$

The new Hilbert space is the tensorial product of position space and spin space. The *radial* Hamiltonian for the hydrogen atom including the centrifugal term and the spin-orbit coupling now takes the form:

$$\hat{H} = \frac{p^2}{2m} + V(r) + \frac{\mathbf{I}^2}{2m_e r^2} + \xi(r)\mathbf{l} \cdot \mathbf{s}. \quad (8.125)$$

We may again consider the energy term  $V_{\ell s}$  as a small perturbation, and calculate it using unperturbed wavefunctions,

$$\Delta E_{\ell s} = \langle n, \ell, s, m_\ell, m_s | V_{\ell s} | n, \ell, s, m_\ell, m_s \rangle = \langle n, \ell | \xi(r) | n, \ell \rangle \langle \ell, s, m_\ell, m_s | \mathbf{s} \cdot \mathbf{l} | \ell, s, m_\ell, m_s \rangle. \quad (8.126)$$

Assuming a Coulombian potential, we first look at the radial part (8.123), which can easily be calculated using the formulae (4.53),

$$\langle n, \ell | \xi(r) | n, \ell \rangle = \frac{E_n Z^2 \alpha^2 n^2}{\hbar^2} \frac{1}{n^3 \ell (\ell + \frac{1}{2})(\ell + 1)}. \quad (8.127)$$

To diagonalize the angular part of the Hamiltonian, we need the common wavefunctions of  $\mathbf{I}^2$  and  $\mathbf{l} \cdot \mathbf{s}$ . We can rewrite the coupling term as:

$$\mathbf{l} \cdot \mathbf{s} = \frac{1}{2}(\mathbf{j}^2 - \mathbf{l}^2 - \mathbf{s}^2). \quad (8.128)$$

In the common eigensystem of  $\mathbf{j}^2$ ,  $\mathbf{l}^2$ , and  $\mathbf{s}^2$  the Hamiltonian, therefore, is diagonal. We know the basis of this system from the theory of the addition of angular momenta. The states of the basis are linear combinations of the functions  $|n, \ell, m_\ell, m_s\rangle$ . Since the spins precess around each other,  $\ell_z$  and  $s_z$  are not good observables, the non-coupled base is not appropriate. But  $\mathbf{s}^2$ ,  $\mathbf{l}^2$ , and  $\mathbf{j}^2$  are good observables. In the coupled basis  $\{n, (\ell, s)j, m_j\}$ ,

$$\langle n, (\ell, s)j, m_j | \mathbf{s} \cdot \mathbf{l} | n, (\ell, s)j, m_j \rangle = \frac{\hbar^2}{2} [j(j+1) - \ell(\ell+1) - s(s+1)]. \quad (8.129)$$

Since  $j = \ell \pm 1/2$ , we find that every level splits into two levels, one with the energy  $E_{n\ell} + \ell\zeta_{n\ell}$  and the degeneracy  $2\ell+2$  and the other with the degeneracy  $E_{n\ell} - (\ell+1)\zeta_{n\ell}$  with the degeneracy  $2\ell$ , where we introduced the abbreviation,

$$\zeta_{n\ell} \equiv \frac{\hbar^2}{2} \langle \xi(r) \rangle. \quad (8.130)$$

All in all, we get an energy correction due to the spin-orbit interaction of,

$$\Delta E_{\ell s} = -E_n (Z\alpha)^2 \frac{j(j+1) - \ell(\ell+1) - \frac{3}{4}}{2n\ell(\ell+1/2)(\ell+1)}. \quad (8.131)$$

Note, that the coupling  $\mathbf{l} \cdot \mathbf{s}$  lifts the degeneracy with respect to  $\mathbf{l}$ , but not with respect to  $\ell_z$  (see Fig. 8.1). As we have already seen in Exc. 8.1.5.6, in the presence of an energy associated with the coupling  $\mathbf{l} \cdot \mathbf{s}$ , only the total angular momentum  $\mathbf{l} + \mathbf{s}$  is a constant of motion.

### 8.2.3 Non-local electron-core interaction

Let us now discuss the third correction in the expression (8.109). The electron-nucleus interaction that we have considered so far is *local*, that is, the interaction at the point  $\mathbf{r}$  sensed by the electron depends essentially on the field at that point in space. However, when relativistic theory is correctly applied, the electron-nucleus interaction becomes *non-local*, and the electron is then affected by all values of the nuclear field in a region around  $\mathbf{r}$ <sup>11</sup>. The size of this region is of the order of the *Compton wavelength* of the electron,  $\lambda_C/2\pi \equiv \hbar/m_e c$ . This correction was introduced by *Sir Charles Galton Darwin* through a substitution in the Dirac equation that solved the problem of normalization of the wavefunction.

Imagine that instead of the potential  $V(\mathbf{r})$ , the potential of the electron is given by the integral,

$$\int f(r')V(\mathbf{r} + \mathbf{r}')d^3r' , \quad (8.132)$$

where  $f(r')$  is a radially symmetric and normalized density-type function that takes significant values only in the vicinity of  $\mathbf{r}$  within a volume  $(\lambda_C/2\pi)^3$  centered at  $\mathbf{r}' = 0$ . Expanding the potential  $V(\mathbf{r} + \mathbf{r}')$  near the origin,

$$V(\mathbf{r} + \mathbf{r}') = V(\mathbf{r}) + [\mathbf{r}' \cdot \nabla_r]V(\mathbf{r}) + \frac{1}{2!}[\mathbf{r}' \cdot \nabla_r]^2V(\mathbf{r}) + \dots , \quad (8.133)$$

and inserting into the integral,

$$\begin{aligned} & \int f(r')V(\mathbf{r} + \mathbf{r}')d^3r' \\ &= V(\mathbf{r}) \int f(r')d^3r' + \int \mathbf{r}' f(r')d^3r' \cdot \nabla_r V(\mathbf{r}) + \frac{1}{2!} \int r'^2 f(r')[\hat{\mathbf{e}}_{r'} \cdot \nabla_r]^2 d^3r' V(\mathbf{r}) + \dots \\ &= V(\mathbf{r}) + 0 + \frac{1}{2!} \int r'^2 f(r')d^3r' \nabla^2 V(\mathbf{r}) + \dots \end{aligned} \quad (8.134)$$

The second term is null due to the parity of  $f(r')$  and the third produces the Darwin correction using  $V(\mathbf{r}) = V(r)$ . Letting the function be constant within the volume,  $f(\mathbf{r}) \simeq f_0$ , and with the normalization,

$$1 = \int_{-\hbar/2m_e c}^{\hbar/2m_e c} \int_{-\hbar/2m_e c}^{\hbar/2m_e c} \int_{-\hbar/2m_e c}^{\hbar/2m_e c} f(r) dx dy dz = f_0 \left( \frac{\hbar}{m_e c} \right)^3 , \quad (8.135)$$

we get the integral

$$\int r^2 f(r) d^3r = \int_{-\hbar/2m_e c}^{\hbar/2m_e c} \int_{-\hbar/2m_e c}^{\hbar/2m_e c} \int_{-\hbar/2m_e c}^{\hbar/2m_e c} f(r) r^2 dx dy dz = \left( \frac{\hbar}{2m_e c} \right)^2 . \quad (8.136)$$

Also,

$$\nabla^2 V(\mathbf{r}) = -e \nabla^2 \frac{Ze}{4\pi\epsilon_0 r} = -e \frac{\rho(\mathbf{r})}{\epsilon_0} = -\frac{Ze^2 \delta^3(\mathbf{r})}{\epsilon_0} . \quad (8.137)$$

Hence,

$$\int f(r')V(\mathbf{r} + \mathbf{r}')d^3r' = -\frac{Ze^2}{4\pi\epsilon_0 r} + \frac{\pi\hbar^2}{2m_e^2 c^2} \frac{Ze^2}{4\pi\epsilon_0} \delta^3(\mathbf{r}) + \dots , \quad (8.138)$$

<sup>11</sup>The smearing out of the electron's position is also known as *Zitterbewegung*. See Exc. 8.1.5.2.

which is precisely the electrostatic energy with the Darwin correction in the expressions (8.86) and (8.109).

To estimate the importance of this effect we insert the wavefunctions (4.52) evaluated at the origin,

$$\begin{aligned} \langle \hat{H}_{dw} \rangle &= \int d^3r \psi_{n\ell m}^*(\mathbf{r}) \frac{\pi \hbar^2}{2m_e^2 c^2} \frac{Ze^2}{4\pi\epsilon_0} \delta^3(\mathbf{r}) \psi_{n\ell m}(\mathbf{r}) \\ &= \frac{\pi \hbar^2}{2m_e^2 c^2} \frac{Ze^2}{4\pi\epsilon_0} |\psi_{n00}(0)|^2 \delta_{\ell 0} \delta_{m0} = \frac{\pi \hbar^2}{2m_e^2 c^2} \frac{Ze^2}{4\pi\epsilon_0} \frac{Z^3}{\pi n^3 a_B^3} \delta_{\ell 0}. \end{aligned} \quad (8.139)$$

We obtain,

$$\frac{H_{dw}}{H_0} = \frac{\frac{\pi \hbar^2}{2m_e^2 c^2} \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{\pi a_B^3}}{\frac{e^2}{4\pi\epsilon_0 a_B}} = \frac{\hbar^2}{2m_e^2 c^2} \frac{Z}{a_B^2} = \frac{\alpha^2}{2} \approx 0.01\%. \quad (8.140)$$

Darwin's correction vanishes for angular momentum  $\mathbf{l} > 0$ , such that,

$$\Delta E_{dw} = \langle \hat{H}_{dw} \rangle = -E_n \frac{(Z\alpha)^2}{n} \delta_{\ell 0}. \quad (8.141)$$

### 8.2.4 Summary of the corrections

Combining the  $\mathbf{l} \cdot \mathbf{s}$  and relativistic corrections, we obtain,

$$\begin{aligned} \Delta E_{fs} &= \Delta E_{rl} + \Delta E_{\ell s} + \Delta E_{dw} \\ &= E_n (Z\alpha)^2 \left[ \frac{1}{n(j + \frac{1}{2})} - \frac{3}{4n^2} \right] - E_n (Z\alpha)^2 \frac{j(j+1) - \ell(\ell+1) - \frac{3}{4}}{2n\ell(j + \frac{1}{2})(\ell+1)} - E_n (Z\alpha)^2 \\ &= E_n (Z\alpha)^2 \begin{cases} \frac{1}{nj} - \frac{3}{4n^2} - \frac{j(j+1) - (j - \frac{1}{2})(j + \frac{1}{2}) - \frac{3}{4}}{2n(j - \frac{1}{2})j(j + \frac{1}{2})} - 1 & \text{para } \ell = j - \frac{1}{2} \\ \frac{1}{n(j+1)} - \frac{3}{4n^2} - \frac{j(j+1) - (j + \frac{1}{2})(j + \frac{3}{2}) - \frac{3}{4}}{2n(j + \frac{1}{2})(j+1)(j + \frac{3}{2})} - 1 & \text{para } \ell = j + \frac{1}{2} \end{cases} \\ &= E_n (Z\alpha)^2 \left[ \frac{1}{n(j + \frac{1}{2})} - \frac{3}{4n^2} - 1 \right]. \end{aligned} \quad (8.142)$$

That is, the levels are now degenerate in  $j$  (see Fig. 8.1)<sup>12</sup>. Obviously the levels which are most affected by relativistic corrections are those with low values of  $n$  and  $\ell$ .

The levels are labeled by  $n\ell j$ . For example, the state  $3d_{5/2}$  has the main quantum number  $n = 3$ , the orbital angular momentum  $\ell = 2$ , and the total angular momentum  $j = 5/2$ . For large  $n$  or  $j$  the fine structure disappears. The new energy scheme is shown in Fig. 8.1. We note that, taking into account all relativistic corrections (but without the Lamb shift), we still have a partial degeneracy of the quantum number  $j$ . For example, the states  $^2s_{1/2}$  and  $^2p_{1/2}$  have the same energy. This is a particularity of the hydrogen atom.

<sup>12</sup>It is interesting that the quantum treatment presented here, including relativistic corrections, coincidentally agrees with the corrections of *Arnold Johannes Wilhelm Sommerfeld*.

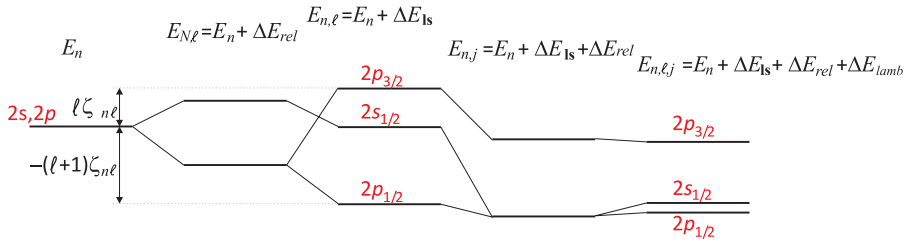


Figure 8.1: Hydrogen levels.

### 8.2.5 Lamb shift

Only remains to discuss the fourth correction,  $\hat{H}_{Lamb}$  in the expression (8.6). The origin of the *Lamb shift* lies in quantum electrodynamics. Being due to the quantum nature of the electromagnetic field, this correction is not predicted within the Dirac equation.

We may imagine the Coulomb force between charged particles being mediated by a continuous exchange of virtual photons. But each isolated charge also continuously emits and reabsorbs virtual photons, with the result that the position of the electron is smeared over a region of 0.1 fm. This reduces the overlap between the electronic orbits and the nucleus. Hence, the Lamb shift causes corrections that are stronger for small  $n$  and small  $\ell$ . For example in hydrogen, the  $2p_{1/2}$  is  $4.4 \cdot 10^{-6}$  eV = 1 GHz below the  $2s_{1/2}$  (see Fig. 8.1).

### 8.2.6 Exercises

#### 8.2.6.1 Ex: The Darwin term

Show that the expressions for the Darwin correction (8.86) and (8.109) are equivalent.

## 8.3 Hyperfine structure

Rutherford's measurements suggested a point-like and infinitely heavy atomic nucleus. In fact, the mass is finite and the nuclear charge is distributed over a finite volume and often in a non-isotropic manner, which leads to multipolar interactions with the electrons. In addition, many nuclei have a spin that can interact with the magnetic moment of the electrons. The energy corrections due to these effects are called *hyperfine structure*<sup>13</sup>.

Because many of the following considerations will remain valid for many-electron systems to be discussed later, we will switch to a notation denoting by  $\mathbf{L}$  the total orbital angular momentum of the electronic shell,  $\mathbf{S}$  the total spin of the electronic shell, and  $\mathbf{J}$  the total angular momentum of the electronic shell, remembering that for hydrogen  $\mathbf{S} = \frac{\hbar}{2}\vec{\sigma}$ .

<sup>13</sup>See [141] p. 1229 and [695] p. 23 for further reading.

### 8.3.1 Coupling to the nuclear spin

#### 8.3.1.1 Dipole moment of the nuclear spin

The nucleus may also have an angular momentum interacting with the angular momentum of the electrons. However, the momentum depends inversely on the masses. That is, the angular momentum of the nucleus is  $\mu_N/\mu_B = m_e/m_p \simeq 10^{-3}$  times smaller, where  $\mu_N = \hbar e/2m_p$  is an abbreviation called *nuclear magneton*. Thus, we can assume that the interaction between the nucleus and the electron will not interfere with the  $\mathbf{L} \cdot \mathbf{S}$ -coupling between the orbital angular momentum and the spin of the electron. The spin of the nucleus will be oriented along the total momentum of the electrons  $\mathbf{J}$ . However, this interaction will have the ability to lift the hydrogen degeneracy, even though the *splitting* will only be *hyperfine*. Indeed, the order of magnitude of *hyperfine splitting* is  $10^{-6}$  eV.

Analogously to the expressions (8.94) and (8.97), we write the dipole moment of the nucleus,

$$\boxed{\frac{\vec{\mu}_I}{\mu_N} = \frac{e}{2m_p\mu_N} g_p \mathbf{I} = g_p \frac{\mathbf{I}}{\hbar}}, \quad (8.143)$$

where  $g_p \equiv \mu_I/I$  is once again a factor taking into account possible corrections between the classical derivation and quantum mechanics<sup>14</sup>.

#### 8.3.1.2 Hyperfine splitting

In the derivation of the Pauli equation (8.90) from the Dirac equation (8.77) we discarded non-relativistic terms and reintroduced electronic spin-orbit coupling by hand allowing for  $\mathbf{A}(\mathbf{r}, t) \neq 0$ . By an analogous calculation directly applied to the Dirac equation we may unravel the *hyperfine structure*. Instead of setting the vector potential to  $\mathbf{A}(\mathbf{r}, t) = 0$ , as we did in (8.46), we now generalize the Dirac equation (8.77),

$$E' \vec{\phi} = qU(\mathbf{r})\vec{\phi} + \vec{\sigma} \cdot \vec{\pi} \frac{1}{2m_e} \left( 1 + \frac{E' - U(\mathbf{r})}{2m_e c^2} \right)^{-1} \vec{\sigma} \cdot \vec{\pi} \vec{\phi}. \quad (8.144)$$

Assuming  $\langle q\mathbf{A} \rangle \ll \langle \mathbf{p} \rangle$ , we may only retain terms to the lowest order in  $\mathbf{A}$  and neglect terms containing  $q\mathbf{A} \frac{E' - U(\mathbf{r})}{2m_e c^2}$ . Using the result of the calculation (8.88),

$$(\vec{\sigma} \cdot \vec{\pi})(\vec{\sigma} \cdot \vec{\pi}) = [\mathbf{p} - q\mathbf{A}]^2 - \hbar q \vec{\sigma} \cdot \vec{\mathcal{B}}, \quad (8.145)$$

we find the generalization of the total energy (8.86),

$$\hat{H} \simeq \frac{[\mathbf{p} - q\mathbf{A}(\mathbf{r})]^2}{2m_e} - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} - \frac{\mathbf{p}^4}{8m_e^3 c^2} - \frac{e}{2m_e^2 c^2} \frac{1}{r} \frac{\partial U}{\partial r} \mathbf{S} \cdot \mathbf{L} - \frac{\hbar^2 e}{4m_e^2 c^2} \frac{\partial U}{\partial r} \frac{\partial}{\partial r} - \frac{\hbar q}{2m_e} \vec{\sigma} \cdot \vec{\mathcal{B}}(\mathbf{r}), \quad (8.146)$$

and expanding the bracket

$$[\mathbf{p} - q\mathbf{A}]^2 \simeq \mathbf{p}^2 - q\mathbf{p} \cdot \mathbf{A} - q\mathbf{A} \cdot \mathbf{p} = \mathbf{p}^2 - 2q\mathbf{A} \cdot \mathbf{p} \quad (8.147)$$

<sup>14</sup>In fact, the proton factor  $g$  is anomalous,  $g_p = 5.58$ , which reduces the fraction  $\mu_I/\mu_N$ . For the neutron we have:  $g_n = -3.83$



in the Coulomb gauge, we see that two new terms are added to the energy called the hyperfine structure,

$$\boxed{\begin{aligned} \hat{H} &= \hat{H}_B + \hat{H}_{fs} + \hat{H}_{hfs} \\ \text{with } \hat{H}_{hfs} &= \hat{H}_{LI} + \hat{H}_{SI} = \frac{e}{m_e} \mathbf{A}(\mathbf{r}) \cdot \mathbf{p} + \frac{2\mu_B}{\hbar} \mathbf{S} \cdot \vec{\mathcal{B}}(\mathbf{r}) \end{aligned}}, \quad (8.148)$$

with  $\vec{\mu}_S = -\frac{e}{m_e} \mathbf{S}$ .

Up to now we did not say anything about the origin of the magnetic field. We only notice that any magnetic field will interact with the electron's orbit and with its spin. We now make use of our knowledge that the proton has a spin of its own which produces, at the position of the electrons, a magnetic vector potential,

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \frac{\vec{\mu}_I \times \mathbf{r}}{r^3}, \quad (8.149)$$

interacting with the angular momentum of the electron  $\mathbf{L}$  in the form,

$$\begin{aligned} \hat{H}_{LI} &= \frac{e}{m_e} \mathbf{A} \cdot \hat{\mathbf{p}} = \frac{e}{m_e} \frac{\mu_0}{4\pi r^3} (\vec{\mu}_I \times \mathbf{r}) \cdot \mathbf{p} \\ &= \frac{e}{m_e} \frac{\mu_0}{4\pi r^3} \frac{\mu_N}{\hbar} g_p (\mathbf{I} \times \mathbf{r}) \cdot \mathbf{p} = \frac{\mu_0}{2\pi r^3} \frac{\mu_B}{\hbar} \frac{\mu_N}{\hbar} g_p \mathbf{L} \cdot \mathbf{I}, \end{aligned} \quad (8.150)$$

using the definition of Bohr's magneton.

In addition, the potential vector (8.149) generated by the nuclear spin produces a magnetic field [361],

$$\vec{\mathcal{B}} = \nabla \times \mathbf{A} = \frac{\mu_0}{4\pi r^3} [3(\vec{\mu}_I \cdot \hat{\mathbf{r}}) \hat{\mathbf{r}} - \vec{\mu}_I] + \frac{2}{3} \mu_0 \vec{\mu}_I \delta^3(\mathbf{r}), \quad (8.151)$$

as will be shown in Exc. 8.3.3.1. This field interacts with the spin of the electron  $\mathbf{S}$  in the form,

$$\begin{aligned} \hat{H}_{SI} &= -\vec{\mu}_S \cdot \vec{\mathcal{B}} = -\frac{\mu_0}{4\pi r^3} [3(\vec{\mu}_I \cdot \hat{\mathbf{r}})(\vec{\mu}_S \cdot \hat{\mathbf{r}}) - (\vec{\mu}_S \cdot \vec{\mu}_I)] - \frac{2}{3} \mu_0 \vec{\mu}_S \cdot \vec{\mu}_I \delta^3(\mathbf{r}) \\ &= \frac{\mu_0}{4\pi r^3} \frac{\mu_B}{\hbar} g_e \frac{\mu_N}{\hbar} g_p [3(\mathbf{I} \cdot \hat{\mathbf{r}})(\mathbf{S} \cdot \hat{\mathbf{r}}) - (\mathbf{S} \cdot \mathbf{I})] + \frac{2}{3} \mu_0 g_e \mu_B \frac{\mathbf{S}}{\hbar} \cdot g_p \mu_N \frac{\mathbf{I}}{\hbar} \delta^3(\mathbf{r}), \end{aligned} \quad (8.152)$$

inserting the expressions (8.97) and (8.143). The first term gives the energy of the nuclear dipole in the field due to the electronic orbital angular momentum. The second term gives the energy of the 'finite distance' interaction of the nuclear dipole with the field due to the electron spin magnetic moments. The final term, often known as the *Fermi contact term* relates to the direct interaction of the nuclear dipole with the spin dipoles and is only non-zero for states with a finite electron spin density at the position of the nucleus (those with unpaired electrons in  $s$ -subshells).

We now discuss the two cases in which  $L = 0$  or  $L \neq 0$  separately in the following subsections [141, 596, 361].

### 8.3.1.3 Orbital angular momentum $L = 0$

For vanishing orbital angular momenta,  $L = 0$ , we only need to consider the contribution  $\hat{H}_{SI}$ . Furthermore, this contribution will be dominated by the Dirac term,

because the  $s$ -orbitals have a high probability at the nuclear region, but fall off quickly at larger distances. Hence,

$$\hat{H}_{SI} \simeq \frac{2}{3}\mu_0 g_e \mu_B \frac{\mathbf{S}}{\hbar} \cdot g_p \mu_N \frac{\mathbf{I}}{\hbar} \delta^3(\mathbf{r}) . \quad (8.153)$$

Defining the complete total angular momentum of the atom,

$$\mathbf{F} \equiv \mathbf{I} + \mathbf{S} , \quad (8.154)$$

we calculate from (8.152),

$$\begin{aligned} \Delta E_{hfs}^{\ell=0} &= \langle (S, I)F, m_F | \hat{H}_{SI} | (S, I)F, m_F \rangle = \frac{2\mu_0 g_e g_p \mu_B \mu_N}{3\hbar^2} \langle \mathbf{S} \cdot \mathbf{I} \rangle \langle \delta^3(\mathbf{r}) \rangle \quad (8.155) \\ &= \frac{2}{3}\mu_0 g_e g_p \mu_B \mu_N [F(F+1) - I(I+1) - S(S+1)] \int \psi_{n00}^*(\mathbf{r}) \delta^3(\mathbf{r}) \psi_{n00}(\mathbf{r}) d^3r \\ &= \frac{2}{3}\mu_0 g_e g_p \mu_B \mu_N [F(F+1) - I(I+1) - S(S+1)] \left| \frac{1}{\sqrt{\pi}} \left( \frac{Z}{na_B} \right)^{3/2} \right|^2 . \end{aligned}$$

As an example consider the hyperfine structure of the state  $1s_{1/2}$  of the hydrogen atom. With  $J = I = \frac{1}{2}$  and  $Z = n = 1$  we obtain (see Exc. 8.3.3.2),

$$\begin{aligned} \Delta E_{hfs}^{L=0}(F=1) - \Delta E_{hfs}^{\ell=0}(F=0) &= \frac{2}{3}\mu_0 g_e \mu_B g_p \mu_N 2 \frac{1}{\pi} \left( \frac{Z}{na_B} \right)^3 \quad (8.156) \\ &= \frac{2g_e g_p m_e^2 c^2}{3m_p} \alpha^4 \approx (2\pi\hbar) \cdot 1.420 \text{ GHz} . \end{aligned}$$

The experimental value is 1.4204057518 GHz. This frequency corresponds to the spectral line used in radio astronomy, where the measurement of the angular distribution of this radiation allows the mapping of the spatial distribution of interstellar hydrogen.

#### 8.3.1.4 Orbital angular momenta $L \neq 0$

In the case  $L \neq 0$  both contributions,  $\hat{H}_{SI}$  and  $\hat{H}_{LI}$  have to be considered, however, we may neglect the Dirac term, because the orbitals with orbital angular momentum have vanishing probabilities at the nuclear region. Combining the two terms (8.150) and (8.152), we obtain,

$$\begin{aligned} \hat{H}_{JI} &= \hat{H}_{LI} + \hat{H}_{SI} = \frac{\mu_0}{4\pi r^3} \frac{\mu_B}{\hbar} g_e \frac{\mu_N}{\hbar} g_p [3(\mathbf{I} \cdot \hat{\mathbf{r}})(\mathbf{S} \cdot \hat{\mathbf{r}}) + \mathbf{L} \cdot \mathbf{I} - \mathbf{S} \cdot \mathbf{I}] \quad (8.157) \\ &= \frac{\mu_0}{4\pi r^3} \frac{\mu_B}{\hbar} g_e \frac{\mu_N}{\hbar} g_p \mathbf{N} \cdot \mathbf{I} , \end{aligned}$$

introducing  $\mathbf{N}$  as a quantity that only depends on the electronic shell:

$$\mathbf{N} \equiv 3(\mathbf{S} \cdot \hat{\mathbf{r}})\hat{\mathbf{r}} + \mathbf{L} - \mathbf{S} . \quad (8.158)$$

Generalizing the complete total angular momentum of the atom (8.154),

$$\mathbf{F} \equiv \mathbf{I} + \mathbf{J} , \quad (8.159)$$

is useful for calculating the coupling  $\mathbf{I} \cdot \mathbf{J} = \frac{1}{2}(\mathbf{F}^2 - \mathbf{I}^2 - \mathbf{J}^2)$ . Now, as the  $\mathbf{L} \cdot \mathbf{S}$ -coupling is strong, we project the two angular momenta onto the total electronic angular momentum  $\mathbf{J}$ ,

$$\mathbf{N} \longrightarrow \frac{\mathbf{N} \cdot \mathbf{J}}{|\mathbf{J}|} \frac{\mathbf{J}}{|\mathbf{J}|}, \quad \mathbf{I} \longrightarrow \frac{\mathbf{I} \cdot \mathbf{J}}{|\mathbf{J}|} \frac{\mathbf{J}}{|\mathbf{J}|}. \quad (8.160)$$

We get for the coupling between the projected spins (8.160) of the electronic layer and the nucleus,

$$\mathbf{N} \cdot \mathbf{I} \longrightarrow \frac{(\mathbf{N} \cdot \mathbf{J})(\mathbf{I} \cdot \mathbf{J})}{|\mathbf{J}|^2} = \frac{(\mathbf{N} \cdot \mathbf{J})(\mathbf{F}^2 - \mathbf{I}^2 - \mathbf{J}^2)}{2|\mathbf{J}|^2}. \quad (8.161)$$

We calculate

$$\begin{aligned} \Delta E_{hfs}^{L \neq 0} &= \langle ((L, S)J, I)F, m_F | \hat{H}_{JI} | ((L, S)J, I)F, m_F \rangle \\ &= \frac{\mu_0 \mu_B}{4\pi} \frac{\mu_B}{\hbar} g_e \frac{\mu_N}{\hbar} g_p \left\langle \frac{\mathbf{N} \cdot \mathbf{I}}{r^3} \right\rangle \\ &\longrightarrow \frac{\mu_0 \mu_B}{4\pi} \frac{\mu_B}{\hbar} g_e \frac{\mu_N}{\hbar} g_p \frac{\mathbf{N} \cdot \mathbf{J} [F(F+1) - I(I+1) - J(J+1)]}{2J(J+1)} \left( \frac{Z}{a_B} \right)^3 \frac{n}{n^4 L(L + \frac{1}{2})(L+1)}. \end{aligned} \quad (8.162)$$

Introducing the *interval factor*,

$$A_J \equiv \frac{\mu_0 \mu_B}{4\pi} \frac{\mu_B}{\hbar} g_e \frac{\mu_N}{\hbar} g_p \left( \frac{Z}{a_B} \right)^3 \frac{\mathbf{N} \cdot \mathbf{J}}{2J(J+1)} \frac{n}{n^4 L(L + \frac{1}{2})(L+1)}, \quad (8.163)$$

as a quantity that only depends on the electronic shell, we can write

$$\Delta E_{hfs}^{L \neq 0} = \frac{A_J}{2} [F(F+1) - J(J+1) - I(I+1)]. \quad (8.164)$$

Note, that the  $\mathbf{J} \cdot \mathbf{I}$ -coupling breaks the degeneracy of  $\mathbf{J}$  in the hydrogen atom, but not of  $J_z$ . We can derive the following *interval rule*,

$$\Delta E_{F+1} - \Delta E_F = A_J(F+1). \quad (8.165)$$

Besides the magnetic interaction between the angular momenta of the nucleus and the electronic shell there is an interaction between the nucleus, when it is not spherically symmetric, and the shell. This interaction causes deviations from the interval rule and an additional splitting of the hyperfine states.

### 8.3.2 Electric quadrupole interaction

The fact that the nucleus is not perfectly spherical gives rise to new electron-nucleus corrections that are called *quadrupolar interaction*. The starting point is,

$$\hat{H}_{qud} = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{|\mathbf{r}_e - \mathbf{r}_N|} - \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\mathbf{r}_e|}, \quad (8.166)$$

Table 8.1: List of atomic data [657] showing the natural linewidth of the  $D_2$  line, frequencies of the  $D_1$  and  $D_2$  lines, and the hyperfine splitting.

Element	$\gamma_{D_2}/2\pi$ [ MHz ]	$D_1$ [ $\text{cm}^{-1}$ ]	$D_2$ [ $\text{cm}^{-1}$ ]	$\nu_{HFS}[S_{1/2}]$ [ MHz ]
$^1\text{H}$	99.58	82264.000	82264.366	1420.4
$^2\text{H}$	99.58	82264.000	82264.366	
$^6\text{Li}$	5.92	14901.000	14901.337	228.2
$^7\text{Li}$	5.92	14901.000	14901.337	803.5
$^{23}\text{Na}$	10.01	16956.000	16973.190	1771.6
$^{39}\text{K}$	6.09	12985.170	13042.876	461.7
$^{40}\text{K}$	6.09	12985.170	13042.876	-1285.8
$^{41}\text{K}$	6.09	12985.170	13042.876	254.0
$^{85}\text{Rb}$	5.98	12578.920	12816.469	3035.7
$^{87}\text{Rb}$	5.98	12578.920	12816.469	6834.7
$^{133}\text{Cs}$	5.18	11182.000	11737.000	9192.6
$^{135}\text{Cs}$	5.18	11182.000	11737.000	

where  $\mathbf{r}_e$  is the electronic coordinate and  $\mathbf{r}_N$  is the nuclear coordinate, both having their origin in the center mass of the nucleus. For  $\mathbf{r}_e > \mathbf{r}_N$  this interaction can be obtained after several mathematical steps as [466],

$$\hat{H}_{qud} = B_J \frac{3(\hat{\mathbf{I}} \cdot \hat{\mathbf{J}})(2\hat{\mathbf{I}} \cdot \hat{\mathbf{J}} + 1) - 2\hat{\mathbf{I}}^2\hat{\mathbf{J}}^2}{2I(I-1)2J(J-1)}, \quad (8.167)$$

where  $B_J$  is called the *constant of the quadrupolar electron-nucleus interaction*. With this expression we can calculate,

$$\Delta E_{qud} = \langle IJKm_K | \hat{H}_{qud} | IJKm_K \rangle = B_J \frac{\frac{3}{2}K(K+1) - 2I(I+1)J(J+1)}{2I(2I-1)2J(2J-1)}, \quad (8.168)$$

where  $K \equiv 2(\hat{\mathbf{J}} \cdot \hat{\mathbf{I}}) = F(F+1) - I(I+1) - J(J+1)$ . It is important to remember that a nucleus with  $I = 0$  or  $I = \frac{1}{2}$  has no quadrupole moment,  $B_J = 0$ . Also for  $J = \frac{1}{2}$  there will be no contribution.

Joining the contributions  $\hat{\mathbf{J}} \cdot \hat{\mathbf{I}}$  of Eq. (8.164) and the quadrupolar contribution (8.168), the hyperfine structure can be described by,

$$\begin{aligned} \Delta E_{hfs} &= \Delta E_{JI} + \Delta E_{qud} \\ &= \frac{A_J}{2}K + \frac{B_J}{8IJ(2I-1)(2J-1)}[3K(K+1) - 4I(I+1)J(J+1)], \end{aligned} \quad (8.169)$$

where the constants  $A_J$  and  $B_J$  depend on the atom and the total electronic angular momentum.

Table 8.2: Hyperfine constants of some alkaline atoms.

atom	$n$	$A_J(n^2S_{1/2})$ [MHz·h]	$A_J(n^2P_{1/2})$ [MHz·h]	$A_J(n^2P_{3/2})$ [MHz·h]	$B_J(n^2P_{3/2})$ [MHz·h]
$^1\text{H}, I = \frac{1}{2}$	1	1420	46.17	-3.07	-0.18
$^7\text{Li}, I = \frac{3}{2}$	2	401.75	46.17	-3.07	-0.18
	3		13.5	-0.96	
$^{23}\text{Na}, I = \frac{3}{2}$	3	885.82	94.3	18.65	2.82
	4	202	28.85	6.00	0.86
$^{85}\text{Rb}, I = \frac{5}{2}$	5	1011.9	120.7	25.029	26.03
	6	239.3	39.11	8.25	8.16
$^{87}\text{Rb}, I = \frac{3}{2}$	5	3417.3	409.1	84.852	12.510
	6	809.1	132.5	27.70	3.947

In Excs. 8.3.3.3 and 8.3.3.4 we determine the hyperfine structures of sodium and rubidium atoms.

### 8.3.3 Exercises

#### 8.3.3.1 Ex: Field of a magnetic moment

a. Calculate the vector potential  $\mathbf{A}(\mathbf{r})$  and the magnetic dipole moment  $\vec{\mu}$  produced by an orbiting electron by Biot-Savart's law using the expansion of  $|\mathbf{r} - \mathbf{r}'|^{-1}$  in Legendre polynomials.

b. Calculate the magnetic field  $\vec{B}(\mathbf{r})$ .

#### 8.3.3.2 Ex: Probability for finding the electron near the nucleus

Calculate the expectation value  $\langle \delta^{(3)}(\mathbf{r}) \rangle_{n\ell m}$  for encountering the electron of a hydrogen atom close to the nucleus.

#### 8.3.3.3 Ex: Hyperfine structure of sodium

Determine the hyperfine structure of the  $^2S$  and  $^2P$  states of the sodium atom including energy shifts. See Tab. 13.1 for the hyperfine constants  $A_J$  and  $B_J$ .

#### 8.3.3.4 Ex: Hyperfine structure of rubidium

Given the following energy distances  $\nu_{F,F'}$  of the hyperfine levels of the rubidium isotopes  $^{87}\text{Rb}$  and  $^{85}\text{Rb}$  [51],

$$^{87}\text{Rb}, S_{1/2} \quad \text{splits into} \quad \nu_{1,2} = 6834.7 \text{ MHz}$$

$$^{87}\text{Rb}, P_{3/2} \quad \text{splits into} \quad \nu_{0,1} = 72.3 \text{ MHz}, \nu_{1,2} = 157.1 \text{ MHz}, \nu_{2,3} = 267.2 \text{ MHz}$$

$$^{85}\text{Rb}, S_{1/2} \quad \text{splits into} \quad \nu_{1,2} = 3035.7 \text{ MHz}$$

$$^{85}\text{Rb}, P_{3/2} \quad \text{splits into} \quad \nu_{1,2} = 29.4 \text{ MHz}, \nu_{2,3} = 63.4 \text{ MHz}, \nu_{3,4} = 120.7 \text{ MHz} ,$$

calculate the positions of the barycenters.

### 8.3.3.5 Ex: Two particles

Consider a two-particle system of masses  $\mu_1$  and  $\mu_2$ , exposed to a central potential  $V(r)$  and an interaction potential  $V(|\mathbf{r}_1 - \mathbf{r}_2|)$  which only depends on the distance between the particles. The Hamiltonian of the system in the interaction representation is  $H = H_1 + H_2 + V(|\mathbf{r}_1 - \mathbf{r}_2|)$  with  $H_\ell = -\frac{\hbar^2}{2\mu_\ell} \nabla_\ell^2 + V(r_\ell)$ ,  $\ell = 1, 2, \dots$ . Show that the individual angular momenta  $\mathbf{L}_\ell$  are not, in general, constants of the motion, unlike the *total* angular momentum  $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$ .

## 8.4 Exotic atoms

'Normal' atoms consist of a nucleus made of protons and neutrons and an electronic shell. But other two-particle systems are possible, e.g. where the nucleus or electron is replaced by another hadron or lepton (anti-proton, positron, muon, etc.). Such a system is called *exotic atom*. Atoms in Rydberg states also belong to this category.

### 8.4.1 Positronium and muonium

Positronium ( $e^+e^-$ ) is a hydrogen-like system consisting of leptons, that is, an electron and a positron, which is the antiparticle of the electron. The muonium ( $\mu^+e^-$ ) is similar to positronium, except that here the positron is replaced by a muon whose mass is  $m_{\mu^+} = 207m_e$ . Leptons are, according to the present understanding, particles without internal structure. Both systems are unstable: the two particles annihilate each other producing  $\gamma$ -photons. The energy levels and orbits of the two particles are similar to that of the hydrogen atom. However, because of the reduced mass, the frequencies of the spectral lines are less than half of the corresponding hydrogen lines.

The fundamental state of positronium, like that of hydrogen, has two possible configurations depending on the relative orientation of the electron and positron spins. The singlet state with antiparallel spins ( $S = 0$ ,  $M_s = 0$ ) is known as para-positronium (p-Ps) and denoted by  $^1S_0$ . It has an average lifetime of

$$\tau = \frac{2\hbar}{m_e c^2 \alpha^5} = 124.4 \text{ ps} \quad (8.170)$$

and decays preferably in two gamma rays with energy of 511 keV each (in the center-of-mass). The triplet state with parallel spins ( $S = 1$ ,  $M_s = -1, 0, 1$ ) is known as ortho-positronium (o-Ps) and denoted as  $^3S_1$ . It has an average life of 138.6 ns, and the most common form of decay produces three photons. Other forms of decay are negligible. For example, the decay channel producing five photons is  $10^{-6}$  times less likely. Measurements of these lifetimes and the positronium energy levels have been used in precision tests of quantum electrodynamics.

While the precise calculation of the positronium energy levels is based on the Bethe-Salpeter equation, the similarity between positronium and hydrogen allows for an approximate estimate. In this approach, the energy levels are supposed to be

different from those of hydrogen because of the difference in the value of the reduced mass  $\mu$ , used in the energy equation. Since  $\mu = m_e/2$  for positronium, we have

$$E_n = -\frac{\mu q_e^4}{8h^2\epsilon_0^2} \frac{1}{n^2} = -\frac{1}{2} \frac{m_e q_e^4}{8h^2\epsilon_0^2} \frac{1}{n^2} = \frac{-6.8\text{eV}}{n^2}. \quad (8.171)$$

A di-positronium molecule, that is, a system of two bound positronium atoms, has already been observed. Positronium in high energy states has been conjectured to become the dominant form of atomic matter in the universe in the very distant future if the proton decay becomes tangible.

### 8.4.2 Hadronic atoms

In contrast to *leptons* (such as the electron  $e^-$ , the positron  $e^+$  and the muons  $\mu^+$  and  $\mu^-$ ) that participate only in electromagnetic interactions and weak interactions, *hadrons* also participate in strong (nuclear type) interactions. There are two types of hadrons, *baryons* (such as the proton  $p$  and antiproton  $\bar{p}$ , the neutron  $n$  and antineutron  $\bar{n}$ , hyperons  $\Sigma$ ,  $\Xi$ , ...) that have semi-integer spin and behave like fermions and *mesons* (like the  $\pi$ -meson,  $K$ -meson, ...) that have an integer spin. Every negatively charged hadron can be used to form a hydrogen-type *hadronic atom*. These systems contain a nucleus and negative hyperon and are known as hyperonic atoms. All of these are unstable and due to the fact that they have a sufficiently long lifetime, some of their spectral lines have now been observed.

Since the hadrons interact strongly with the nucleus, the theory developed for hydrogen systems (in which only exist Coulomb interaction) can not be directly applied. In this way the values shown in Tab. 8.3 give only an estimate of the 'radius' and the ionization potential of the hadronic atoms  $p\pi^-$ ,  $p\kappa^-$ ,  $p\bar{p}$  and  $p\Sigma^-$ .

Table 8.3: *Main features of some exotic atoms.*

system	reduced mass	radius 'a'	$I_p$
$pe^-$	$1836/1837 \approx 1$	$\approx a_B = 1$	$e^2/2a_B \approx 0.5$
$e^+e^-$	0.5	2	0.25
$\mu^+e^-$	$207/208 \approx 1$	1	0.5
$p\mu^-$	$\approx 186$	$5.4 \cdot 10^{-3}$	93
$p\pi^-$	$\approx 238$	$4.2 \cdot 10^{-3}$	119
$p\kappa^-$	$\approx 633$	$1.6 \cdot 10^{-3}$	317
$p\bar{p}$	$\approx 928$	$1.1 \cdot 10^{-3}$	459
$p\Sigma^-$	$\approx 1029$	$9.7 \cdot 10^{-3}$	515

### 8.4.3 Muonic hydrogen

The muon mass is  $m_\mu = 207m_e$ . When a muon is attached to a proton we have *muonic hydrogen*. Its size is smaller because of the reduced mass  $a_\mu = a_B \frac{1/m_e}{1/m_\mu + 1/m_p}$

and the binding energy and the energies of excitation are greater for the same reason. F.ex. while for  $H = p^+e^-$  the transition  $2S - 2P_{1/2}$  is at  $10\text{ eV} \triangleq 121\text{ nm}$ , for  $p^+\mu^-$  it is at  $1900\text{ eV}$ . Muonic atoms are interesting because they have amplified Lamb shifts, hyperfine interactions, and quantum electrodynamical corrections. Therefore, the displacement due to the finite distribution of charges in the proton  $r_p = 0.8\text{ fm}$  should influence the spectrum. While in  $p^+e^-$  the  $2S$  level is shifted upward by the Lamb shift by a value of  $4.4 \times 10^{-6}\text{ eV}$ , in  $p^+\mu^-$  it is shifted down by a value of  $0.14\text{ eV}$ . In Exc. 8.4.5.2 we calculate the spectrum of the muonic hydrogen and in Exc. 6.1.3.3 we compare the energy corrections due to the finite extension of the nuclei for muonic and for standard hydrogen in first order TIPT.

### 8.4.4 Rydberg atoms

An atom excited to a state whose main quantum number is very high is called *Rydberg atom*. These atoms have a number of peculiar properties, including high sensitivity to electric and magnetic fields, long decay times, and wavefunctions that approximate classical electron orbits. The inner electrons protect the outer electron from the electric field of the nucleus such that, from a distance, the electric potential looks identical to that seen by the electron of a hydrogen atom.

Despite its flaws, Bohr's atom model is useful in explaining these properties. In Exc. 1.1.6.6 we derive Bohr's expression for the orbital radius in terms of the principal quantum number  $n$ :

$$r = \frac{4\pi\epsilon_0 n^2 \hbar^2}{e^2 m} . \quad (8.172)$$

Thus, it is clear why Rydberg atoms have peculiar properties: the radius goes as  $n^2$  (such that for example the state with  $n = 137$  of hydrogen has a radius of  $\sim 1\text{ mm}$ ) and the geometric cross section goes as  $n^4$ . Thus, Rydberg atoms are extremely large, with loosely bound valence electrons that are easily perturbed or ionized by collisions or external fields.

Since the binding energy of a Rydberg electron is proportional to  $1/r$ , and therefore falls as  $1/n^2$ , the spacing between energy levels falls as

$$\Delta E = E_1 \left( \frac{1}{(n+1)^2} - \frac{1}{n^2} \right) \xrightarrow{n \rightarrow \infty} E_1 \left( -\frac{2}{n^3} + \frac{3}{n^4} + \dots \right) \quad (8.173)$$

leading to less and less spaced levels. These Rydberg states form the *Rydberg series*.

#### 8.4.4.1 Correspondence principle in Rydberg atoms

To calculate the oscillation frequency of an electron confined to a proton, we use the classical planetary model,

$$m\omega_n^2 = \frac{e^2}{4\pi\epsilon_0 r} \quad \text{and} \quad m\omega r^2 = n\hbar . \quad (8.174)$$

Eliminating  $r$ ,

$$\omega_n = \frac{me^4}{(4\pi\epsilon_0)^2 n^3 \hbar^3} . \quad (8.175)$$



Radiation of this frequency will be emitted by an atomic antenna. On the other hand, the Bohr model predicts frequencies between orbitals,

$$\omega_n = \frac{E_{n+1} - E_n}{\hbar} = \frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2} \left( \frac{1}{(n+1)^2} - \frac{1}{n^2} \right) \xrightarrow{n \rightarrow \infty} \frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2} \frac{2}{n^3}. \quad (8.176)$$

#### 8.4.4.2 Production of Rydberg atoms

In the hydrogen atom only the ground state ( $n = 1$ ) is actually stable. Other states must be excited by various techniques such as electron impact or charge exchange. In contrast to these methods, which produce a distribution of excited atoms at various levels, the optical excitation method allows to produce specific states, but only for alkali metals whose transitions fall into frequency regimes which are accessible to lasers.

#### 8.4.4.3 Potential in a Rydberg atom

The valence electron in a Rydberg atom with  $Z$  protons in the nucleus and  $Z - 1$  electrons in closed layers sees a spherically symmetric Coulomb potential:

$$U_{cou} = -\frac{e^2}{4\pi\epsilon_0 r}. \quad (8.177)$$

The similarity of the effective potential 'seen' by the outer electron and the authentic hydrogen potential suggests a classical treatment within the planetary model. There are three notable exceptions:

- An atom can have two (or more) electrons in highly excited states with comparable orbital radii. In this case, the electron-electron interaction gives rise to a significant deviation from the hydrogen potential. For an atom in a multiple Rydberg state the additional term  $U_{ee}$  includes a sum over each pair of highly excited electrons:

$$U_{ee} = \frac{e^2}{4\pi\epsilon_0} \sum_{i < j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (8.178)$$

- If the valence electron has very low angular momentum (interpreted classically as an extremely eccentric elliptical orbit), it can pass close enough to the nucleus to polarize it, giving rise to an additional term,

$$U_{pol} = -\frac{e^2\alpha_d}{(4\pi\epsilon_0)^2 r^4}. \quad (8.179)$$

- If the outer electron penetrates the inner electronic shells, it *sees* more of the charge of the nucleus and therefore feels a larger force. In general, the modification of the potential energy is not simple to calculate and should be based on some knowledge of the nucleus' geometry.

In hydrogen the binding energy is given by:

$$E_B = -\frac{E_1}{n^2}. \quad (8.180)$$

The binding energy is weak at high values of  $n$ , which explains the fragility of the Rydberg states that can easily be ionized, e.g. by collisions.

Additional terms modifying the potential energy of a Rydberg state require the introduction of a *quantum defect*,  $\delta\ell$ , in the expression for the binding energy:

$$E_B = -\frac{E_1}{(n - \delta\ell)^2} . \quad (8.181)$$

The long lifetimes of Rydberg states with high orbital angular momentum can be explained in terms of overlapping wavefunctions. The wavefunction of an electron in a state with high  $\ell$  (large angular momentum, 'circular orbit') has little overlap with the wavefunctions of the internal electrons and therefore stays relatively unperturbed. Also, the small energy difference between adjacent Rydberg states decreased the decay rate according to the result (13.37).

#### 8.4.4.4 Rydberg atoms in external fields

The large distance between the electron and ionic nucleus in a Rydberg atom gives rise to an extremely large electric dipole moment  $d$ . There is an energy associated with the presence of an electric dipole in an electric field  $\vec{\mathcal{E}}$ , known as *Stark shift*,

$$E_S = -\mathbf{d} \cdot \vec{\mathcal{E}} . \quad (8.182)$$

Depending on the sign of the projection of the dipole moment onto the vector of the local electric field, the energy of a state increases or decreases with the intensity of the field. The narrow spacing between adjacent levels  $n$  in the Rydberg series means that the states can approach degeneracy even for relatively weak fields. Theoretically, the force of the field in which a level crossing would occur (assuming no coupling between the states) is given by the *Inglis-Teller limit*,

$$F_{IT} = \frac{e}{12\pi\epsilon_0 a_0^2 n^5} . \quad (8.183)$$

In hydrogen the pure Coulomb potential does not couple the Stark states of an  $n$  level, which results in a *real crossover*. In other elements, deviations from the ideal  $1/r$ -potential allow for *avoided crossings*.

### 8.4.5 Exercises

#### 8.4.5.1 Ex: Positronium

Calculate and compare the fine and hyperfine structure of positronium.

#### 8.4.5.2 Ex: Muonic hydrogen

Muonic hydrogen consists of a proton and a negatively charged muon. Calculate the binding energy of the ground state of muonic hydrogen in eV and write down the ground state's wavefunction.

## 8.5 Further reading

et al., [\[DOI\]](#)



# Chapter 9

## Atoms with spin in external fields

The atomic fine structure was derived in the last chapter under the assumption that all electric and magnetic fields arise from the motion and spin of the electrons in the atomic shell and the nuclear spin. In this chapter, we will extend the treatment to include the reaction of the electrons to external electrostatic or electromagnetic fields. In this context, we will discuss the Zeeman and the Stark effect.

### 9.1 Charged particles in electromagnetic fields

#### 9.1.1 Lagrangian and Hamiltonian of charged particles

A charge subject to an electromagnetic field feels the Lorentz force,

$$\mathbf{F} = q\vec{\mathcal{E}} + q\dot{\mathbf{r}} \times \vec{\mathcal{B}}, \quad (9.1)$$

where

$$\vec{\mathcal{E}} = -\nabla\Phi - \frac{\partial\mathbf{A}}{\partial t} \quad \text{and} \quad \vec{\mathcal{B}} = \nabla \times \mathbf{A}, \quad (9.2)$$

where  $\Phi$  and  $\mathbf{A}$  are called scalar and vector potential, respectively.

It is important to realize here, that the momentum  $\mathbf{p}$  not only involves the momentum of the particle  $m\mathbf{v}$ , but the field also carries a momentum  $q\mathbf{A}(\mathbf{r})$ . As we learned in electrodynamics it is possible to derive this force from a Lagrangian for the electronic motion,

$$\mathcal{L}(r_i, \dot{r}_i) = \frac{m}{2}\dot{\mathbf{r}}^2 - q\Phi(\mathbf{r}) + q\dot{\mathbf{r}} \cdot \mathbf{A}(\mathbf{r}). \quad (9.3)$$

With this aim we first determine the momentum by,

$$p_i = \frac{\partial\mathcal{L}}{\partial\dot{r}_i} = m\dot{r}_i + qA_i, \quad (9.4)$$

and the Hamiltonian by,

$$\mathcal{H} = \sum_i p_i\dot{r}_i - \mathcal{L}(r_i, \dot{r}_i) = (m\mathbf{v} + q\mathbf{A}) \cdot \dot{\mathbf{r}} - \frac{m}{2}\dot{\mathbf{r}}^2 + q\Phi - q\dot{\mathbf{r}} \cdot \mathbf{A} = \frac{m}{2}\mathbf{v}^2 + q\Phi. \quad (9.5)$$

That is,

$$\boxed{\mathcal{H}(r_i, p_i) = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\Phi} . \quad (9.6)$$

The following equations hold,

$$\dot{r}_i = \frac{\partial \mathcal{H}}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial r_i} . \quad (9.7)$$

The first equation is easily verified by inserting the Hamiltonian (9.5). The second leads to the Lorentz force,

$$F_i = m\dot{v}_i = \dot{p}_i - q\dot{A}_i = -\frac{\partial \mathcal{H}}{\partial r_i} - q\dot{A}_i = q\mathcal{E}_i + q(\mathbf{v} \times \vec{\mathcal{B}})_i , \quad (9.8)$$

where the last step of the derivation will be shown in the Exc. 9.1.3.1 using the Coulomb gauge  $\nabla \cdot \mathbf{A} = 0$ .

### 9.1.2 Minimal coupling

Note that the same result (9.6) can be obtained by a canonical substitution,

$$m\mathbf{v} \longrightarrow \mathbf{p} - q\mathbf{A} \quad \text{and} \quad \mathcal{H} \longrightarrow \mathcal{H} + q\Phi . \quad (9.9)$$

This substitution rule, called *minimal coupling*, can be applied in quantum mechanics,

$$m\hat{\mathbf{v}} \longrightarrow -i\hbar\nabla - q\mathbf{A} \quad \text{and} \quad \hat{H} \longrightarrow \hat{H} + q\Phi . \quad (9.10)$$

In the case of the electron ( $q = -e$ ) trapped in a central Coulomb potential  $q\Phi = -\frac{Ze^2}{4\pi\epsilon_0 r}$  and in the presence of any magnetic potential  $\mathbf{A}$ , we thus obtain,

$$\boxed{\hat{H} = \frac{m_e}{2}\hat{\mathbf{v}}^2 + q\Phi = \frac{-\hbar^2}{2m_e}\nabla^2 - \frac{i\hbar e}{2m_e}\mathbf{A} \cdot \nabla - \frac{i\hbar e}{2m_e}\nabla \cdot \mathbf{A} + \frac{e^2\mathbf{A}^2}{2m_e} + q\Phi} . \quad (9.11)$$

The fourth term called *diamagnetic term* is quadratic in  $\mathbf{A}$  and usually so small that it can be neglected. The second and third terms describe the interaction of the electron through its momentum  $\hat{\mathbf{p}}$  with the potential vector  $\mathbf{A}$  produced by magnetic moments inside the atom or outer magnetic fields. Within the Coulomb gauge we have  $(\nabla \cdot \mathbf{A})\psi = (\mathbf{A} \cdot \nabla)\psi + \psi(\nabla \cdot \mathbf{A}) = (\mathbf{A} \cdot \nabla)\psi$ , such that,

$$\boxed{\hat{H}_{int} = \frac{e}{m_e}\mathbf{A} \cdot \hat{\mathbf{p}}} . \quad (9.12)$$

**Example 46 (Interaction Hamiltonian in dipolar approximation):** Note that the Hamiltonian (9.11) has been obtained from a gauge transformation in (2.205). With the particular choice for the gauge field,

$$\chi(\mathbf{r}, t) \equiv -\mathbf{A}(\mathbf{r}, t) \cdot \mathbf{r} ,$$

assuming that the potential only weakly varies in space, such that,

$$\nabla\chi(\mathbf{r}, t) \simeq -\mathbf{A}(\mathbf{r}, t) \quad \text{and} \quad \frac{\partial\chi(\mathbf{r}, t)}{\partial t} = -\mathbf{r} \cdot \frac{\partial\mathbf{A}(\mathbf{r}, t)}{\partial t} = -\mathbf{r} \cdot \vec{\mathcal{E}}(\mathbf{r}, t) ,$$

we get with  $\mathbf{d} \equiv q\mathbf{r}$ ,

$$\begin{aligned}\hat{H} &= \frac{1}{2m_e}(\hat{\mathbf{p}} - q\mathbf{A} + \nabla\chi)^2 + q\Phi + q\frac{\partial\chi(\mathbf{r}, t)}{\partial t} \\ &\simeq \frac{\hat{\mathbf{p}}^2}{2m_e} + q\Phi - \mathbf{d} \cdot \vec{\mathcal{E}}(\mathbf{r}, t),\end{aligned}\quad (9.13)$$

with  $\mathbf{d} \equiv q\mathbf{r}$ . This is the interaction Hamiltonian in the dipolar approximation.

### 9.1.3 Exercises

#### 9.1.3.1 Ex: Lagrangian of an electron in the electromagnetic field

- Show that the Lagrangian (9.3) reproduces the Lorentz force (9.1).
- Show that the Hamiltonian (9.5) reproduces the Lorentz force (9.1).

## 9.2 Interaction with magnetic fields

### 9.2.1 Normal Zeeman effect of the fine structure

The dipole moments of atoms can interact with external magnetic fields. The interaction leads to a shift of levels, which depends on the magnetic quantum number. Thus, the ultimate degeneracy in the energetic structure of the atom is lifted. This is called *Zeeman splitting*. We consider a uniform magnetic field  $\vec{\mathcal{B}} = \mathcal{B}\hat{\mathbf{e}}_z$  with the potential vector,

$$\mathbf{A} = \frac{1}{2}\vec{\mathcal{B}} \times \mathbf{r} = -\frac{\mathcal{B}}{2}(-y\hat{\mathbf{e}}_x + x\hat{\mathbf{e}}_y). \quad (9.14)$$

Thus the interaction energy between the electron and the field is given by the Hamiltonian (9.12),

$$\begin{aligned}\hat{V}_{zee}(B) &= -\frac{i\hbar e}{m_e}\mathbf{A} \cdot \nabla = -\frac{i\hbar e}{2m_e}(\vec{\mathcal{B}} \times \mathbf{r}) \cdot \nabla = -\frac{i\hbar e}{2m_e}\vec{\mathcal{B}} \cdot (\mathbf{r} \times \nabla) \\ &= -\frac{e}{2m_e}\vec{\mathcal{B}} \cdot \hat{\mathbf{L}} = -\frac{\mu_B}{\hbar}g_L\hat{\mathbf{L}} \cdot \vec{\mathcal{B}} = -\vec{\mu}_L \cdot \vec{\mathcal{B}} = -\frac{\mu_B}{\hbar}\hat{L}_z\mathcal{B},\end{aligned}\quad (9.15)$$

with  $g_L = 1$  using the relation (8.94),  $\vec{\mu}_L = \frac{e}{2m_e}\mathbf{L}$ , between the angular momentum of the electron and the resulting magnetic moment. This relationship holds for an atom without spin (two electrons can couple their spins to a singlet state) and no hyperfine structure (or an unresolved hyperfine structure). The energies are therefore,

$$\boxed{\Delta E_{zee}(\mathcal{B}) = -\frac{\mu_B}{\hbar}\mathcal{B}\langle n, L, m_L | \hat{L}_z | n, L, m_L \rangle = -\mu_B m_L \mathcal{B}}. \quad (9.16)$$

In the Excs. 9.2.8.1 and 9.2.8.2 we represent the interaction between an atomic angular momentum and a magnetic field in different bases characterized by different quantization axes.

### 9.2.2 Anomalous Zeeman effect

The anomalous Zeeman effect occurs when the ensemble of electrons has a spin. Using the already known expressions for the dipole moments of the orbital momentum and the spin of the electron, we obtain for the magnetic dipole moment,

$$\vec{\mu}_J = \vec{\mu}_L + \vec{\mu}_S = \frac{\mu_B}{\hbar} g_L \hat{\mathbf{L}} + \frac{\mu_B}{\hbar} g_S \mathbf{S} = \frac{\mu_B}{\hbar} (\hat{\mathbf{L}} + 2\hat{\mathbf{S}}), \quad (9.17)$$

with  $g_L = 1$  and  $g_S = g_e = 2$ . We can see that the dipole moment of the atom is not parallel to the total momentum,  $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ .

When the magnetic field is weak,  $\hat{V}_{ls} \gg \hat{V}_{zee}(\mathcal{B})$ , the total momentum  $\hat{\mathbf{J}}$  will be a good observable. Therefore, we must first project the momenta  $\hat{\mathbf{L}}$  and  $\hat{\mathbf{S}}$  onto  $\hat{\mathbf{J}}$ ,

$$\hat{\mathbf{L}} \longrightarrow \left( \hat{\mathbf{L}} \cdot \frac{\hat{\mathbf{J}}}{|\hat{\mathbf{J}}|} \right) \frac{\hat{\mathbf{J}}}{|\hat{\mathbf{J}}|} \quad \text{and} \quad \hat{\mathbf{S}} \longrightarrow \left( \hat{\mathbf{S}} \cdot \frac{\hat{\mathbf{J}}}{|\hat{\mathbf{J}}|} \right) \frac{\hat{\mathbf{J}}}{|\hat{\mathbf{J}}|}, \quad (9.18)$$

before projecting the result onto the  $\vec{\mathcal{B}}$ -field. The potential is,

$$\begin{aligned} \hat{V}_{zee}(\mathcal{B}) &= -\vec{\mu}_J \cdot \vec{\mathcal{B}} = -\frac{\mu_B}{\hbar} (\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) \cdot \vec{\mathcal{B}} \longrightarrow -\frac{\mu_B}{\hbar} \left[ \left( \hat{\mathbf{L}} \cdot \frac{\hat{\mathbf{J}}}{|\hat{\mathbf{J}}|} \right) \frac{\hat{\mathbf{J}}}{|\hat{\mathbf{J}}|} \cdot \vec{\mathcal{B}} + 2 \left( \hat{\mathbf{S}} \cdot \frac{\hat{\mathbf{J}}}{|\hat{\mathbf{J}}|} \right) \frac{\hat{\mathbf{J}}}{|\hat{\mathbf{J}}|} \cdot \vec{\mathcal{B}} \right] \\ &= -\frac{\mu_B}{\hbar |\hat{\mathbf{J}}|^2} \left[ \hat{\mathbf{L}} \cdot \hat{\mathbf{J}} + 2\hat{\mathbf{S}} \cdot \hat{\mathbf{J}} \right] \hat{\mathbf{J}} \cdot \vec{\mathcal{B}} = -\frac{\mu_B}{\hbar |\hat{\mathbf{J}}|^2} \frac{1}{2} \left[ \hat{\mathbf{J}}^2 + \hat{\mathbf{L}}^2 - \hat{\mathbf{S}}^2 + 2(\hat{\mathbf{J}}^2 + \hat{\mathbf{S}}^2 - \hat{\mathbf{L}}^2) \right] \hat{\mathbf{J}} \cdot \vec{\mathcal{B}} \\ &= -\frac{\mu_B}{\hbar} \frac{1}{2} \frac{3\hat{\mathbf{J}}^2 - \hat{\mathbf{L}}^2 + \hat{\mathbf{S}}^2}{|\hat{\mathbf{J}}|^2} \hat{\mathbf{J}} \cdot \vec{\mathcal{B}}. \end{aligned} \quad (9.19)$$

And the energy is,

$$\Delta E_{zee}(\mathcal{B}) = \left\langle \frac{\mu_B}{\hbar} \left( 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)} \right) \hat{\mathbf{J}} \cdot \vec{\mathcal{B}} \right\rangle. \quad (9.20)$$

Introducing the *Landé factor*,

$$g_J \equiv 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}, \quad (9.21)$$

we can write

$$\Delta E_{zee}(\mathcal{B}) = -\frac{\mu_B}{\hbar} g_J \langle \hat{J}_z \rangle \mathcal{B} = -\mu_B g_J m_J \mathcal{B}. \quad (9.22)$$

This expression describes the *anomalous Zeeman effect*, for which  $S \neq 0$ . For the *normal Zeeman effect*, for which the spin is zero, we find again  $g_J = 1$ .

### 9.2.3 Paschen-Back effect and intermediate magnetic fields

A very strong external magnetic field ( $> 1$  T), such that  $\hat{V}_{ls} \ll \hat{V}_{zee}(\mathcal{B})$ , can break the  $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$ -coupling. Both spins  $\hat{\mathbf{L}}$  and  $\hat{\mathbf{S}}$  now couple separately to the field,

$$\hat{\mathbf{L}} \longrightarrow \left( \hat{\mathbf{L}} \cdot \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \right) \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \quad \text{and} \quad \hat{\mathbf{S}} \longrightarrow \left( \hat{\mathbf{S}} \cdot \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \right) \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|}. \quad (9.23)$$

Therefore,

$$\hat{V}_{pb}(\mathcal{B}) = -\frac{\mu_B}{\hbar} (\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) \cdot \vec{\mathcal{B}} \longrightarrow -\frac{\mu_B}{\hbar} \left[ \left( \hat{\mathbf{L}} \cdot \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \right) \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} + 2 \left( \hat{\mathbf{S}} \cdot \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \right) \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \right] \cdot \vec{\mathcal{B}}, \quad (9.24)$$

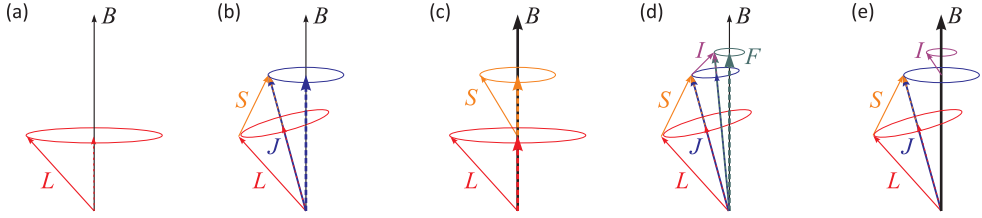


Figure 9.1: Coupling angular momenta for the effect (a) Normal Zeeman effect, (b) anomalous Zeeman effect, (c) Paschen-Back effect, (d) Zeeman effect of the hyperfine structure, and (e) Paschen-Goudsmith effect.

such that

$$\Delta E_{pb}(\mathcal{B}) = -\mu_B(m_L + 2m_S)\mathcal{B} . \quad (9.25)$$

This is the *Paschen-Back effect*.

The derivations we have made so far have focused on simple situations well described by CSCOs in various coupling schemes. The projections on the different quantization axes [the total spin (9.18) in the Zeeman case or the applied magnetic field (9.23) in the Paschen-Back case] ensure that the Hamiltonians  $\hat{V}_{ls}$  and  $\hat{V}_{zee}(\mathcal{B})$  in these CSCOs are described by diagonal matrices. However, in regimes *intermediate* between Zeeman and Paschen-Back,  $\hat{V}_{ls} \simeq \hat{V}_{zee}(\mathcal{B})$ , it is generally not possible to find a diagonal representation.

In order to calculate the energy spectrum in intermediate regimes we must, therefore, determine all the components of the matrix,

$$\hat{V}_{ls} + \hat{V}_{zee}(\mathcal{B}) = \xi(r)\hat{\mathbf{L}} \cdot \hat{\mathbf{S}} + \frac{\mu_B}{\hbar}(\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) . \quad (9.26)$$

Using  $\hat{L}_{\pm} \equiv \hat{L}_x \pm i\hat{L}_y$  and  $\hat{S}_{\pm} \equiv \hat{S}_x \pm i\hat{S}_y$ , we can easily rewrite the energy in the following way,

$$\hat{V}_{ls} + \hat{V}_{zee}(\mathcal{B}) = \xi(r) \left( \hat{L}_z \hat{S}_z + \frac{1}{2} \hat{L}_+ \hat{S}_- + \frac{1}{2} \hat{L}_- \hat{S}_+ \right) + \frac{\mu_B}{\hbar} (\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) \cdot \vec{\mathcal{B}} . \quad (9.27)$$

This operator acts on the uncoupled states,

$$\begin{aligned} \Delta E_{ls} + \Delta E_{zee}(\mathcal{B}) &= \langle L' m'_L; S' m'_S | \xi_{nl} (\hat{L}_z \hat{S}_z + \frac{1}{2} \hat{L}_+ \hat{S}_- + \frac{1}{2} \hat{L}_- \hat{S}_+) + \mu_B (\hat{L}_z + 2\hat{S}_z) \mathcal{B} | L m_L; S m_S \rangle \\ &= \hbar^2 \xi_{nl} \left( m_L m_S \delta_{m_L, m'_L} \delta_{m_S, m'_S} + \frac{1}{2} L_+ S_- \delta_{m_L, m'_L-1} \delta_{m_S-1, m'_S} + \frac{1}{2} L_- S_+ \delta_{m_L-1, m'_L} \delta_{m_S, m'_S-1} \right) \\ &\quad + \hbar \mu_B (m_L + 2m_S) \mathcal{B} \delta_{m_L, m'_L} \delta_{m_S, m'_S} , \end{aligned} \quad (9.28)$$

with the abbreviations  $L_{\pm} \equiv \sqrt{L(L+1) - m_L(m_L \pm 1)}$ . The energies are now the eigenvalues of this matrix. The factor  $\xi_{nl}$  is usually determined experimentally by letting  $\mathcal{B} = 0$ . In Exc. 9.2.8.3 we calculate the re-coupling of the spins of two electrons in an external magnetic field.



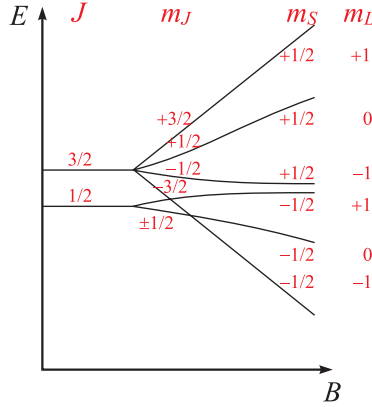


Figure 9.2: Transition between the Zeeman regime and the Paschen-Back regime for the case  $L = 1$  and  $S = 1/2$ .

### 9.2.4 Zeeman effect of the hyperfine structure

When the energy of the interaction with the magnetic field is comparable to the hyperfine interactions, but much weaker than that of the fine interactions, the fields do not disturb the coupling between the total electronic momentum  $\hat{\mathbf{J}}$  and the spin of the nucleus  $\hat{\mathbf{I}}$ . Hence,  $J, I, F$ , and  $m_F$  are good quantum numbers. Therefore, to calculate the interaction energy,

$$\hat{V}_{hfs} + \hat{V}_{zee}(\mathcal{B}) = \hat{V}_{hfs} - \vec{\mu}_F \cdot \vec{\mathcal{B}}, \quad (9.29)$$

where  $\vec{\mu}_F$  is the total magnetic momentum,

$$\vec{\mu}_F = \vec{\mu}_J + \vec{\mu}_I = -\frac{\mu_B}{\hbar} g_J \hat{\mathbf{J}} + \frac{\mu_N}{\hbar} g_p \hat{\mathbf{I}}. \quad (9.30)$$

we project the nuclear spin and the total electronic momentum separately in the direction of  $\hat{\mathbf{F}}$ ,

$$\hat{\mathbf{J}} \longrightarrow \left( \hat{\mathbf{J}} \cdot \frac{\hat{\mathbf{F}}}{|\mathbf{F}|} \right) \frac{\hat{\mathbf{F}}}{|\mathbf{F}|} \quad \text{and} \quad \hat{\mathbf{I}} \longrightarrow \left( \hat{\mathbf{I}} \cdot \frac{\hat{\mathbf{F}}}{|\mathbf{F}|} \right) \frac{\hat{\mathbf{F}}}{|\mathbf{F}|}. \quad (9.31)$$

Note the negative sign in (9.30) due to the negative charge of the electron. The Landé factor  $g_J$  [see (9.21)] is the one caused by the coupling of the orbital angular momentum  $\hat{\mathbf{L}}$  and the electron spin  $\hat{\mathbf{S}}$  and depends on the state under consideration. Thereby,

$$\begin{aligned} \hat{V}_{zee}(\mathcal{B}) &= \left[ -\frac{\mu_B}{\hbar} g_J \left( \hat{\mathbf{J}} \cdot \frac{\hat{\mathbf{F}}}{|\mathbf{F}|} \right) \frac{\hat{\mathbf{F}}}{|\mathbf{F}|} + \frac{\mu_N}{\hbar} g_p \left( \hat{\mathbf{I}} \cdot \frac{\hat{\mathbf{F}}}{|\mathbf{F}|} \right) \frac{\hat{\mathbf{F}}}{|\mathbf{F}|} \right] \vec{\mathcal{B}} \\ &= \left( -\frac{\mu_B}{\hbar |\mathbf{F}|^2} g_J \hat{\mathbf{J}} \cdot \hat{\mathbf{F}} + \frac{\mu_N}{\hbar |\mathbf{F}|^2} g_p \hat{\mathbf{I}} \cdot \hat{\mathbf{F}} \right) (\mathcal{B} \cdot \hat{F}_z). \end{aligned} \quad (9.32)$$

Using  $\hat{\mathbf{J}} \cdot \hat{\mathbf{F}} = \frac{1}{2}(\hat{\mathbf{F}}^2 + \hat{\mathbf{J}}^2 - \hat{\mathbf{I}}^2)$  and  $\hat{\mathbf{I}} \cdot \hat{\mathbf{F}} = \frac{1}{2}(\hat{\mathbf{F}}^2 - \hat{\mathbf{J}}^2 + \hat{\mathbf{I}}^2)$  we write,

$$\hat{V}_{zee}(\mathcal{B}) = -\frac{\mu_B}{\hbar} g_J \frac{\hat{\mathbf{F}}^2 + \hat{\mathbf{J}}^2 - \hat{\mathbf{I}}^2}{2|\mathbf{F}|^2} \mathcal{B} \hat{F}_z + g_p \frac{\mu_N}{\hbar} \frac{\hat{\mathbf{F}}^2 - \hat{\mathbf{J}}^2 + \hat{\mathbf{I}}^2}{2|\mathbf{F}|^2} \mathcal{B} \hat{F}_z, \quad (9.33)$$

such that

$$\boxed{\Delta E_{hfs} + \Delta E_{zee}(\mathcal{B}) \simeq \Delta E_{hfs} + \mu_B g_F m_F \mathcal{B}}, \quad (9.34)$$

using the *Landé factor*  $g_F$  for the state  $F$ ,

$$g_F \simeq g_J \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)} - g_p \frac{\mu_N}{\mu_B} \frac{F(F+1) - J(J+1) + I(I+1)}{2F(F+1)}, \quad (9.35)$$

where the second term can be neglected.

The splitting of electronic states with the momentum  $\hat{\mathbf{F}}$  into  $2F + 1$  sublevels  $m_F = -F, \dots, F$  is called *Zeeman effect of the hyperfine structure*. The result (9.32) only applies to weak magnetic fields. For strong fields the Zeeman splitting becomes a Paschen-Back splitting of the hyperfine structure.

### 9.2.5 Paschen-Back effect of the hyperfine structure

When the interaction with the magnetic field exceeds the hyperfine interaction, the nuclear spin  $\hat{\mathbf{I}}$  decouples from the total momentum  $\hat{\mathbf{J}}$ , and both couple separately to the external magnetic field,

$$\hat{\mathbf{J}} \longrightarrow \left( \hat{\mathbf{J}} \cdot \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \right) \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \quad \text{and} \quad \hat{\mathbf{I}} \longrightarrow \left( \hat{\mathbf{I}} \cdot \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|} \right) \frac{\vec{\mathcal{B}}}{|\vec{\mathcal{B}}|}. \quad (9.36)$$

The Zeeman effect of the hyperfine structure becomes a hyperfine structure of the Zeeman effect, also called *Paschen-Back effect of the hyperfine structure* or *Paschen-Goudsmith effect*. We can diagonalize the potential on a basis, where  $I, m_I, J$ , and  $m_J$  are good quantum numbers. Using the expression (8.169) but disregarding the quadrupolar contribution to the hyperfine interaction,  $B_J \simeq 0$ , we obtain,

$$\begin{aligned} \hat{V}_{hfs} + \hat{V}_{zee}(\mathcal{B}) &= \hat{V}_{hfs} - (\vec{\mu}_J + \vec{\mu}_I \overset{\simeq 0}{\longrightarrow}) \cdot \vec{\mathcal{B}} \simeq \frac{A_J}{\hbar^2} \hat{\mathbf{J}} \cdot \hat{\mathbf{I}} - \vec{\mu}_J \cdot \vec{\mathcal{B}} \\ &\longrightarrow \frac{A_J}{\hbar^2} \left( \hat{\mathbf{J}} \cdot \frac{\vec{\mathcal{B}}}{\mathcal{B}} \right) \frac{\vec{\mathcal{B}}}{\mathcal{B}} \cdot \left( \hat{\mathbf{I}} \cdot \frac{\vec{\mathcal{B}}}{\mathcal{B}} \right) \frac{\vec{\mathcal{B}}}{\mathcal{B}} - \mu_{Jz} \mathcal{B} = \frac{A_J}{\hbar^2} \hat{J}_z \hat{I}_z + \frac{\mu_B}{\hbar} g_J \hat{J}_z \mathcal{B}, \end{aligned} \quad (9.37)$$

where we neglect the interaction of the dipole moment of the nucleus with the external magnetic field,  $\vec{\mu}_I \simeq 0$ . We obtain for strong magnetic fields,

$$\boxed{\Delta E_{hfs} + \Delta E_{zee}(\mathcal{B}) \simeq A_J m_J m_I + \mu_B g_J m_J \mathcal{B}}. \quad (9.38)$$

The re-coupling of the state  $|F m_F\rangle$  to  $|m_I m_J\rangle$  in strong magnetic fields is described by Clebsch-Gordan coefficients,

$$|F m_F\rangle = \sum_{m_I + m_J = m_F} |m_I m_J\rangle \langle m_I m_J | F m_F\rangle. \quad (9.39)$$

**Example 47 (Nuclear magnetic resonance):** In Eq. (9.37) we have neglected the nuclear dipole moment for being small in comparison to the electronic one. Taking it into account, we get an additional term  $\hat{V}_{nmr}$ ,

$$\hat{V}_{hfs} + \hat{V}_{zee} + \hat{V}_{nmr} = \frac{A_J}{\hbar^2} \hat{\mathbf{J}} \cdot \hat{\mathbf{I}} + \vec{\mu}_J \cdot \vec{\mathcal{B}} + \vec{\mu}_I \cdot \vec{\mathcal{B}} = \frac{A_J}{\hbar^2} \hat{J}_z \hat{I}_z + \mu_{Jz} \mathcal{B} + \mu_{Iz} \mathcal{B}. \quad (9.40)$$

Considering a hydrogen atom  $^1\text{H}$  in a  $\vec{\mathcal{B}} = 10\text{ T}$  strong magnetic field, we have the following hierarchy of energies:

$$\begin{aligned}\Delta E_{zee}(\mathcal{B}) &= \mu_B g_e m_J \simeq h \cdot 140\text{ GHz} \\ \Delta E_{hfs}(\mathcal{B}) &\simeq h \cdot 1.4\text{ GHz} \\ \Delta E_{nmr}(\mathcal{B}) &= \mu_N g_p m_I \simeq h \cdot 213\text{ MHz} ,\end{aligned}\tag{9.41}$$

where  $g_e = 2.002..$  is the g-factor of the electron and  $g_p = 5.586..$  of the proton. Now, in large molecules the most electrons are paired, such that  $\hat{\mathbf{J}} = 0$ . In that case, we are left with the interaction between the nuclear spin and the applied magnetic field,

$$\Delta E_{nmr}(\mathcal{B}) = \mu_N g_I m_I \mathcal{B} ,\tag{9.42}$$

where the g-factor of the nucleus  $g_I$  must be looked up in data tables. This is the regime where *nuclear magnetic resonances* (NMR) can be excited with a large variety of applications in spectroscopy and imaging.

## 9.2.6 Hyperfine structure in the intermediate field regime

Knowing the dipolar magnetic  $A_J$  and quadrupolar  $B_J$  interval factors, it is possible to calculate the Zeeman shift of the hyperfine structure in magnetic fields intermediate between the Zeeman and Paschen-Back regimes. For this, we must determine all the components of the matrix  $\hat{V}_{hfs} + \hat{V}_{zee}(\mathcal{B})$  and calculate the eigenvalues. The relevant terms of the Eqs. (8.169) and the Eq. (9.36) are,

$$\hat{V}_{hfs} + \hat{V}_{zee}(\mathcal{B}) = \frac{A_J}{\hbar^2} \hat{\mathbf{I}} \cdot \hat{\mathbf{J}} + \frac{B_J}{\hbar^2} \frac{6(\hat{\mathbf{I}} \cdot \hat{\mathbf{J}})^2 + 3\hat{\mathbf{I}} \cdot \hat{\mathbf{J}} - 2\hat{\mathbf{J}}^2 \hat{\mathbf{I}}^2}{2I(2I-1)2J(2J-1)} + g_J \mu_B \vec{\mathcal{B}} \cdot \hat{\mathbf{J}} - g_I \mu_N \vec{\mathcal{B}} \cdot \hat{\mathbf{I}} .\tag{9.43}$$

We develop the complete matrix representation of this Hamiltonian within the uncoupled base, where  $m_J, m_I$  are good quantum numbers, introducing the abbreviations  $I_{\pm} \equiv \sqrt{I(I+1) - m_I(m_I \pm 1)}$  and  $I_{\pm\pm} \equiv \sqrt{I(I+1) - (m_I \pm 1)(m_I \pm 2)}$ . The SU(2) algebra provides useful expressions,  $\hat{\mathbf{I}} \cdot \hat{\mathbf{J}} = \hat{I}_z \hat{J}_z + \frac{1}{2}(\hat{I}_+ \hat{J}_- + \hat{I}_- \hat{J}_+)$ . The elements of the matrix are,

$$\begin{aligned}\langle m'_I m'_J | H_{hfs} + H_B | m_I m_J \rangle &= \left[ A_J + \frac{3B_J}{2I(2I-1)2J(2J-1)} \right] \times \\ &\times \left\{ m_I m_J \delta_{m'_I m_I} \delta_{m'_J m_J} + \frac{1}{2} I_+ J_- \delta_{m'_I m_I+1} \delta_{m'_J m_J-1} + \frac{1}{2} I_- J_+ \delta_{m'_I m_I-1} \delta_{m'_J m_J+1} \right\} \\ &+ \frac{6B_J}{2I(2I-1)2J(2J-1)} \langle m'_I m'_J | \left( \frac{\hat{\mathbf{I}} \cdot \hat{\mathbf{J}}}{\hbar} \right)^2 | m_I m_J \rangle \\ &+ \left[ -\frac{B_J 2I(I+1)J(J+1)}{2I(2I-1)2J(2J-1)} + (g_J m_J - g_I \mu_N m_I) \mu_B \mathcal{B} \right] \delta_{m'_I m_I} \delta_{m'_J m_J}\end{aligned}\tag{9.44}$$

where

$$\begin{aligned}\langle m'_I m'_J | \left( \frac{\hat{\mathbf{I}} \cdot \hat{\mathbf{J}}}{\hbar} \right)^2 | m_I m_J \rangle &= [(m_I m_J)^2 + \frac{1}{4} I_-^2 J_+^2 + \frac{1}{4} I_+^2 J_-^2] \delta_{m'_I m_I} \delta_{m'_J m_J} + \\ &+ \frac{1}{2} (m'_I m'_J + m_I m_J) I_+ J_- \delta_{m'_I m_I+1} \delta_{m'_J m_J-1} + \\ &+ \frac{1}{2} (m'_I m'_J + m_I m_J) I_- J_+ \delta_{m'_I m_I-1} \delta_{m'_J m_J+1} + \\ &+ \frac{1}{4} I_+ J_- I_{++} J_{--} \delta_{m'_I m_I+2} \delta_{m'_J m_J-2} + \\ &+ \frac{1}{4} I_- J_+ I_{--} J_{++} \delta_{m'_I m_I-2} \delta_{m'_J m_J+2} .\end{aligned}\tag{9.45}$$

The matrix  $\langle m'_I m'_J | H_{hfs} + H_B | m_I m_J \rangle$  is divided into  $2F + 1$  diagonal blocks, each labeled  $m_F$ . The total number of levels is,

$$\sum_{F=|I-J|, \dots, I+J} 2F+1 = (2I+1)(2J+1) = \sum_{m_F=-F, \dots, F} \left( \sum_{\substack{m_I=-I, \dots, I, \\ m_J=-J, \dots, J, \\ m_I+m_J=m_F}} 1 \right).$$

In this form the matrix can be programmed, e.g. using computational software such as MATLAB, and all eigenvalues of the Hamiltonian for any state  $^{2S+1}X_J$  and nuclear spin  $I$  can be calculated numerically. Obviously, the eigenvalues follow from a diagonalization of the matrix and do not depend on the chosen base. Fig. 9.3 shows the result obtained for  ${}^6\text{Li}$  ( $I = \frac{3}{2}$ ) in the state  $2s\ ^2P_{3/2}$  knowing that  $A_J/h = -1.17$  MHz and  $B_J = 0$ .

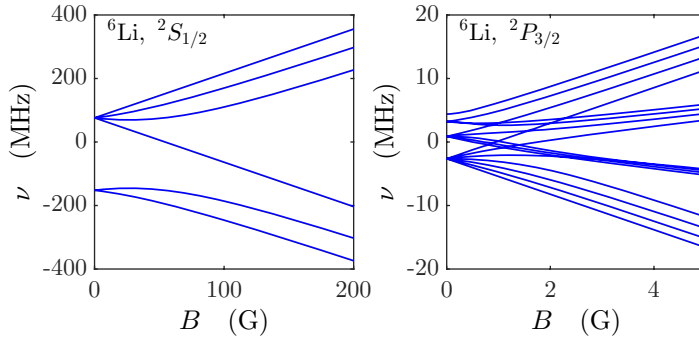


Figure 9.3: (code) Hyperfine and Zeeman structure of the state  ${}^2P_{3/2}$  of  ${}^6\text{Li}$ .

**Example 48 (Fully stretched states):** It is interesting to analyze the so-called *fully stretched Zeeman states* defined by  $F = I + J$  and  $|m_F| = F$ . For these states, the spin  $K$  defined in (8.168) becomes,

$$\begin{aligned} K &\equiv 2(\hat{\mathbf{J}} \cdot \hat{\mathbf{I}}) = F(F+1) - I(I+1) - J(J+1) \\ &= (I+J)(I+J+1) - I(I+1) - J(J+1) = 2JI, \end{aligned}$$

and the hyperfine structure (8.169) becomes,

$$\Delta E_{hfs} = \frac{A_J}{2} K + \frac{B_J}{8I(2I-1)J(2J-1)} [3K(K+1) - 4I(I+1)J(J+1)] = A_J IJ + \frac{B_J}{4}.$$

That is, the hyperfine structure does not depend on the  $F$  quantum number at any  $\mathcal{B}$ -field amplitude, which means that the  $m_J$ ,  $m_I$ , and  $m_F$  will be good quantum numbers at arbitrary  $\mathcal{B}$ -field strengths. So see this, we calculate the Landé-factor (9.35),

$$g_F = g_J \frac{J}{F} - g_J \frac{\mu_N}{\mu_B} \frac{I}{F},$$

and consider the particular Zeeman state  $m_F = F$ ,  $m_J = J$ , and  $m_I = I$ ,

$$\begin{aligned} \hat{V}_{hfs} + \hat{V}_{ze}(\mathcal{B}) &= A_J IJ + \frac{B_J}{4} + g_J \mu_B \vec{\mathcal{B}} \cdot \hat{\mathbf{J}} - g_I \mu_N \vec{\mathcal{B}} \cdot \hat{\mathbf{I}} \\ &= A_J IJ + \frac{B_J}{4} + \mu_B g_F m_F \mathcal{B} = A_J IJ + \frac{B_J}{4} + (\mu_B g_J J - \mu_N g_J I) \mathcal{B}. \end{aligned}$$

The energy displacement of the fully stretched states is always linear in the magnetic field. We can also look at the matrix elements  $I_+ = 0$  and  $I_- = \sqrt{2I}$  and note that all non-diagonal terms vanish.

When one of the spins,  $J$  or  $I$ , is equal to  $1/2$  only two possible hyperfine states exist:  $F = I \pm J$ . For this case there is an approximate analytic formula called the *Breit-Rabi formula* [42], which will be derived in Exc. 9.2.8.4,

$$\begin{aligned} \Delta E_{hfs} + \Delta E_{zee}(\mathcal{B}) &= \langle \frac{A_J}{\hbar^2} \hat{\mathbf{I}} \cdot \hat{\mathbf{J}} + g_J \mu_B \vec{\mathcal{B}} \cdot \hat{\mathbf{J}} - g_I \mu_N \vec{\mathcal{B}} \cdot \hat{\mathbf{I}} \rangle \\ &= -\frac{A_J}{4} + \mu_N g_N m_F \mathcal{B} \pm \frac{A_J(I + \frac{1}{2})}{2} \sqrt{1 + \frac{4m_F}{2I + 1} x + x^2}, \end{aligned} \quad (9.46)$$

with the abbreviation  $x \equiv \frac{2(\mu_B g_J - \mu_N g_I) \mathcal{B}}{A_J}$ . Resolve also Exc. 9.2.8.5.

Atoms with paired electrons have no spin and therefore no magnetic dipole moment. For example, helium or strontium in their ground state  $^1S_0$ . These systems are diamagnetic due to the Hamiltonian term (9.11) being quadratic in  $\vec{\mathcal{B}}$ , as we shall see in Exc. 9.2.8.6.

## 9.2.7 Landau levels in two-dimensional systems subject to magnetic fields

Magnetic field can also have interesting effects in *artificial atoms*, e.g. quantum dots. An important example is the formation of *Landau levels*. We consider a two-dimensional system of non-interacting particles with charge  $q$  and spin  $S$  confined to an area  $A = L_x L_y$  in the  $x$ - $y$  plane. We apply a uniform magnetic field,

$$\vec{\mathcal{B}} = \mathcal{B} \hat{e}_z \quad (9.47)$$

along the  $z$  axis. The Hamiltonian of this system is,

$$\hat{H} = \frac{1}{2m} (\hat{\mathbf{p}} - q \hat{\mathbf{A}})^2, \quad (9.48)$$

where  $\hat{\mathbf{p}}$  is the operator of the canonical momentum and  $\hat{\mathbf{A}}$  is the potential vector, related to the magnetic field by  $\vec{\mathcal{B}} = \nabla \times \hat{\mathbf{A}}$ . The vector potential,

$$\mathbf{A} = \frac{1}{2} \begin{pmatrix} -\mathcal{B}y \\ \mathcal{B}x \\ 0 \end{pmatrix} \quad (9.49)$$

reproduces the field (9.47). However, we have the freedom in choosing the potential vector, given by the gauge transformation, to add the gradient of a scalar field, for example,

$$\chi \equiv \frac{1}{2} \mathcal{B}xy \quad \Rightarrow \quad \nabla \chi = \frac{1}{2} \begin{pmatrix} \mathcal{B}y \\ \mathcal{B}x \\ 0 \end{pmatrix} \quad \Rightarrow \quad \mathbf{A}' \equiv \mathbf{A} + \nabla \chi = \mathcal{B}x \hat{e}_y. \quad (9.50)$$

The potential vector  $\mathbf{A}'$  gives the same magnetic field and only changes the general phase of the wavefunction, but the physical properties do not change. In this gauge,

which is called *Landau gauge*, the Hamiltonian is,

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2m} \left( \hat{p}_y - \frac{q\mathcal{B}}{c} \hat{x} \right)^2 . \quad (9.51)$$

The operator  $\hat{p}_y$  commutes with this Hamiltonian, since the  $\hat{y}$  operator is absent due to the choice of the gauge. Thus, the operator  $\hat{p}_y$  can be replaced by its eigenvalue  $\hbar k_y$ . Hence, by introducing the *cyclotron frequency*,

$$\omega_c \equiv \frac{q\mathcal{B}}{mc} , \quad (9.52)$$

we obtain,

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{m\omega_c^2}{2} \left( \hat{x} - \frac{\hbar k_y}{m\omega_c} \right)^2 . \quad (9.53)$$

This is exactly the Hamiltonian of the quantum harmonic oscillator, except that the minimum of the potential is displaced in position space by the value,

$$x_0 \equiv \frac{\hbar k_y}{m\omega_c} . \quad (9.54)$$

To find the energies, we note that the translation of the potential of the harmonic oscillator does not affect the energies. The energies of this system are therefore identical to those of the standard quantum harmonic oscillator,

$$E_n = \hbar\omega_c \left( n + \frac{1}{2} \right) , \quad (9.55)$$

for  $n \geq 0$ . Since the energy does not depend on the quantum number  $k_y$ , we will have degeneracy. To derive the wavefunctions, we remember that  $\hat{p}_y$  commutes with the Hamiltonian. Then the wavefunction splits into a product of eigenstates of the momentum in  $y$ -direction and eigenstates of the harmonic oscillator  $|\phi_n\rangle$  shifted by a value  $x_0$  in  $x$ -direction:

$$\Psi(x, y) = e^{ik_y y} \phi_n(x - x_0) . \quad (9.56)$$

That is, the state of the electron is characterized by two quantum numbers,  $n$  and  $k_y$ .

Each set of wavefunctions with the same  $n$  is called *Landau level*. Effects due to Landau levels are only observed, when the average thermal energy is lower than the separation of the energy levels, which means that low temperatures and strong magnetic fields are required. Each Landau level is degenerate, because of the second quantum number  $k_y$ , which can adopt the values,

$$k_y = \frac{2\pi N}{L_y} , \quad (9.57)$$

with  $N \in \mathbb{N}$ . The allowed values of  $N$  are further restricted by the condition that the center of mass of the oscillator,  $x_0$ , must be physically inside the system,  $0 \leq x_0 < L_x$ . Using (9.54) this gives the following range for  $N$ ,

$$0 \leq N < \frac{m\omega_c L_x L_y}{2\pi\hbar} . \quad (9.58)$$

For particles with charge  $q = Ze$ , the upper limit in  $N$  can simply be written as a ratio of fluxes,

$$Z \frac{\Phi}{\Phi_0} = \frac{ZBL_xL_y}{(hc/e)} = N_{max} , \quad (9.59)$$

where  $\Phi_0 = h/2e$  is the fundamental *flux quantum* and  $\Phi = \mathcal{B}A$  the flux through the system (with area  $A = L_xL_y$ ). Thus, for particles with spin  $S$ , the maximum number of particles per Landau level is,

$$N_{max} = Z(2S + 1) \frac{\Phi}{\Phi_0} . \quad (9.60)$$

### 9.2.7.1 Integer and fractional quantum Hall effect

In general, Landau levels are observed in electronic systems with  $Z = 1$  and  $S = 1/2$ . As the magnetic field increases, more and more electrons can fit a certain Landau level. The occupation of the highest Landau level ranges from entirely full to entirely empty, leading to oscillations in various electronic properties (see *de Haas-van Alphen effect*, *Shubnikov-de Haas effect* and *quantum Hall effect*). The most direct observation

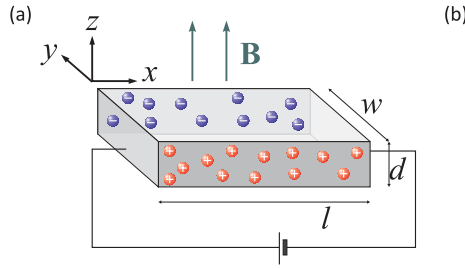


Figure 9.4: Scheme of the Quantum Hall effect.

of the Landau levels is done via the quantum Hall effect. To discuss this effect let us briefly recapitulate the Hall effect. In the scheme of Fig. 9.4, charges are deviated by the Lorentz force exerted by an applied magnetic field  $\vec{\mathcal{B}}$  from a driven current density  $j_x$  into a current density  $j_y$  until a sufficient amount of surface charge density has accumulated to generate an electric field exerting a Coulomb force on the charges which neutralizes the Lorentz force,  $\mathbf{F} = q(\vec{\mathcal{E}} + \mathbf{v} \times \vec{\mathcal{B}}) = 0$ . Resolving this condition by  $\mathbf{v}$ , we obtain for the current density,

$$\mathbf{j} = \rho q \mathbf{v} = \rho q \frac{\mathcal{E}}{\mathcal{B}} \hat{\mathbf{e}}_x = \varsigma \vec{\mathcal{E}} , \quad (9.61)$$

where the last equation is Ohm's law and

$$\varsigma = \begin{pmatrix} \varsigma_{xx} & \varsigma_{xy} \\ -\varsigma_{xy} & \varsigma_{yy} \end{pmatrix} \quad \text{and} \quad \rho = \varsigma^{-1} = \frac{1}{\varsigma_{xx}^2 + \varsigma_{yy}^2} \begin{pmatrix} \varsigma_{xx} & -\varsigma_{xy} \\ \varsigma_{xy} & \varsigma_{yy} \end{pmatrix} \quad (9.62)$$

the conductivity and the resistivity, respectively. The Hall resistivity does therefore depend linearly on the magnetic field,

$$\rho_{xy} = \frac{\mathcal{E}}{j} = \frac{\mathcal{B}}{\rho q} . \quad (9.63)$$

In two-dimensional systems this is, however, not observed. Instead, plateaus emerge whenever the magnetic field is ramped across a value where a new Landau level is possible binding one more electron,

$$\rho_{xy} = \frac{2\pi\hbar}{e^2} \frac{1}{\nu} \quad \text{with} \quad \nu \in \mathbb{Z}. \quad (9.64)$$

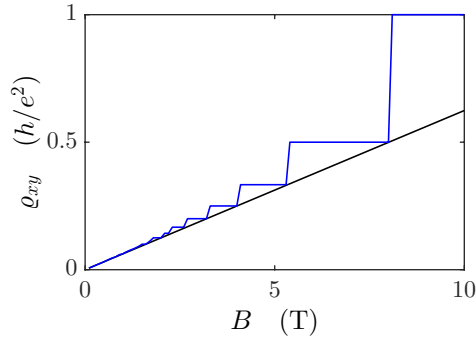


Figure 9.5: (code) Scheme of the quantum Hall effect.

## 9.2.8 Exercises

### 9.2.8.1 Ex: Zeeman effect with different quantization axes

The Zeeman effect can be described in several ways depending on the choice of the quantization axis. Consider a magnetic field  $\vec{\mathcal{B}} = \mathcal{B}_x \hat{e}_x$  and calculate the interaction Hamiltonian  $V(\mathcal{B}) = -\vec{\mu}_J \cdot \vec{\mathcal{B}}$

- choosing the quantization axis  $\hat{e}_x$  in the direction of the magnetic field,
- choosing the quantization axis  $\hat{e}_z$  perpendicular to the direction of the magnetic field.

### 9.2.8.2 Ex: Zeeman shift and quantization axes

Choosing the fixed quantization axis  $\hat{e}_z$  and a magnetic field  $\vec{\mathcal{B}}$  in an arbitrary direction, calculate the Hamiltonian of the Zeeman interaction with an angular momentum  $J = 1$  and show that the energy shift depends only on absolute value  $|\vec{\mathcal{B}}|$ .

### 9.2.8.3 Ex: Coupling of two electrons

Consider a two-electron system.

- Show that the operator  $(\hbar A / \hbar^2) \hat{s}_1 \cdot \hat{s}_2$  distinguishes the triplet from the singlet states.
- Consider now, that the electrons are exposed to a magnetic field  $B$  applied in the direction  $\hat{e}_z$ , so that they acquire the interaction energies with the field  $(\mu_B \mathcal{B} / \hbar)(g_1 \hat{s}_{1z} + g_2 \hat{s}_{2z})$ . Obtain the matrix associated with the total Hamiltonian and demonstrate that in the regime  $\hbar A \gg \mu_B \mathcal{B}$ , the representation that favors the total momentum is



more adequate.

c. Show that in the regime  $\hbar A \ll \mu_B \mathcal{B}$ , it is convenient to use the representation that privileges the *individual* spins of the total momentum.

d. Analyze the intermediate regime  $\hbar A \simeq \mu_B \mathcal{B}$ .

#### 9.2.8.4 Ex: Breit-Rabi formula

Derive the analytical Breit-Rabi formula for the hyperfine structure (9.46) supposing  $J = \frac{1}{2}$ .

#### 9.2.8.5 Ex: Reciprocal pollution of the Paschen-Back and Zeeman regimes

a. Determine the interaction matrix  $\langle \tilde{m}_J \tilde{m}_I | \hat{V}_{hfs} + \hat{V}_{zee}(B) | m_J m_I \rangle$  of an atom with electron spin  $\mathbf{J}$  and nuclear spin  $\mathbf{J}$  in the decoupled base without considering the quadrupolar terms.

b. Determine the interaction matrix explicitly for the case of  ${}^6\text{Li}$  ( $I = 1$ ) in its ground state  ${}^2S_{1/2}$  ( $A_J = h \cdot 152.137$  MHz) for a magnetic field of  $\mathcal{B} = 100$  G.

c. For the system defined in (b) determine the eigenvalues  $E(\mathcal{B})$  of the interaction matrix and the eigenvectors  $|\alpha(\mathcal{B})\rangle$  on the decoupled base  $|m_J m_I\rangle$ .

d. For the system defined in (c) determine the eigenvectors  $|\alpha(\mathcal{B})\rangle$  in the coupled base  $|F m_F\rangle$ .

e. How good are the selection rules for transitions  $S_{1/2} - P_{3/2}$  in the intermediate regime between Zeeman and Paschen-Back? We start by calculating the Zeeman shifts for both levels ( $s$  denotes the structure  $S_{1/2}$ ,  $p$  the structure  $P_{3/2}$ )

$$\begin{aligned} {}_B \langle m_J^s m_I^s | H_{hfs} + H_B | m_J^s m_I^s \rangle_B &= E^s(\mathcal{B}) \\ {}_B \langle m_J^p m_I^p | H_{hfs} + H_B | m_J^p m_I^p \rangle_B &= E^p(\mathcal{B}) . \end{aligned}$$

For the level  $P_{3/2}$  the interval factor is less. In particular for  ${}^6\text{Li}$  it is so small that we are immediately in the Paschen-Back scheme. This means that the matrix  ${}_\infty \langle \tilde{m}_J^p \tilde{m}_I^p | m_J^p m_I^p \rangle_B = \delta_{m_J^p, \tilde{m}_J^p} \delta_{m_I^p, \tilde{m}_I^p}$  is diagonal. The element of the transition matrix is then,

$$\begin{aligned} &{}_B \langle m_J^p m_I^p | T_q^{(E\kappa)} | m_J^s m_I^s \rangle_B \\ &= \sum_{\tilde{m}_J^s, \tilde{m}_I^s} \sum_{\tilde{m}_J^p, \tilde{m}_I^p} \overline{\langle \tilde{m}_J^p \tilde{m}_I^p | m_J^p m_I^p \rangle_B} \langle \tilde{m}_J^s \tilde{m}_I^s | m_J^s m_I^s \rangle_B \langle \tilde{m}_J^p \tilde{m}_I^p | T_q^{(E\kappa)} | \tilde{m}_J^s \tilde{m}_I^s \rangle_\infty \\ &= \sum_{\tilde{m}_J^s, \tilde{m}_I^s} \langle \tilde{m}_J^s \tilde{m}_I^s | m_J^s m_I^s \rangle_B \langle m_J^p m_I^p | T_q^{(E\kappa)} | \tilde{m}_J^s \tilde{m}_I^s \rangle_\infty . \end{aligned}$$

The matrix elements in the pure Zeeman regime can be expressed by [Deh07, unpublished],

$$\begin{aligned} \langle F^p m_F^p | T_q^{(E\kappa)} | F^s m_F^s \rangle_0 &= \langle m_J^p m_I^p | T_q^{(E\kappa)} | m_J^s m_I^s \rangle_0 \\ &= \begin{pmatrix} J^s & \kappa & J^p \\ m_J^s & \text{sign}(m^p - m^s) & -m_J^p \end{pmatrix}^2 \begin{Bmatrix} J^p & J^s & \kappa \\ F^s & F^p & I \end{Bmatrix}^2 \frac{(2F^s + 1)(2J^p + 1)(2\kappa + 1)}{2I + 1} . \end{aligned}$$

Discuss the pure Paschen-Back regime via  ${}_\infty \langle m_J^p m_I^p | T_q^{(E\kappa)} | m_J^s m_I^s \rangle_\infty$ .

### 9.2.8.6 Ex: Diamagnetism of the ground states of H atoms

Calculate the quadratic Zeeman effect for the ground state of the hydrogen atom caused by the (usually neglected) diamagnetic term of the Hamiltonian in first order TPIIT. Write down the energy shift as  $\Delta E = -\frac{\chi}{2}\mathcal{B}^2$  assuming a constant magnetic field in order to obtain the diamagnetic susceptibility  $\chi$ .

## 9.3 Interaction with electric fields

### 9.3.1 Stark Effect

Electric fields interact with the electrons of the atom. Describing the atom by its dipole moment, according to (9.13), the interaction energy is,

$$\hat{V}_{stark} = -\hat{\mathbf{d}} \cdot \vec{\mathcal{E}} . \quad (9.65)$$

This is the *Stark effect*. This effect is usually weak, and its observation requires strong fields or high spectral resolution. Stationary perturbation theory TIPT gives,

$$E_n^{(1)} = \langle \psi_n^{(0)} | -\hat{\mathbf{d}} \cdot \mathcal{E} | \psi_n^{(0)} \rangle = e\mathcal{E}_z \int_{\mathbb{R}^3} z |\psi_n^{(0)}|^2 d^3r = 0 , \quad (9.66)$$

with  $\mathbf{d} = -e\mathbf{r}$  and  $\vec{\mathcal{E}}_z = \mathcal{E}_z \hat{\mathbf{e}}_z$ . This only applies when the states have well-defined parity and are NOT degenerate in  $\ell$ . When they ARE degenerate in  $\ell$ , which is the case of hydrogen, the states have no defined parity  $(-1)^\ell$ . For example, the states  $s$  and  $p$  contributing to the same state  $|\psi_{n,j}\rangle$  have different parities. In this case, the condition (9.66) is not automatically satisfied, and the first perturbation order yields a value. This is the case of the *linear Stark effect*. In the Excs. 9.3.2.1 and 9.3.2.2 we explicitly calculate the Stark energy shift for a hydrogen atom subject to an electric field.

Other atoms do not have this degeneracy, and we must calculate the *quadratic Stark effect* in second order TIPT,

$$|\psi_n^{(1)}\rangle = e\mathcal{E}_z \sum_{n' \neq n} |\psi_{n'}^{(0)}\rangle \frac{\langle \psi_{n'}^{(0)} | \hat{z} | \psi_n^{(0)} \rangle}{E_n - E_{n'}} . \quad (9.67)$$

and

$$E_n^{(2)} = e^2 \mathcal{E}_z^2 \sum_{n' \neq n} \frac{|\langle \psi_{n'}^{(0)} | \hat{z} | \psi_n^{(0)} \rangle|^2}{E_n - E_{n'}} . \quad (9.68)$$

To simplify the matrix elements, we separate the radial part from the angular part,

$$\langle \psi_{n'}^{(0)} | \hat{z} | \psi_n^{(0)} \rangle = \langle n' J' m'_J | \hat{z} | n J m_J \rangle = \int_0^\infty r^3 R_{n' J'} R_{n J} dr \int Y_{J' m'_J}^* \frac{z}{r} Y_{J m_J} d\Omega . \quad (9.69)$$

The radial part, written as

$$\langle n' J' | | \hat{z} | | n J \rangle \equiv \int_0^\infty r^3 R_{n' J'} R_{n J} dr , \quad (9.70)$$

and called the *irreducible matrix element*, no longer depends on the magnetic quantum number. On the other hand, the angular part may be expressed by Clebsch-Gordan coefficients, as will be discussed more extensively in Sec. 13.2.3. The result is called *Wigner-Eckart theorem*,

$$\frac{\langle n'_J J' m'_J | \hat{z} | n_J J m_J \rangle}{\langle n'_J J' || \hat{z} || n_J J \rangle} = \int Y_{J' m'_J}^* \frac{\hat{z}}{r} Y_{J m_J} d\Omega = \frac{1}{2J'+1} \begin{pmatrix} J & 1 & J' \\ m_J & 0 & -m'_J \end{pmatrix}. \quad (9.71)$$

With  $[\hat{z}, \hat{L}_z] = 0$ , which was shown in Exc. 4.3.4.2, and obviously  $[\hat{z}, \hat{S}_z] = 0$  we find,

$$0 = \langle J' m'_J | [\hat{z}, \hat{J}_z] | J m_J \rangle = (m_J - m'_J) \langle J' m'_J | \hat{z} | J m_J \rangle. \quad (9.72)$$

This means that for  $m_J \neq m'_J$ , the matrix elements  $\langle J' m'_J | \hat{z} | J m_J \rangle$  should disappear. Therefore, the matrix is diagonal in  $m_J$ . We consider dipole transitions with  $|J - J'| \leq 1$ <sup>1</sup>,

$$\begin{pmatrix} J & 1 & J+1 \\ m_J & 0 & -m_J \end{pmatrix} = \frac{(J+1)^2 - m_J^2}{(2J+1)(J+1)}, \quad (9.73)$$

$$\begin{pmatrix} J & 1 & J \\ m_J & 0 & -m_J \end{pmatrix} = \frac{m_J^2}{J(J+1)},$$

$$\begin{pmatrix} J & 1 & J-1 \\ m_J & 0 & -m_J \end{pmatrix} = \frac{J^2 - m_J^2}{J(2J+1)}.$$

States with the same  $|m_J|$  lead to the same quadratic Stark effect,

$$\Delta E \sim A + B|m_J|^2. \quad (9.74)$$

The factors  $A$  and  $B$  depend on the main quantum number  $n$  and also on  $L, S, J$ . Moreover, they depend on the energy distance of all contributing levels, because of the denominator in the perturbation equation (9.67). Only levels with different parity  $(-1)^L$  contribute. The formulae (9.73) will be derived explicitly in Exc. 9.3.2.3.

## 9.3.2 Exercises

### 9.3.2.1 Ex: Stark effect in hydrogen

Consider the hydrogen atom immersed in a uniform electric field  $\vec{\mathcal{E}}$  applied along the  $\hat{\mathbf{e}}_z$ -direction. The term corresponding to this interaction in the total Hamiltonian is  $\hat{H}^{(1)} = -e\vec{\mathcal{E}}\hat{z}$ . For typical electric fields produced in laboratory, the condition  $\hat{H}^{(1)} \ll \hat{H}_0$ , which allows the use of TIPT, is satisfied. The effect of the perturbation  $\hat{H}^{(1)}$ , called Stark effect, is the removal of the degeneracy of some of the hydrogen atom states. Calculate the Stark effect for the state  $n = 2$ .

### 9.3.2.2 Ex: Stark effect in the 1s hydrogen level

Calculate the Stark shift of the hydrogen ground state by taking into account the contributions of the excited states  $n = 2, 3, \dots$

<sup>1</sup>For it is possible to show that  $\langle n'_J J' || \hat{z} || n_J J \rangle = 0$  for  $|J - J'| > 1$ .

**9.3.2.3 Ex: Stark effect**

Derive the Eqs. (9.73) from the formula (7.4).

## 9.4 Further reading

et al., [\[DOI\]](#)



# Chapter 10

## Atoms with many electrons

### 10.1 Symmetrization of bosons and fermions

Quantum mechanics must be formulated in a way to avoid any possibility of distinguishing identical particles. However, the language of mathematics automatically assigns a particle to a wavefunction; for example,  $\psi_a(x_1)$  is the wavefunction  $a$  of particle 1 and  $\psi_b(x_2)$  the wavefunction  $b$  of particle 2. In the absence of interactions, the total wavefunction,  $\Psi = \psi_a(x_1)\psi_b(x_2)$ , solves the Schrödinger equation of two particles. Now, by changing the coordinates of the particles we get a different state  $\Psi' = \psi_a(x_2)\psi_b(x_1)$ <sup>1</sup>. This erroneously suggests that the wavefunction of a particle plays the role of a *label* (or 'soul') characterizing the particle beyond its set of quantum numbers. Why this is a problem, we will see in the following example<sup>2</sup>.

**Example 49 (Indistinguishability of particles):** We consider a system of two non-interacting spinless particles in an infinite potential well. The total wavefunction is,

$$\Psi^{(1,2)} \equiv \psi_a(x_1)\psi_b(x_2) = C \cos \frac{n_a \pi x_1}{L} \cos \frac{n_b \pi x_2}{L} \quad (10.1)$$

with the energy,

$$E_{a,b} = \frac{\pi^2 n_a^2}{2mL^2} + \frac{\pi^2 n_b^2}{2mL^2} .$$

For observable quantities, such as  $|\Psi^{(1,2)}|^2$ , we must ensure,  $|\Psi^{(1,2)}|^2 = |\Psi^{(2,1)}|^2$ , that is,

$$C^2 \cos^2 \frac{n_a \pi x_1}{L} \cos^2 \frac{n_b \pi x_2}{L} = C^2 \cos^2 \frac{n_a \pi x_2}{L} \cos^2 \frac{n_b \pi x_1}{L} ,$$

---

<sup>1</sup>We note that the states are orthogonal, because

$$\begin{aligned} \int \Psi^{*(1,2)} \Psi^{(2,1)} dx_1 dx_2 &= \int \psi_a^*(x_1)\psi_b^*(x_2)\psi_a(x_2)\psi_b(x_1) dx_1 dx_2 \\ &= \int \psi_a^*(x_1)\psi_b(x_1) dx_1 \int \psi_b^*(x_2)\psi_a(x_2) dx_2 = \delta_{n_a, n_b} . \end{aligned}$$

<sup>2</sup>Ultimately, all this is simply a consequence of the uncertainty principle, which forbids us to specify a wavefunction as a function of two non-commuting coordinates: We have to choose one coordinate on which the wavefunction depends and treat the other as a quantum number, for example,  $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$  or  $\psi_n(x) = \cos \frac{n\pi x}{L}$ . When we now exchange the coordinates of two particles without changing their quantum numbers, we get obviously different states. In classical physics, the wavefunction of a particle would be written  $\psi(x, p)$ . If two classical particles are not distinct by any other mean, an exchange of *all* their coordinates would reproduce exactly the same state.

but this is not valid for  $n_a \neq n_b$ . If  $n_a = n_b$ , we have  $\psi_a = \psi_b$ . That is, the particles stay in the same state, and we do not need to worry about indistinguishability:

$$\Psi^{(2,1)} = \psi_a(x_2)\psi_b(x_1) = \Psi^{(1,2)} \quad \text{and} \quad E_{a,b} = E_{b,a} .$$

However, the fact that this state is never observed with two electrons shows, that theory must be corrected to allow a true description of reality. Will deepen this argument in Exc. 10.1.3.1.

We need to construct the total wavefunction in another way. Let us consider linear combinations of  $\Psi^{(1,2)}$ ,

$$\Psi^{S,A} \equiv \frac{1}{\sqrt{2}}(\Psi^{(1,2)} \pm \Psi^{(2,1)}) = \frac{1}{\sqrt{2}} [\psi_a(x_1)\psi_b(x_2) \pm \psi_a(x_2)\psi_b(x_1)] . \quad (10.2)$$

This *symmetrized wavefunction* (or anti-symmetrized) represents a trick to eradicate the *label* sticking to the particles. For, under position exchange described by the operator  $\mathcal{P}_x\psi_a(x_1)\psi_b(x_2) \equiv \psi_a(x_2)\psi_b(x_1)$ , the (anti-)symmetrized functions behave like <sup>3</sup>,

$$\mathcal{P}_x\Psi^{S,A} = \pm\Psi^{S,A} \quad \text{while} \quad \mathcal{P}_x\Psi^{(1,2)} = \Psi^{(2,1)} \neq \mp\Psi^{(1,2)} . \quad (10.3)$$

The (anti-)symmetrized function solves the Schrödinger equation, as well. As  $[\hat{H}, \mathcal{P}_x] = 0$ , we can say that the system exhibits an *exchange symmetry* or *exchange degeneracy* upon particle exchange. Observables such as  $\Psi^{*S,A}\Psi^{S,A}$  stay conserved, for example, the probability

$$\begin{aligned} |\Psi^{S,A}|^2 &= \frac{1}{2} [|\psi_a(x_1)\psi_b(x_2)|^2 + |\psi_a(x_2)\psi_b(x_1)|^2] \\ &\pm \frac{1}{2} [\psi_a^*(x_1)\psi_b^*(x_2)\psi_a(x_2)\psi_b(x_1) + \psi_a^*(x_2)\psi_b^*(x_1)\psi_a(x_1)\psi_b(x_2)] = \mathcal{P}_x|\Psi^{S,A}|^2 \end{aligned} \quad (10.4)$$

does not change, when we exchange  $x_1$  for  $x_2$ . For  $x_1 = x_2$ , we observe,

$$|\Psi^{S,A}|^2 = |\psi_a(x)\psi_b(x)|^2 \pm |\psi_a(x)\psi_b(x)|^2 . \quad (10.5)$$

That is, for a symmetric system, the probability of finding two particles at the same location is doubled, whereas for an anti-symmetric system, this probability is zero.

Wolfgang Pauli showed that the (anti-)symmetric character is related to the spin of the particles. Particles with *integer spin* called *bosons* must be symmetric. Particles with *semi-integer spin* called *fermions* must be anti-symmetric. Electrons are fermions. Therefore, in an atom, they can not be in the same state (location), but must be distributed over a complicated shell of orbitals. We note, that this applies not only to elementary particles, but also to composed particles such as, for example, atoms. We will determine in Exc. 10.1.3.2 the bosonic or fermionic character of several atomic species.

### 10.1.1 Pauli's Principle

Two electrons with anti-parallel spins can be separated by inhomogeneous magnetic fields, even if they are initially in the same place. Therefore, they are distinguishable

<sup>3</sup>To guarantee  $|\mathcal{P}_x\Psi^{(1,2)}|^2 = |\Psi^{(1,2)}|^2$ , we have  $\mathcal{P}_x\Psi^{(1,2)} = e^{i\phi}\Psi^{(1,2)}$ . From this,  $\mathcal{P}_x\mathcal{P}_x\Psi^{(1,2)} = e^{2i\phi}\Psi^{(1,2)} = \Psi^{(1,2)}$ . Hence,  $\mathcal{P}_x\Psi^{(1,2)} = \pm\Psi^{(1,2)}$ .

and the wavefunction need not be anti-symmetric. But if we exchange the spin along with the position, the particles must be indistinguishable. This must be taken into account in the wavefunction by assigning a spin coordinate,  $\psi_a(x_1, s_1)$ . The exchange operator should now be generalized,

$$\mathcal{P}_{x,s}\Psi^{(1,2)} \equiv \mathcal{P}_{x,s}\psi_a(x_1, s_1)\psi_b(x_2, s_2) = \psi_a(x_2, s_2)\psi_b(x_1, s_1) = \Psi^{(2,1)}. \quad (10.6)$$

We now assume that the electrons not only do *not* interact with each other, but there is also *no interaction* between the position and the spin of each electron. That is, for a while we will discard  $\mathbf{L} \cdot \mathbf{S}$ -coupling<sup>4</sup>. We can then write the total wavefunction of an electron as the *product* of a spatial function,  $\psi(x)$ , and a spin function,  $\chi(s) = \alpha \uparrow + \beta \downarrow$ , where  $\alpha$  and  $\beta$  are probability amplitudes of finding the electron in the respective spin state, such that,

$$\psi(x, s) = \psi(x)\chi(s). \quad (10.7)$$

For two particles, the total spin function is,

$$X^{(1,2)} = \chi_a(s_1)\chi_b(s_2). \quad (10.8)$$

The (anti-)symmetrized version is

$$X^{S,A} = \frac{1}{\sqrt{2}}(X^{(1,2)} \pm X^{(2,1)}) = \frac{1}{\sqrt{2}}[\chi_a(s_1)\chi_b(s_2) \pm \chi_a(s_2)\chi_b(s_1)], \quad (10.9)$$

as we have already seen in Sec. 4.4.1. Since there are only two spin directions, there are four possibilities to attribute the spins  $\uparrow$  and  $\downarrow$  to the functions  $\chi_m(s_n)$ ,

$$X^S = \begin{cases} \uparrow\uparrow & = \chi_{1,1} \\ \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) & = \chi_{1,0} \\ \downarrow\downarrow & = \chi_{1,-1} \end{cases} \quad \text{and} \quad X^A = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) = \chi_{0,0} \quad (10.10)$$

For the total wavefunction, which must be anti-symmetric for electrons, there are two possibilities,

$$\Theta^A = \begin{cases} \Psi^S X^A = \frac{1}{2}(\Psi^{(1,2)} + \Psi^{(2,1)})(X^{(1,2)} - X^{(2,1)}) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) + \psi_a(x_2)\psi_b(x_1)]\chi_{0,0} \\ \Psi^A X^S = \frac{1}{2}(\Psi^{(1,2)} - \Psi^{(2,1)})(X^{(1,2)} + X^{(2,1)}) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) - \psi_a(x_2)\psi_b(x_1)] \end{cases} \begin{cases} \chi_{1,1} \\ \chi_{1,0} \\ \chi_{1,-1} \end{cases}. \quad (10.11)$$

That is, the two electrons may be in a *triplet* state with the anti-symmetric spatial wavefunction, or in a *singlet* state with the symmetric spatial wavefunction<sup>5</sup>.

How to generalize these considerations to  $N$  particles? The symmetric wavefunctions contain all permutations of the label  $a_k$ , where we understand by  $a_k$  the set of quantum numbers unambiguously specifying the state of the particle  $k$ ,

$$\Theta^S = \mathcal{N} \sum_{\mathcal{P}_{x,s,a_k}} \psi_{a_1}(x_1)\dots\psi_{a_N}(x_N), \quad (10.12)$$

<sup>4</sup>In the case of  $\mathbf{L} \cdot \mathbf{S}$ -coupling, the total wavefunction can not be written as a product of spatial and spin functions, but it must be anti-symmetric anyway.

<sup>5</sup>In the coupled image, the total spin  $\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2$  can have the following values  $S = |s_1 - s_2|, \dots, s_1 + s_2 = 0, 1$ . In the case  $S = 0$  the magnetic quantum number can only have one value (singlet),  $m_S = 0$ . In the case  $S = 1$  it can have three values  $m_S = -1.0, +1$  (triplet) (see Exc. 9.2.8.3).



with a normalization factor  $\mathcal{N}$ <sup>6</sup>. The (anti-)symmetrized wavefunction is obtained from the *Slater determinant*,

$$\Theta^A = \frac{1}{N!} \det \psi_{a_k}(x_n) = \frac{1}{N!} \begin{vmatrix} \psi_{a_1}(x_1) & \cdots & \psi_{a_1}(x_N) \\ \vdots & \ddots & \vdots \\ \psi_{a_N}(x_1) & \cdots & \psi_{a_N}(x_N) \end{vmatrix}. \quad (10.13)$$

This function satisfies

$$\mathcal{P}_{x,s} \Theta^{A,(1,\dots,i,j,\dots,N)} = \Theta^{A,(1,\dots,j,i,\dots,N)} = -\Theta^{A,(1,\dots,i,j,\dots,N)}. \quad (10.14)$$

The Slater determinant is zero, when two sets of quantum numbers are identical,  $a_i = a_j$ . For example, for two electrons in an electronic shell,  $|n_i, l_i, m_i, s_i\rangle = |n_j, l_j, m_j, s_j\rangle$ . This is *Pauli's strong exclusion principle*:

*The total wavefunction must be antisymmetric with respect to the exchange of any pair of identical fermions and symmetrical with respect to exchange of any pair of identical bosons.*

*Pauli's weak exclusion principle* (usually sufficient for qualitative considerations) says that two fermions in identical states can not occupy the same region in space. That is, their Broglie waves interfere destructively, as if Pauli's principle exerted a repulsive interaction on the particles. This 'force' has a great impact on the phenomenology of the bonds between atoms, as we will discuss in the following sections.

## 10.1.2 Consequences for quantum statistics

The indistinguishability of quantum particles has interesting consequences on the statistical behavior of bosons and fermions. This becomes obvious when we consider two particles 1 and 2 being able to adopt two different states  $a$  and  $b$ . Distinguishable particles can be in one of the following four states,

$$\Psi = \{\psi_a(x_1)\psi_a(x_2), \psi_a(x_1)\psi_b(x_2), \psi_b(x_1)\psi_a(x_2), \psi_b(x_1)\psi_b(x_2)\} \quad (10.15)$$

with the same probability of  $p = 1/4$ . When the quantum particles approach each other,  $x_1 \simeq x_2$ , they must become indistinguishable. Bosonic indistinguishable particles can stay in one of the following three states,

$$\Psi = \{\psi_a(x_1)\psi_a(x_2), \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) + \psi_b(x_1)\psi_a(x_2)], \psi_b(x_1)\psi_b(x_2)\} \quad (10.16)$$

with the same probability of  $p = 1/3$ . Finally, fermionic indistinguishable particles can only be in one state,

$$\Psi = \{\frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) - \psi_b(x_1)\psi_a(x_2)]\} \quad (10.17)$$

with the probability of  $p = 1$ . We see that a simple two-particle system already exhibits qualitative modifications of its statistical behavior. These differences generate

<sup>6</sup>It is possible to show  $\mathcal{N} = \sqrt{\frac{\prod_{k=1}^m n_k!}{N!}}$ , where  $n_k$  is the population of state  $\psi_{a_k}$ , that is, the number of particles with the same set of quantum numbers  $a_k$ .

different physics as we deal with systems of large numbers of particles, as we can see in the cases of the free electron gas and the Bose-Einstein condensate.

We finally note a result of the standard model of particle physics assigning a fermionic character to all fundamental constituent particles of matter while the mediators of fundamental forces are always bosons.

### 10.1.3 Exercises

#### 10.1.3.1 Ex: Indistinguishability of particles

Consider the observable quantity  $\int_0^{L/2} \int_0^{L/4} |\Psi(x_1, x_2)|^2 dx_1 dx_2$  for the case of the wavefunction defined in (10.1) and show, that it *does* depend on particle exchange.

#### 10.1.3.2 Ex: Bosonic and fermionic isotopes

Consulting an isotope table determine the bosonic or fermionic character of the following atomic species:  $^{87}\text{Sr}$ ,  $^{86}\text{Sr}$ ,  $^{87}\text{Rb}$ ,  $^{39}\text{K}$ , and  $^{40}\text{K}$ .

#### 10.1.3.3 Ex: Interference of bosons and fermions

a. Consider two clouds of ultracold bosonic atoms (BECs at temperature  $T = 0$ ) moving into opposite direction with velocities  $v_{\pm} = \pm v$ , respectively. Describe the matter wave interference pattern.

b. Repeat the consideration for the case of (i) fermionic clouds and (ii) only two counterpropagating atoms. Is matter wave interference possible at all for fermions?

## 10.2 Helium

The simplest atom to discuss Pauli's principle is helium. The helium atom has a charged nucleus  $Z = +2e$  and mass  $m_{He} \approx 4m_H$ .

### 10.2.1 The ground state

The ground state of the *helium* atom brings together the two electrons, that is,  $(1s)^2$ . To treat the helium atom, we can, as a first trial, describe the atom by the Bohr model, assuming independent electrons. Neglecting the electronic repulsion term (which depends on  $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ ), we can separate the total wavefunction:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \Psi_1(\mathbf{r}_1)\Psi_2(\mathbf{r}_2) , \quad (10.18)$$

and we get two Schrödinger equations, the Hamiltonian being equal to the one of hydrogen-like atoms:

$$\left[ -\frac{\hbar^2}{2\mu} \nabla_i^2 - \frac{e^2}{4\pi\epsilon_0} \frac{Z}{r_i} \right] \Psi_i(\mathbf{r}_i) = E_n^{(i)} \Psi_i(\mathbf{r}_i) , \quad (10.19)$$

with  $i = 1, 2$ . For hydrogen-like atoms we have,

$$E = E_n^{(1)} + E_n^{(2)} = E_B Z^2 \left( \frac{1}{n_1^2} + \frac{1}{n_2^2} \right) , \quad (10.20)$$

with  $E_B = -13.6$  eV. With this, we get the energy for the ground state:

$$E_{He}(1s) = -2Z^2 E_B = -108.8 \text{ eV} . \quad (10.21)$$

The value predicted by Bohr's model is far from experimental reality: The ionization energy measured for the first electron is 24.6 eV, for the second 54.4 eV, totalizing a binding energy for two electrons of  $-78.983$  eV . This corresponds to an error of about 38%. The lower energy of the first electron is due to the shielding of the nucleus by the second.

### 10.2.1.1 First-order perturbation of the energy

Treating the repulsion term between the electrons as a perturbation [28] and using the eigenfunctions of hydrogen atoms  $|n, \ell, m_\ell\rangle$ , the total wavefunction is  $|n_1, \ell_1, m_{\ell_1}; n_2, \ell_2, m_{\ell_2}\rangle$ , we obtain as first order TIPT correction for the energy:

$$\Delta E = \langle n_1, \ell_1, m_{\ell_1}; n_2, \ell_2, m_{\ell_2} | \frac{e^2}{4\pi\epsilon_0 r_{12}} | n_1, \ell_1, m_{\ell_1}; n_2, \ell_2, m_{\ell_2} \rangle . \quad (10.22)$$

This correction is called the *Coulomb integral* and has the value:

$$\Delta E = \frac{e^2}{4\pi\epsilon_0} \int |\Psi_{n_1, \ell_1, m_{\ell_1}}(\mathbf{r}_1)|^2 \left( \frac{1}{r_{12}} \right) |\Psi_{n_2, \ell_2, m_{\ell_2}}(\mathbf{r}_2)|^2 dV_1 dV_2 . \quad (10.23)$$

This integral is always positive. The term  $|\Psi_{n_1, \ell_1, m_{\ell_1}}(\mathbf{r}_1)|^2 dV_1$  is the probability of finding the electron inside the volume element  $dV_1$  and, when multiplied by  $-e$ , gives the charge associated with that region. Thus, the integral represents the Coulombian interaction energy of the confined charges within the two volume elements  $dV_1$  and  $dV_2$ .  $\Delta E$  is the total contribution to the potential energy. Calculating the Coulomb integral for the ground state, which will be done in Exc. 10.2.3.1, we obtain,

$$\Delta E = \frac{5Z}{4} \left( \frac{e^2}{4\pi\epsilon_0 2a_B} \right) = \frac{5Z}{4} E_B , \quad (10.24)$$

with  $a_B$  the Bohr radius.  $\Delta E$  corresponds to 34 eV. Thus, the ground state energy is  $E_{He}(1s) = -108.8 \text{ eV} + 34 \text{ eV} = -74.8 \text{ eV}$ . Comparing with the experimental value of  $-78.983$  eV we have an error around 5.3%.

### 10.2.1.2 Shielding of the nuclear charge

We can make the approximation in which we consider that each electron moves in a Coulombian potential, with respect to the nucleus, shielded by the charge distribution of the other electron [187]. The resulting potential will be generated by an effective charge  $\zeta e \equiv (Z - B)e$ . The quantity  $B \in [0, 1]$  is called the shielding constant.

The first electron feels a total nuclear charge  $Ze$ , while the second feels an effective nuclear charge  $\zeta e$ . We exchange  $Z$  for  $\zeta$  in the energy term for hydrogen-like atoms,

$$E_n = -\zeta \frac{E_B}{n^2} , \quad (10.25)$$

and the energy for the ground state becomes, assuming total shielding,  $B = 1$ ,

$$E = E_1 + E_2 = -Z^2 E_B - \zeta^2 E_B = -4E_B - E_B = -5E_B = -67.5 \text{ eV} . \quad (10.26)$$

Comparing with the experimental value of  $-78.983 \text{ eV}$  we have an error around 15%. For a shielding constant of around  $B = 0.656$  the experimental value is reproduced. This means that the effective nuclear charge felt by the second electron is only *partly* shielded by the former. The TPIT method (10.22) and the shielding concept (10.25) can be combined in a variational calculation, where the effective charge  $\zeta$  is the variational parameter. In Exc. 10.2.3.2 we study the reciprocal shielding of the electrons at the example of the helium-type ion  $\text{H}^-$ .

### 10.2.2 Excited states

Let us now investigate the excited states of helium, in particular those, where *only one electron* is excited, the other one being in the ground state,  $(1s)^1(2s)^1$  and  $(1s)^1(2p)^1$ . All energies are considerably higher (weaker binding) than predicted by Bohr's model with  $Z = 2$ , because of the interaction with the other electron. Also, the  $(2s)$  and  $(2p)$  levels are no longer degenerate, because the electrostatic potential is no longer Coulombian (see Fig. 10.1).

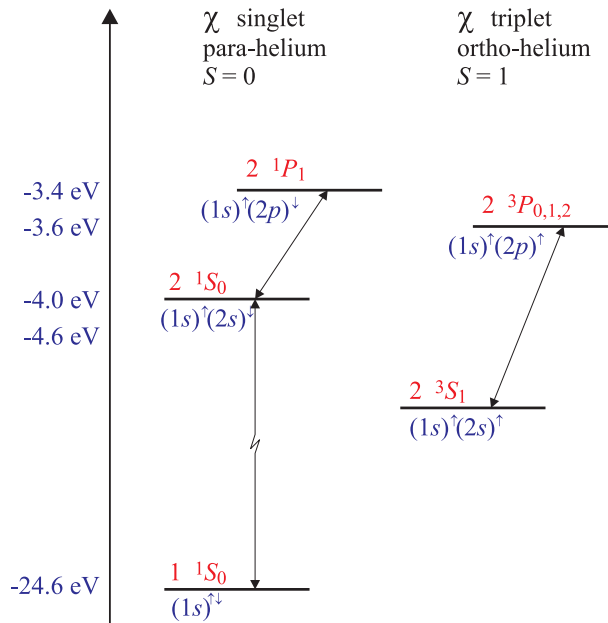


Figure 10.1: Helium levels for the excitation of the first electron and allowed singlet and triplet transitions. Note that the state  $(1s)^\uparrow\uparrow$  does not exist.

As we have seen in the discussion of the fine structure of hydrogen, the energy of the  $\mathbf{l} \cdot \mathbf{s}$ -coupling given by (8.131) is  $\propto E_n(Z\alpha)^2 \propto Z^4$ . For helium which still has a small  $Z$ , the energy of the coupling is weak ( $\sim 10^{-4} \text{ eV}$ ), so that we can count on a direct coupling of the spins of the two electrons. If in an excited state the

orbits of the electrons are different, we can construct combinations of symmetric **or** antisymmetric spatial wavefunctions  $\Psi^{S,A}$ , are therefore combinations  $X^{A,S}$  of antiparallel or parallel spins. When the spins are parallel ( $S = 1$ ), the spatial wavefunction is antisymmetric, when they are antiparallel ( $S = 0$ ), it is symmetric. From the symmetry of the wavefunction depends the energy of the Coulombian interelectronic interaction, because in the symmetric state the average distance of the electrons is much smaller than in the antisymmetric state, where *the total spatial function disappears for zero distance*. Consequently, the configuration  $(1s)^1(2s)^1$  has two states with  $S = 0$  and  $S = 1$ , with energy  $E_{S=0} > E_{S=1}$ . Likewise, all configurations are split, as shown in Fig. 10.1. The energy difference ( $\sim 0.6$  eV) is considerable and larger than the energy of fine structure interaction. This explains why the two spins first couple to a total spin,  $\mathbf{s}_1 + \mathbf{s}_2 = \mathbf{S}$ , before this spin couples to the total orbital angular momentum,  $\mathbf{S} + \mathbf{L} = \mathbf{J}$ . This is the  $\mathbf{L} \cdot \mathbf{S}$ -coupling.

### 10.2.2.1 Exchange energy

The energy difference between the two states  $S = 0$  and  $S = 1$  is called *exchange energy*. It comes out of a first-order perturbation calculation. For example, for the two possible states  $(1s)^1(2s)^1$ , we write the total anti-symmetric wavefunctions,

$$\Theta_{\pm}^A = \frac{1}{\sqrt{2}} [\psi_{100}(\mathbf{r}_1)\psi_{200}(\mathbf{r}_2) \pm \psi_{100}(\mathbf{r}_2)\psi_{200}(\mathbf{r}_1)] \cdot \chi^{A,S}, \quad (10.27)$$

where the (+) sign holds for  $\chi^A$  ( $S = 0$ ) and the (-) sign for  $\chi^S$  ( $S = 1$ ). The energies are,

$$\begin{aligned} \Delta E^{S,A} &= \frac{1}{2} \int dr_1^3 \int dr_2^3 \Theta_{\pm}^{*A} \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} \Theta_p m^A \quad (10.28) \\ &= \frac{1}{2} \int dr_1^3 \int dr_2^3 \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} [|\psi_{100}(\mathbf{r}_1)|^2 |\psi_{200}(\mathbf{r}_2)|^2 + |\psi_{100}(\mathbf{r}_2)|^2 |\psi_{200}(\mathbf{r}_1)|^2] \\ &\quad \pm \frac{1}{2} \int dr_1^3 \int dr_2^3 \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} 2\psi_{100}^*(\mathbf{r}_1)\psi_{200}^*(\mathbf{r}_2)\psi_{100}(\mathbf{r}_2)\psi_{200}(\mathbf{r}_1) \\ &\equiv \Delta E_{coulomb} \pm \Delta E_{exchange}. \end{aligned}$$

The first integral,

$$\Delta E_{coulomb} = \int dr_1^3 \int dr_2^3 \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} |\psi_{100}(\mathbf{r}_1)|^2 |\psi_{200}(\mathbf{r}_2)|^2, \quad (10.29)$$

is the Coulomb energy (10.23) between the electronic orbitals. We note that this part can be calculated from the Hamiltonian using *non-symmetrized* orbitals. The second integral,

$$\Delta E_{exchange} = \int dr_1^3 \int dr_2^3 \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} \psi_{100}^*(\mathbf{r}_1)\psi_{200}^*(\mathbf{r}_2)\psi_{100}(\mathbf{r}_2)\psi_{200}(\mathbf{r}_1), \quad (10.30)$$

called *exchange energy* corresponds to the interference terms of the symmetrization and must be added or subtracted according to their symmetry character. It is interesting to note that up to this point the spin does not enter directly into the helium

Hamiltonian,

$$\hat{H}^{S,A} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(r_1) + V(r_2) + V(|\mathbf{r}_1 - \mathbf{r}_2|) \pm \Delta E_{exchange} , \quad (10.31)$$

but only through the symmetry character of the spatial wavefunction. On the other hand, on a much smaller energy scale, the spin enters through the  $\mathbf{L} \cdot \mathbf{S}$ -interaction.

The potential is not spherically symmetric, the term  $r_{12}$  depends on the angle between  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . Thus, the total wavefunction  $\Psi(\mathbf{r}_1, \mathbf{r}_2)$  is not separable into a radial and an angular part. By consequence, unlike for hydrogen, the Schrödinger equation with the Hamiltonian (10.21) has no analytical solution.

**Example 50 (TIPT for excited helium states):** We consider the two electrons of a helium atom occupying different orbits described by wavefunctions denoted by  $\psi_a(1) \equiv \psi_{n_1, \ell_1, m_{\ell_1}}(\mathbf{r}_1)$  and  $\psi_b(2) \equiv \psi_{n_2, \ell_2, m_{\ell_2}}(\mathbf{r}_2)$ . Applying the Hamiltonian without the interelectronic interaction term, the total states  $\Theta = \psi_a(1)\psi_b(2)$  and  $\psi_a(2)\psi_b(1)$  have the same energy  $E_a + E_b$ . To calculate the energy correction, we use TIPT for degenerate states. We have to calculate the secular determinant  $\det(\langle n, \nu | H^{(1)} | n, \mu \rangle - E_n^{(1)} \delta_{\mu, \nu})$ . The terms of the perturbation matrix  $H^{(1)}$  are:

$$\begin{aligned} H_{11}^{(1)} &= \langle \psi_a(1)\psi_b(2) | \frac{e^2}{4\pi\epsilon_0 r_{12}} | \psi_a(1)\psi_b(2) \rangle \\ H_{22}^{(1)} &= \langle \psi_a(2)\psi_b(1) | \frac{e^2}{4\pi\epsilon_0 r_{12}} | \psi_a(2)\psi_b(1) \rangle \\ H_{12}^{(1)} &= \langle \psi_a(1)\psi_b(2) | \frac{e^2}{4\pi\epsilon_0 r_{12}} | \psi_a(2)\psi_b(1) \rangle = H_{21}^{(1)} . \end{aligned}$$

The terms  $J \equiv H_{11}^{(1)} = H_{22}^{(1)}$  are Coulomb integrals. The term  $K \equiv H_{12}^{(1)}$  is called *exchange integral*:

$$K = \frac{e^2}{4\pi\epsilon_0} \langle \psi_a(1)\psi_b(2) | \frac{1}{r_{12}} | \psi_a(2)\psi_b(1) \rangle .$$

Hence, as  $J$  and  $K$  are positive, the determinant is:

$$\begin{vmatrix} J - E & K \\ K & J - E \end{vmatrix} = 0 ,$$

yielding,

$$E^{(1)} = J \pm K .$$

That is, the states that were previously degenerate with energy  $E = E_a + E_b$  are now split into two states with energies  $E = E_a + E_b + J \pm K$ . And the corresponding eigenfunctions are:

$$\Psi^{S,A}(1, 2) = \frac{1}{\sqrt{2}} [\psi_a(1)\psi_b(2) \pm \psi_b(1)\psi_a(2)] .$$

This result shows that the repulsion between the two electrons breaks the degeneracy (of separable functions written in product form) into states with an energy difference  $2K$ . Note that the eigenfunctions are symmetric, which is discussed in the next section.

### 10.2.2.2 The spectrum of helium

So far we have seen that, if the electrons are in the same orbital, we have an energy term  $E = 2E_a + J$  and, when they are in *different orbitals*, we have  $E = E_a + E_b + J \pm K$ , with a separation between levels of  $2K$ .

In practice, we consider only the excitation of *one* electron, because the energy to excite the two electrons exceeds the ionization energy of the helium atom. To find the selection rules for transitions between symmetric and antisymmetric states, we calculate the dipole moment of the transition. For a two-electron system the dipole moment is  $\hat{\mathbf{d}} = -e\mathbf{r}_1 - e\mathbf{r}_2$ , which is symmetric with respect to a permutation of the two electrons. The matrix element for the dipolar transition is:

$$\langle \Psi^A | \hat{\mathbf{d}} | \Psi^S \rangle = -e \int \Psi^{*A}(\mathbf{r}_1, \mathbf{r}_2) (\mathbf{r}_1 + \mathbf{r}_2) \Psi^S(\mathbf{r}_1, \mathbf{r}_2) dV_1 dV_2 . \quad (10.32)$$

If we exchange the electrons, the above integral changes sign, because  $\Psi^A(\mathbf{r}_1, \mathbf{r}_2)$  changes sign. But the integral can not depend on the nomenclature of the integration variables, so *it must be zero*. The transition between a symmetric and an antisymmetric state can not occur. Looking at the spin wavefunction in  $\Theta = \Psi^S \chi^A$  or  $\Psi^A \chi^S$ , we find that transitions are only allowed between singlet states or between triplet states. That is, there is a *selection rule* for the spin postulating  $\Delta S = 0$ <sup>7,8</sup>.

Because of the differences observed in the singlet and the triplet spectrum of helium, illustrated in Fig. 10.1, it was first believed that they belong to different atomic species, called *para-helium* and *ortho-helium*. A chemical analysis showed later that it was the same element.

## 10.2.3 Exercises

### 10.2.3.1 Ex: Helium atom

Compare the measured binding energy with the prediction of Bohr's model considering the inter-electronic interaction up to first order TIPT.

### 10.2.3.2 Ex: Shielding in helium

The helium atom (or helium-like atoms such as  $H^-$ ) has two interacting electrons in its composition, which means that these systems have no exact solution. To circumvent this problem we have to come up with a series of approximate methods for calculating their eigenstates and their respective eigenenergies. Among these methods, a widely used one, due mainly to its ease and practicality, is the variational method, in which we

<sup>7</sup>Moreover, transitions between the states  $^1S_0$  and  $^3S_1$  are impossible, because they violate the selection rule for the angular momentum,  $\Delta L = \pm 1$ .

<sup>8</sup>We can understand the selection rules as follows: As long as the wavefunction can be written as a product,  $\Theta = \Psi(x)\chi(s)$ , the symmetry character is preserved for the two functions separately. The eigenvalues of the operators  $\mathcal{P}_x$  and  $\mathcal{P}_s$  are then good quantum numbers. But this only holds for weak  $\mathbf{L} \cdot \mathbf{S}$ -coupling. The electric dipole operator for the transition does not act on the spin (which prevents the recoupling  $S = 1 \leftrightarrow S = 0$  via  $E1$ -radiation) and also does not act on the symmetry character of the orbitals (which prevents transitions  $\Psi^S \leftrightarrow \Psi^A$ ).

In principle, this holds for any species of atoms with two valence electrons. In reality however, the influence of the  $\mathbf{L} \cdot \mathbf{S}$ -coupling grows with  $Z$ , which weakens the interdiction of the intercombination transition. In this case, only the operator  $\mathcal{P}_{x,s}$  yields good eigenvalues.

calculate the fundamental state of a given problem through a test function that is not a solution of the original problem. This method, when applied to a helium atom, uses as test function the solution of the problem without coulombian interaction between the electrons, which only feel the interaction with the original charge of the nucleus. However, this method could be further improved if we considered an effective nuclear charge, due to its interaction with the electrons themselves, and then obtaining the test function. Apply this correction to the case of helium. Interpret the result. **Help:**

$$\int \frac{\sin \theta_2}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_2}} d\theta_2 = \frac{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_2}}{r_1 r_2} \quad \text{and} \quad \left\langle \frac{1}{r} \right\rangle = \frac{Z}{a_B} .$$

## 10.3 Electronic shell structure

The interelectronic interaction and the need to antisymmetrize the wavefunction of the electrons both contribute to excessively increase the complexity of multielectronic atoms. The Hamiltonian describing a multielectronic atom of atomic number  $Z$ ,

$$\hat{H} = E_{kin} + V_{ncl-ele} + V_{ele-ele} = \sum_{i=1}^Z \frac{p_i^2}{2m} - \sum_{i=1}^Z \frac{Ze^2}{4\pi\epsilon_0|\mathbf{r}_i|} + \sum_{i<j=1}^Z \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} , \quad (10.33)$$

is extremely complicated to solve, even for the simplest case ( $Z = 2$ ) we must use approximation methods.

### 10.3.1 TIPT method

Note that, if we assume independent electrons ( $V_{ele-ele} = 0$ ), that is, each electron moves independently of the others within the electrostatic potential generated by the nucleus and the other  $Z - 1$  electrons, the problem would be solvable: We could solve the Schrödinger equation for a product state of all the electronic wavefunctions, and we would know the eigenfunctions and individual eigenenergies of each electron (as for the hydrogen atom). In principle, we should use antisymmetric wavefunctions, but as a first approach we can choose to only respect Pauli's weak principle, that is, assign an *individual and unique* set of quantum numbers to each electron. The total energy would be the sum of the energy of every electron, and the associated physical eigenstates would be obtained by means of an antisymmetrization of the tensor product of the multielectronic state.

Thus, as a first approximation, we use the states of individual electrons (orbital approximation) and consider  $V_{ele-ele}(|\mathbf{r}_i - \mathbf{r}_j|)$  as a perturbation making use of *time-independent perturbation theory*. However, this term is not small enough to justify this procedure, since approximating

$$V_{ncl-ele} \simeq \frac{Z^2 e^2}{a_B} \quad \text{and} \quad V_{ele-ele} \simeq \frac{Z(Z-1)e^2}{2a_B} , \quad (10.34)$$

we realize that  $V_{ele-ele}/V_{ncl-ele}$  varies between  $\frac{1}{4}$  for  $Z = 2$  and  $\frac{1}{2}$  for  $Z \gg 1/2$ . For this reason the use of alternative methods to describe multielectronic atoms is



necessary. Nevertheless, the set of quantum numbers derived from Bohr's atomic model are still the same as those used for many-electron atoms, and the orbitals are used as starting points for more sophisticated methods.

To calculate most of the atomic properties we need reasonably realistic potentials. The most important terms of the Hamiltonian are the Coulombian potential between the nucleus and the electrons,  $V_{ne}$ , being naturally spherical, and the interaction potentials between the electrons,  $V_{ee}$ , which we will try to approximate by a spherical potential and treat the deviations caused by the approximation afterward. Knowing the effect of the shielding of the nucleus by electronic charges, we already know the asymptotes (see Fig. 10.2),

$$V_{eff} = -\frac{Ze^2}{4\pi\epsilon_0 r} \quad \text{for } r \rightarrow 0 \quad \text{and} \quad V_{eff} = -\frac{e^2}{4\pi\epsilon_0 r} \quad \text{for } r \rightarrow \infty. \quad (10.35)$$

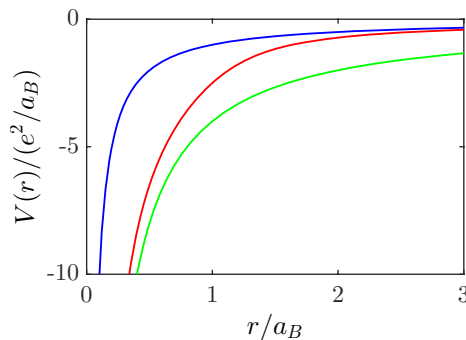


Figure 10.2: (code) External potential (shielded Coulombian)  $V_{cl} \propto \frac{e^2}{r}$  (blue, upper curve), interior potential (non-shielded Coulombian for  $Z = 4$ )  $V_{bl} \propto \frac{Ze^2}{r}$  (green, lower curve), and effective potential (red, middle curve).

### 10.3.2 Thomas-Fermi model for an electron gas

A first approach to getting a reasonable *effective potential*  $V_{eff}$  is provided by the *Thomas-Fermi model*. This is a semi-classical model that aims to roughly describe the total energy of the electrons as a *density functional* of atomic/molecular electrons. It serves as a basis for more sophisticated methods aiming at determining the electronic structure, such as *density functional theory* (DFT), and the wavefunctions determined by this method often serve as a starting point for the Hartree method discussed below. One of the important predictions of the *Thomas-Fermi model* is that the average radius of an atom depends on the nuclear charge as  $\bar{R} \propto Z^{-1/3}$ .

The Thomas-Fermi model allows us to understand the electronic configuration of the fundamental states and provides the basis for the periodic system of elements. In this model, the electrons are treated as independent particles, on one side forming an effective radial electric potential, on the other side being subjected to this potential. Instead of requiring anti-symmetry of the wavefunction, it is only necessary to ensure that all electrons are distinguished by at least one quantum number. The orbitals of

complex atoms are similar to the wavefunctions of hydrogen. So, we can use these quantum numbers  $n$ ,  $\ell$ ,  $m_\ell$ , and  $m_s$  for every electron.

However, the effective radial potential depends very much on the species and is quite different from the Coulomb potential. So, the degeneracy in  $\ell$  is lifted. In general, electrons with small  $\ell$  are more strongly bound, because they have a higher probability of being near the nucleus, where the potential is deeper (see Fig. 10.2). The same argument explains why electrons with small  $n$  are more strongly bound. We will discuss these effects in more depth in Sec. 10.4.1 by comparing the excitation levels of the valence electron in different alkalis.

### 10.3.2.1 Density of states in the Fermi gas model

Even though the real potential sensed by the electrons bound to a nucleus is very different from the three-dimensional well, we can roughly imagine that the atom is subdivided into small volumes, understood as box potentials, all filled with electrons. From this we can calculate the distribution of the electronic charge, such that the average local energy is homogeneous and the electronic cloud in equilibrium. The distribution, in turn, serves to determine the shape of the electrostatic potential which, when subdivided into small volumes filled with electrons, produces the same charge distribution. This principle is called *self-consistency*.

According to the Fermi gas model, we consider an infinite potential well, that we gradually fill up with electrons. The Pauli principle allows us to place at most two electrons in each orbital,

$$\Psi = \psi_{1,\uparrow}(x_1)\psi_{1,\downarrow}(x_2)\psi_{2,\uparrow}(x_3)\psi_{2,\downarrow}(x_4) \cdot \dots \quad (10.36)$$

This total wavefunction satisfies the weak Pauli principle, but is obviously not anti-symmetric. The approximation is good, when the interaction between the electrons is negligible. Otherwise, we need to consider the exchange energy terms. This model, called *Fermi gas model*, is often used to describe the behavior of electrons that can freely move within the conduction band of a metal.

We divide the atom into small volumes (cells) containing uniformly distributed non-interacting electrons, whose total number is  $N$ , and we analyze each cell individually. The whole volume can be modeled by a box potential:  $V(\mathbf{r}) = 0$  for  $0 \leq x, y, z \leq L$  and  $V(\mathbf{r}) = \infty$  in all other places. In this case we find the possible states  $\{n_x, n_y, n_z\}$  with  $n_x, n_y, n_z = 1, 2, 3$  and the single electron energies,

$$E_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2m_e L^2} (n_x^2 + n_y^2 + n_z^2) = \frac{\hbar^2}{2m_e} \mathbf{k}_{n_x, n_y, n_z}^2, \quad (10.37)$$

where  $\mathbf{k}_{n_x, n_y, n_z}^2 = k_x^2 + k_y^2 + k_z^2 = \left(\frac{n_x \pi}{L}\right)^2 + \left(\frac{n_y \pi}{L}\right)^2 + \left(\frac{n_z \pi}{L}\right)^2$ . Each set of values  $\mathbf{k} = (k_x, k_y, k_z)$  corresponds to an accessible state of the system, and each state is associated with a volume element  $(\pi/L)^3$  in  $k$ -space. Defining the density of states  $\eta(E)$ , we can express the total number of states below a particular energy  $E$  by,

$$\begin{aligned} n(E) &= \int_0^E \eta(E') dE' \equiv \frac{1}{(2\pi)^3} \int d^3r d^3k = \frac{L^3}{(2\pi)^3} 4\pi \int k^2 dk \\ &= \frac{L^3}{(2\pi)^3} 4\pi \left(\frac{2m_e}{\hbar^3}\right)^{3/2} \int_0^E \sqrt{E'} dE' = \frac{L^3}{3\pi^2} \left(\frac{2m_e E}{\hbar^3}\right)^{3/2}. \end{aligned} \quad (10.38)$$

$\eta(E)dE$  is the number of states with energies between  $E$  and  $E + dE$ .

At temperature  $T = 0$  K all  $N$  electrons are in their energetically lowest available state, obeying the Pauli exclusion principle and considering the spin. The energy of the  $N$ -th electron (the most energetic one) is then called the *Fermi energy*  $E_F$ . That is, below  $E_F$  all states are occupied, and all states above  $E_F$  are unoccupied. The total energy is given by the sum of the energies of the  $N$  less energetic states, and the final physical state is given by the antisymmetrization of the corresponding wavefunction. With the formula (10.38), we can express the Fermi energy via  $n(E_F) \equiv N$ , such that,

$$E_F = \frac{\hbar^2}{2m_e L^2} (3\pi^2 N)^{2/3} , \quad (10.39)$$

so that the density of states can be expressed as,

$$\boxed{\eta(E) = \frac{dn(E)}{dE} = \frac{L^3}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} E^{1/2} = \frac{3N}{2} \frac{E^{1/2}}{E_F^{3/2}}} . \quad (10.40)$$

### 10.3.2.2 Thomas-Fermi energy

Fermi's box potential trick allowed us to model the impact of Pauli's principle on the spatial distribution of fermions in a restricted volume, but we did not take into account yet the fact that electrons are charged and will interact. Hence, the energy calculated so far is purely kinetic and will have to be complemented by potential energy.

The total kinetic energy of the electrons with the system in its ground state is,

$$\begin{aligned} E_{tot} &= \int_0^{E_F} E \eta(E) dE = \frac{L^3}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} \int_0^{E_F} E^{3/2} dE \\ &= \frac{L^3}{5\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} E_F^{5/2} = \frac{\hbar^2 3^{5/3} \pi^{4/3}}{10m_e} L^3 \left( \frac{N}{L^3} \right)^{5/3} = C L^3 \rho^{5/3} , \end{aligned} \quad (10.41)$$

where  $\rho \equiv N/L^3$  is the density of electrons per unit volume and  $C$  just a proportionality constant. Now understanding  $\rho$  as a quantity depending on position in space, we calculate the total number of electrons as,

$$N = \int_{\mathbb{R}^3} \rho(\mathbf{r}) d^3r , \quad (10.42)$$

and the kinetic energy density by,

$$u_{kin}(\mathbf{r}) = C \rho^{5/3}(\mathbf{r}) , \quad (10.43)$$

such that the total kinetic energy of the electrons in the electronic shell is,

$$T[\rho] = C \int \rho^{5/3}(\mathbf{r}) d^3r . \quad (10.44)$$

The potential associated with the electron-nucleus interaction is,

$$V_{ep}[\rho] = -\frac{Ze^2}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}')}{r'} d^3r' = \int V_p(\mathbf{r}') \rho(\mathbf{r}') d^3r' , \quad (10.45)$$

with the electrical potential generated by the nucleus,

$$\Phi_p(\mathbf{r}) = \frac{V_p(\mathbf{r})}{-e} = \frac{Ze}{4\pi\epsilon_0} \frac{1}{r} \quad (10.46)$$

The potential associated with the electron-electron interaction is,

$$V_{ee}[\rho] = \frac{1}{2} \frac{e^2}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' = \int V_e(\mathbf{r}')\rho(\mathbf{r}')d^3r' , \quad (10.47)$$

with the electrical potential generated by the electron cloud,

$$\Phi_e(\mathbf{r}) = \frac{V_e(\mathbf{r})}{-e} = -\frac{1}{2} \frac{e}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r' \quad (10.48)$$

Thus, the total energy (*Thomas-Fermi energy*) can be written as a functional of the electronic density of the atom,

$$\boxed{H_{TF}[\rho] = T[\rho] + V_{ep}[\rho] + V_{ee}[\rho]} . \quad (10.49)$$

### 10.3.2.3 Electronic density and the Thomas-Fermi equation

Exploiting the variational principle, we are interested in the electronic density  $\rho(\mathbf{r})$  which minimizes the Thomas-Fermi energy. We can perform this process via Lagrange multipliers under the constraint, that the number of electrons remains constant in the atom. Thus,

$$0 = \delta \left\{ H_{TF}[\rho] - \mu \left( \int \rho(\mathbf{r}) d^3r - N \right) \right\} . \quad (10.50)$$

Inserting the Thomas-Fermi energy (10.49) we calculate,

$$\mu = \frac{\delta}{\delta\rho(\mathbf{r})} \left\{ C\rho^{5/3}(\mathbf{r}) + V_p(\mathbf{r})\rho(\mathbf{r}) + V_e(\mathbf{r})\rho(\mathbf{r}) \right\} = \frac{5}{3}C\rho^{2/3}(\mathbf{r}) + V_p(\mathbf{r}) + V_e(\mathbf{r}) . \quad (10.51)$$

Resolving for the electronic density,

$$\rho(\mathbf{r}) = \left( \frac{3}{5C} \right)^{3/2} [\mu - V_p(\mathbf{r}) - V_e(\mathbf{r})]^{3/2} . \quad (10.52)$$

The above expression is called the *Thomas-Fermi equation* and describes the electron density of the atom in its ground state. The expression (10.48) can be rewritten as a Poisson equation,

$$\nabla^2 V_e(\mathbf{r}) = \frac{e^2}{2\epsilon_0} \rho(\mathbf{r}) , \quad (10.53)$$

so that,

$$\nabla^2 V_e(\mathbf{r}) = \frac{e^2}{2\epsilon_0} \left( \frac{3}{5C} \right)^{3/2} [\mu - V_p(\mathbf{r}) - V_e(\mathbf{r})]^{3/2} . \quad (10.54)$$

For the effective potential introduced via  $V_{eff} = V_p + V_e$ , we find,

$$\begin{aligned} \nabla^2 V_{eff}(\mathbf{r}) &= \nabla^2 \left( -\frac{Ze^2}{4\pi\epsilon_0} \frac{1}{r} \right) + \nabla^2 V_e(\mathbf{r}) \\ &= -\frac{Ze^2}{\epsilon_0} \delta^3(\mathbf{r}) + \frac{e^2}{2\epsilon_0} \left( \frac{3}{5C} \right)^{3/2} [\mu - V_{eff}(\mathbf{r})]^{3/2} . \end{aligned} \quad (10.55)$$

We note that, with (10.50), we can identify the Lagrange multiplier  $\mu$  as a *chemical potential*. In particular, for non-interacting neutral atoms, we have  $\mu = 0$ . In addition, since for an atom both the potential and the electronic density must have spherical symmetry, we can write for  $r \neq 0$ ,

$$\frac{1}{r} \frac{\partial^2}{\partial r^2} [rV_{eff}(r)] = \frac{e^2}{2\varepsilon_0} \left( \frac{3}{5C} \right)^{3/2} [-V_{eff}(\mathbf{r})]^{3/2}. \quad (10.56)$$

We now make the ansatz,

$$V_{eff}(r) \equiv -\frac{Z}{r} \chi(\alpha r) \quad \text{setting} \quad \alpha \equiv \frac{3e^{4/3}}{5C\varepsilon_0^{2/3}} Z^{1/3}. \quad (10.57)$$

This transforms the expression (10.56) into,

$$\frac{\partial^2}{\partial r^2} \chi(\alpha r) = -\frac{e^2}{Z\varepsilon_0} \left( \frac{3Z}{5C} \right)^{3/2} \frac{\chi^{3/2}(\alpha r)}{r^{1/2}}, \quad (10.58)$$

or, substituting  $x \equiv \alpha r$ ,

$$\frac{d^2 \chi}{dx^2} = -\frac{\chi^{3/2}}{x^{1/2}}. \quad (10.59)$$

It is important to note the last equation does not depend on the parameter  $Z$ , thus being a general result for any neutral atom. The function  $\chi(x)$  is determined numerically, but we can analyze its asymptotic values given the expected behavior of the effective potential  $V_{eff}(r)$ : for  $r \rightarrow 0$  we expect that  $V_{eff}(r) = V_p(r)$ , hence  $\chi(0) = 1$ . On the other hand, for  $r \rightarrow \infty$ , we expect  $V_{eff}(r) = 0$ , hence  $\chi(\infty) = 0$ . Do the Exc. 10.3.5.1.

With  $\chi(x)$  known, we obtain the charge density  $\rho(x)$ , and hence we are able to calculate the total energy of the atom under investigation. Thus, it is possible to show that [28],

$$H_{TF}[\rho] = -0.7687 \frac{e^2}{4\pi\varepsilon_0 a_B} Z^{7/3}. \quad (10.60)$$

It is important to highlight some points:

1. The result holds for neutral atoms.
2. There is no electronic shell structure assumed; apart from the fact that the kinetic energy was derived in a way as to respect Pauli's principle, the whole calculation was done within the laws of classical electromagnetism; no quantum mechanics was involved and, hence, no set of quantum numbers has been found.
3. Apart from the Pauli principle used to calculate the density of states (10.40), quantum statistical effects of identical particles (such as wavefunction antisymmetrization) are not taken into account.

A more refined model which deals with third criticism and, in addition, is closer to density functional theory (DFT) is the Thomas-Fermi-Dirac model.

### 10.3.3 Hartree method

The effective potential obtained from the Thomas-Fermi model can serve as a starting point for quantum treatments. Assuming that all electrons are subject to the same effective potential  $V_{eff}$ , we numerically solve the Schrödinger equation for each electron independently,

$$\hat{H}_i = \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V_{eff} \right) \psi_i(\mathbf{r}_i) = e_i \psi_i(\mathbf{r}_i). \quad (10.61)$$

With this we calculate all energies and eigenfunctions (only the radial parts are of interest) minimizing the total energy and respecting the weak Pauli principle, that is, we classify the states in the order of increasing energies  $e_i$  and fill them successively with electrons. For the total wavefunction we obtain,

$$\left( \sum_{i=1}^N \hat{H}_i \right) \Psi_N = E_n \Psi_N \quad \text{with} \quad \Psi_N = \psi_1 \cdots \psi_N \quad \text{and} \quad E_n = \sum_{i=1}^N e_i. \quad (10.62)$$

With the eigenfunctions we calculate the charge densities  $e|\psi_j(\mathbf{r}_j)|^2$ . We integrate the interaction energy between these charge densities and the potentials exerted by the nucleus and all other electrons  $j \neq i$  to obtain an effective potential that represents an improved estimation for the electronic mean field,

$$V_{eff} \leftarrow -\frac{Ze^2}{4\pi\epsilon_0 r_i} + \sum_{j \neq i} \int d^3r_j \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} |\psi_j(\mathbf{r}_j)|^2. \quad (10.63)$$

We replace that potential in the Schrödinger equation, and repeat the whole process from the beginning, until the total energy  $\sum_i e_i$  does not get any lower. This self-consistent method is called *Hartree method*. Fock improved these calculations using antisymmetric wavefunctions for the valence electrons. This method is called *Hartree-Fock method*.

### 10.3.4 Hartree-Fock method

The Hartree-Fock method used to treat atomic or molecular many-body systems aims at obtaining the electronic wavefunction of the system. Dealing with anti-symmetrized wavefunctions, it represents a refinement of the Hartree method. The method is based on the variational principle and on the assumption that we can write the global wavefunction as a Slater determinant, with each electron occupying a specific orbital state (spin-orbital) and interacting with an effective potential stemming from the electrons which occupy other orbitals. Instead of solving the Schrödinger equation, we must now solve a set of equations called Hartree-Fock equations of the type  $\hat{F}\psi_k(1) = \epsilon_k \psi_k(1)$ . The method is performed iteratively until convergence of the atomic orbitals and their respective energies is reached. The procedure is then called *self-consistent*: Starting from an initial trial global wavefunction we calculate the effective potential in each orbital and a new set of wavefunctions which, in turn, generate a new effective potential. This new potential is then used in a new set of Hartree-Fock equations.

### 10.3.4.1 Hartree-Fock equations

To start with, we write the Hamiltonian (10.33) of a multi-electronic atom as [28],

$$\hat{H} = \sum_{i=1}^Z \hat{h}_i + \frac{1}{2} \sum_{i \neq j} \hat{V}_{ij}, \quad (10.64)$$

where  $\hat{h}_i$  is the Hamiltonian only of the electron  $i$ , and  $\hat{V}_{ij}$  is the interaction term between the electrons  $i$  and  $j$ . To implement the method we must suppose that the multi-electronic state can be written as the product of the individual states of each electron:

$$\Psi'(1, \dots, Z) = \psi_1(1)\psi_2(2)\dots\psi_Z(Z), \quad (10.65)$$

where  $\psi_i(1) = \phi_i(r_1)\chi(\alpha) = \psi_i^\alpha(r_1)$  represents the spin-orbital state of electron 1, that is, the spatial wavefunction of the electron in the state  $i$  and with spin  $\alpha$ . However, due to the symmetrization postulate, the physical state of the system must be expressed by a Slater determinant,

$$\Psi(1, \dots, Z) = \frac{1}{\sqrt{Z!}} \det [\psi_1(1)\psi_2(2)\dots\psi_Z(Z)]. \quad (10.66)$$

Now, we use the variational principle to minimize the expectation value of the ground state energy by varying the functions  $\psi_k(n)$ . In this way, the correct orbitals are those that minimize the energy. The expectation value is written as,

$$E = \langle \Psi | \hat{H} | \Psi \rangle = \langle \Psi | \sum_{i=1}^Z \hat{h}_i | \Psi \rangle + \langle \Psi | \frac{1}{2} \sum_{i \neq j} \hat{V}_{ij} | \Psi \rangle. \quad (10.67)$$

It is possible to show that,

$$\begin{aligned} \langle \Psi | \sum_{i=1}^Z \hat{h}_i | \Psi \rangle &= \sum_{i=1}^Z \langle \psi_i | \hat{h}_i | \psi_i \rangle \quad \text{and} \\ \langle \Psi | \frac{1}{2} \sum_{i \neq j} \hat{V}_{ij} | \Psi \rangle &= \frac{1}{2} \sum_{i,j}^Z [\langle \psi_i \psi_j | \hat{V}_{ij} | \psi_i \psi_j \rangle - \langle \psi_j \psi_i | \hat{V}_{ij} | \psi_j \psi_i \rangle]. \end{aligned} \quad (10.68)$$

Hence,

$$E = \sum_{i=1}^Z \langle \psi_i | \hat{h}_i | \psi_i \rangle + \frac{1}{2} \sum_{i,j}^Z [\langle \psi_i \psi_j | \hat{V}_{ij} | \psi_i \psi_j \rangle - \langle \psi_j \psi_i | \hat{V}_{ij} | \psi_j \psi_i \rangle]. \quad (10.69)$$

The above expression can be minimized via Lagrange multipliers under the constraint that the states are orthogonal  $\langle \psi_i | \psi_j \rangle = \delta_{ij}$ ,

$$\delta \left\{ \langle \Psi | \hat{H} | \Psi \rangle - \sum_{i,j} \epsilon_{ij} [\langle \psi_i \psi_j | \hat{V}_{ij} | \psi_i \psi_j \rangle - \langle \psi_j \psi_i | \hat{V}_{ij} | \psi_j \psi_i \rangle] \right\} \quad (10.70)$$

Thus, we obtain the following set of *Hartree-Fock equations*:

$$\hat{F}\psi_k(1) = \epsilon_k\psi_k(1) \quad \text{where} \quad \hat{F} = \hat{h}_1 + \sum_i (2\hat{J}_i - \hat{K}_i) \quad (10.71)$$

is the Fock operator and  $\epsilon_k$  is the energy associated with the spin-orbital  $\psi_k$ . The operator  $\hat{J}_i$ , called *Coulomb operator*, represents the mean potential sensed by electron 1 in the orbital  $k$  due to the presence of electron 2 in the orbital  $i$ :

$$\hat{J}_i\psi_k(1) = \left\{ \int \psi_i^*(2)V_{12}\psi_i(2)dr_2 \right\} \psi_k(1) . \quad (10.72)$$

The operator  $\hat{K}_i$ , denominated *exchange operator*, is a consequence of the symmetrization process and therefore a purely quantum effect, that is, without classical analogue:

$$\hat{K}_i\psi_k(1) = \left\{ \int \psi_i^*(2)V_{12}\psi_k(2)dr_2 \right\} \psi_k(1) . \quad (10.73)$$

Once we know all wavefunctions, the energies of the orbitals can be obtained in the following way:

$$\int dr_1\psi_k^*(1) \left\{ \hat{h}_1 + \sum_i (2\hat{J}_i - \hat{K}_i) \right\} \psi_k^*(1) = \epsilon_k \int dr_1\psi_k^*(1)\psi_k(1) = \epsilon_k , \quad (10.74)$$

that is,

$$\epsilon_k = \int dr_1\psi_k^*(1)\hat{h}_1\psi_k^*(1) + \sum_i (2\hat{J}_{ki} - \hat{K}_{ki}) , \quad (10.75)$$

where,

$$\begin{aligned} \hat{J}_{ki} &= \int dr_1\psi_k^*(1)\hat{J}_i\psi_k(1) && \text{is the Coulomb integral} \\ \hat{K}_{ki} &= \int dr_1\psi_k^*(1)\hat{K}_i\psi_k(1) && \text{is the exchange integral} . \end{aligned} \quad (10.76)$$

The total atomic energy can be calculated by,

$$E = 2 \sum_k \epsilon_k - \sum_{k,i} (2\hat{J}_{ki} - \hat{K}_{ki}) . \quad (10.77)$$

Furthermore, if assuming that, taking an electron away from the orbital  $\psi_k$  the electronic distribution remains unchanged, it is possible to associate the energy  $\epsilon_k$  with the ionization energy of the electron in this orbital,  $I_k \simeq \epsilon_k$ . This equality is known as *Koopman's theorem*.

## 10.3.5 Exercises

### 10.3.5.1 Ex: Effective potential in the Thomas-Fermi model

Calculate numerically and plot the effective potential in the Thomas-Fermi model from the differential equation (10.59) for  $Z = 40$  [749].



## 10.4 The periodic system of elements

Completely filled principal layers  $n, \ell$  are isotropic,  $\Psi_N(\mathbf{r}) = \Psi(r)$ , as we will show in Exc. 10.4.4.1. It is important to distinguish three different energetic sequences: 1. Tab. 10.5 shows, for a given atom, the excited orbitals of the *last electron*. 2. The energy sequence shown in Tab. 10.6 tells us in which orbital the next electron will be placed, when we go to the *next atom* in the periodic table 10.8 which has one more proton in the nucleus. 3. The inner electrons are subject to different potentials and, hence, follow a different sequence energetic sequence: While for the inner electrons we find,

$$E_{n,\ell} < E_{n,\ell+1} \ll E_{n+1,\ell}, \quad (10.78)$$

the sequence is partially inverted for the outermost electron. Note that it is the outermost electrons that determine the chemical reactivity of the atom. The sequence is illustrated in Fig. 10.4.

Noble gases have small radii, high excitation energies and high ionization energies. The outermost electrons in a noble gas atom must overcome a large energy gap to any higher quantum numbers. Halogens have strong electro-affinities, since the outer electron layer ( $n_{max}$ ) is incomplete and therefore malleable, such that an electron approaching the halogen perceives the nuclear charge through a partially transparent shield. Alkalis are similar to hydrogen and have excitation energies in the optical regime. Their fundamental state  $^2S_{1/2}$  is determined by a single valence electron in the  $\ell = 0$  orbital. Unlike hydrogen, excitation energies are highly dependent on  $\ell$ , since orbits with small  $\ell$  correspond to eccentric ellipses and have higher probabilities to be in the unshielded region  $-Z^2e^2/r$  than orbits with large  $\ell$ , who spend more time in the shielded region  $-e^2/r$ . For the same reason, energies corresponding to larger  $n$  resemble more those of the hydrogen spectrum.

### 10.4.0.1 Inner shell electrons

The interior shell structure of the atoms can be analyzed by X-ray scattering. Electrons decelerated by atoms emit a continuous spectrum called *Bremsstrahlung*, but they can also expel electrons from the inner layers leaving a hole behind. When a hole is filled by cascades of electrons falling down from higher layers, the atom emits a specific X-ray spectrum ( $\approx 10^4$  eV). The selection rules  $\Delta\ell = \pm 1$  and  $\Delta j = \pm 1$  split the lines in two components. X-ray spectra of neighboring elements in the periodic table are very similar, because the inner layers not being shielded, they see a potential close to  $\propto Z^2/r$ . Therefore, the  $Z$ -dependency of inner energy levels along a horizontal rows in the periodic table is more or less  $\omega \propto Z^2$ , as predicted by Bohr's atomic model.

### 10.4.1 Electronic shell model

In the Fermi gas model, each of the energy levels contains several states, and each of these states can be occupied by a single electron, according to the Pauli principle. In this way, we obtain the electronic configuration for the atoms of the periodic system. In this picture, the energies of the ground states of the elements, normalized by  $1/Z^2$ , can be arranged in the scheme of Fig. 10.3.

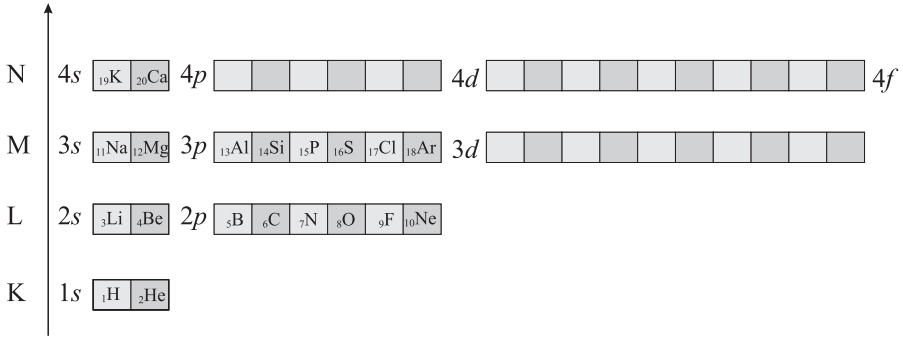


Figure 10.3: Periodic order.

This only works for atoms with up to 18 electrons. When the layer  $3p$  is completely filled, the next to be occupied is not  $3d$  but the  $4s$ . The new scheme is illustrated in Fig. 10.4. The anomalies beginning at  $Z = 18$  arise due to electron-electron interaction. The real potential evolves from one to the other Coulombian potential, as distance from the nucleus is increased, as illustrated in Fig. 10.2. Near the nucleus, the electrons shield the positive charge less than for large distances  $r$ . Thus, those states that have a high probability near the nucleus are energetically lowered. That is,

$$E_{2s} < E_{2p} \quad \text{and} \quad E_{6s} < E_{6p} < E_{6d} . \quad (10.79)$$

The degeneracy of the orbital angular momentum in the Schrödinger model is thus lifted. The shielding is, as can be seen in the example of the excited states of lithium, a large effect in the range of some eV.

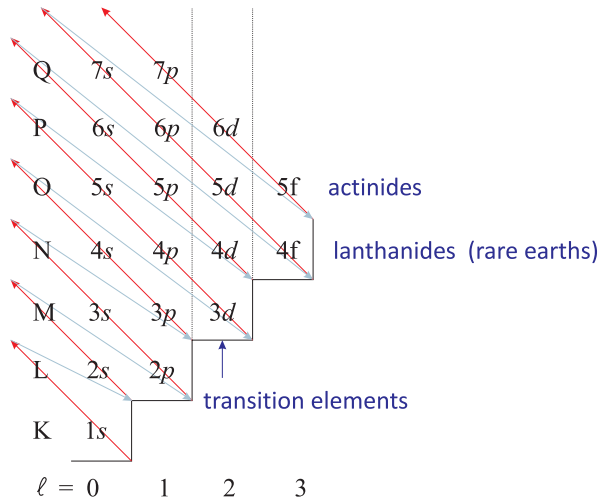


Figure 10.4: Illustration of the sequence of filling the orbitals with electrons.

The shielding also accounts for the anomalies in the periodic system, such as in K or Ca. Since  $E_{4s} < E_{3d}$ , the  $4s$  state is filled before the  $3d$ . Similar anomalies

also occur in Rb (5*s*), Cs (6*s*), and Fr (7*s*). In rare earths the shielding effect is even more pronounced. Here, the energy of the state 6*s* is even below the energy of the 4*f*, which means that the shells 6*s*, 5*s*, 5*p*, and 5*d* protect the 4*f* shell very well <sup>9</sup>. Resolve Exc. 10.4.4.2.

### 10.4.1.1 Alkalines

The electronic shell structure of alkalines consists of a completed noble gas shell and an additional valence electron. Their spectrum is therefore very similar to hydrogen. An empirical approach can be stressed to describe this feature,

$$E_{n,\ell} = -\frac{\mu_{EG}c^2}{2} \frac{Z^2\alpha^2}{(n - \Delta_{n,\ell})^2}, \quad (10.80)$$

where  $\mu_{EG}$  is the reduced mass relative to the noble gas shell and  $\Delta_{n,\ell}$  is called *quantum defect*. The quantum defect is tabulated for most alkaline states and is particularly important for low energy states. For sodium, for example, the values are:

$\ell$	$n = 3$	$n = 4$	$n = 5$	$n = 6$
<i>s</i>	1.37	1.36	1.35	1.34
<i>p</i>	0.88	0.87	0.86	0.86
<i>d</i>	0.10	0.11	0.13	0.11
<i>f</i>	-	0.00	-0.01	0.008

For states with a large angular momentum, the quantum defect disappears. In these states, the electron is far from the nucleus and the potential is similar to that of hydrogen. Alkalines are currently widely studied in quantum optics laboratories, for being comparatively simple, but having a sufficiently rich structure to be interesting. The fundamental electronic transitions typically lie in the visible and near-infrared spectral range and can be excited with comparatively simple laser sources. The lifetime of excited states is typically longer than 20 ns, which corresponds natural linewidths of approximately  $(2\pi) 10$  MHz.

### 10.4.1.2 Excited states

The experimentally easiest and most precise approach to determining orbital energies consists in measuring excitation spectra of valence electrons. The diagram of Fig. 10.5 compares such excitation spectra for various alkaline atoms. Although this is not to be confused with the binding energies of valence electrons of different atoms, it gives us a qualitative idea of the impact of shielding and indicates, which orbital will be occupied by the additional valence electron of the next species in the periodic table.

<sup>9</sup>An example of this is Nd:YAG (Neodymium in Yttrium Aluminum Garnet). In this crystal, optical transitions can be excited within the 4*f* shell of the Nd. However, these transitions are only allowed due to perturbations of the crystalline field. The very strong shielding ensures a long life of the excited state. For this reason this crystal is an excellent laser material.

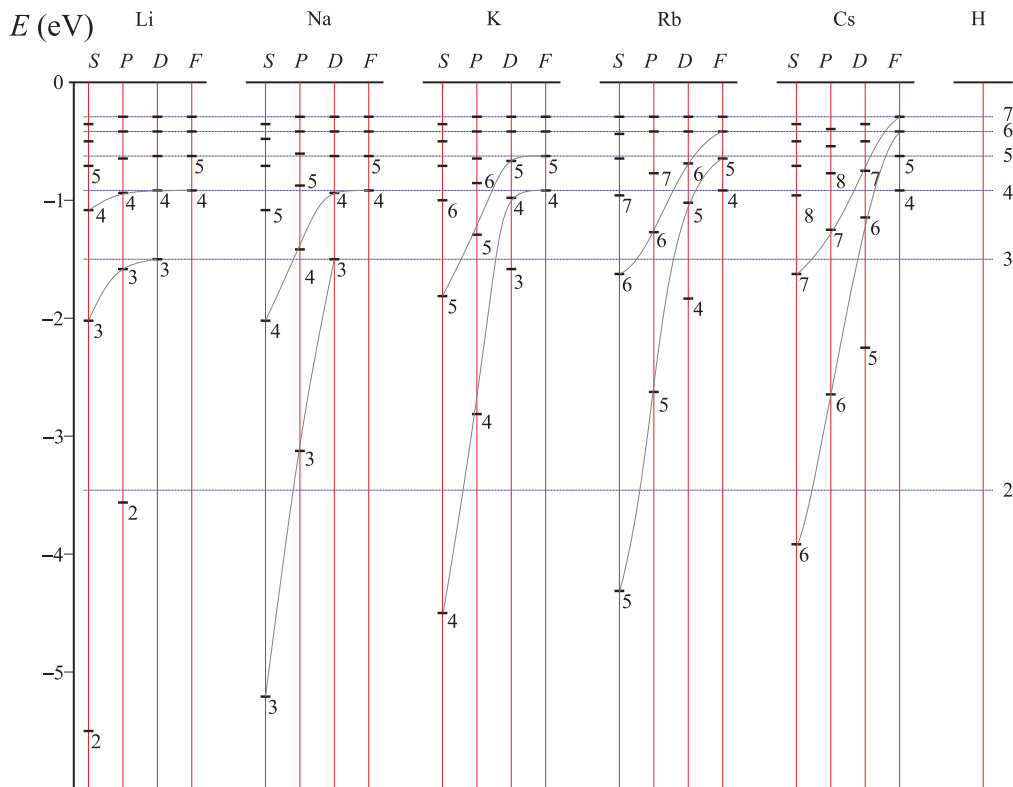


Figure 10.5: Comparison of the excitation energies of the *valence electron* for several alkaline atoms. Grey line are meant to guide the eye.

### 10.4.2 LS and jj-coupling

Following Hund's rule, the  $\mathbf{L} \cdot \mathbf{S}$ -coupling is energetically favorable compared to the  $\mathbf{j} \cdot \mathbf{j}$ -coupling, which means that the spins of the outermost electrons, that is, the electrons outside of filled subshells  $(n, \ell)$ , prefer to orient their spins in parallel in order to anti-symmetrize the spatial wavefunctions and thus maximize the distance between the electrons. Every sub-layer of the series shown in Fig. 10.4 must be filled in the listed order before placing new electrons in the next layer.

In the case of helium, we have seen that the Pauli principle first determines the relative orientation of the electron spins. The spins  $\mathbf{s}_i$  of the individual electrons therefore add up to a total angular momentum  $\mathbf{S}$ . The *orbital* angular momenta  $\mathbf{l}_i$  also adopt a relative orientation. It is determined by a residual spherically non-symmetric Coulomb interaction: A certain combination  $\mathbf{L}$  of orbital angular momenta leads to a certain spatial distribution of the electrons and thus to a certain electrostatic energy distribution.

The total spin  $\mathbf{S}$  and the total orbital angular momentum  $\mathbf{L}$  subsequently couple to a total angular momentum  $\mathbf{J}$  very similar to the  $\mathbf{l} \cdot \mathbf{s}$  spin-orbit coupling in single electron systems. States with different  $\mathbf{J}$  then have the respective energies that the

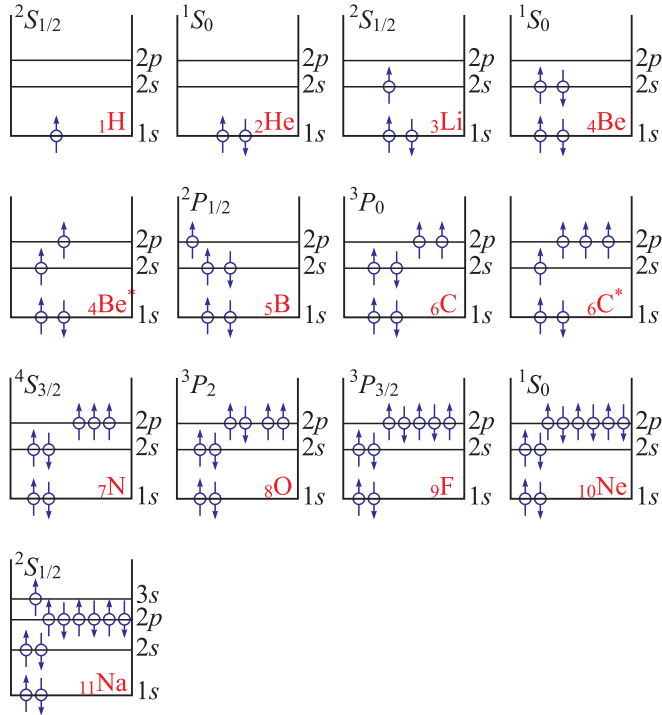


Figure 10.6: Illustration of Hund's rule.

total spin  $\mathbf{S}$  adopts in the field generated by the total orbital angular momentum  $\mathbf{L}$ <sup>10</sup>.

The above coupling scheme is called *Russel-Saunders coupling* or *LS-coupling*. It works well when the spin-orbit coupling of individual electrons is small. In this case, intercombination is forbidden, which means that there can be no electromagnetic transition between states with different spins (see the case of metastable helium in Sec. 10.2.2).

Since  $E_{LS} \simeq (Z\alpha)^4 \simeq Z^4$ , as shown in (8.131), for heavy atoms, the coupling of an electronic spin to its own orbital momentum grows strongly with  $Z$ , as well as the symmetrization and the exchange energy, which mutually orient the spins, and the residual Coulomb interaction, which mutually couples the angular orbital momenta. In this case, the orientation of  $\mathbf{L}_i$  relative to  $\mathbf{S}_i$  delivers more energy than the exchange energy and the residual energy cost. Hence, the spin and the orbital angular momentum of an individual electron couple first,

$$\mathbf{j}_i = \mathbf{l}_i + \mathbf{s}_i . \quad (10.81)$$

We obtain a new Hamiltonian of fine structure of the form,

$$H_{FS} \propto \mathbf{j}_i \cdot \mathbf{j}_j . \quad (10.82)$$

<sup>10</sup>In addition, there are the small contributions due to  $\mathbf{l}_i \cdot \mathbf{l}_j$ -coupling and to  $\mathbf{s}_i \cdot \mathbf{s}_j$ -coupling, where  $i \neq j$ .

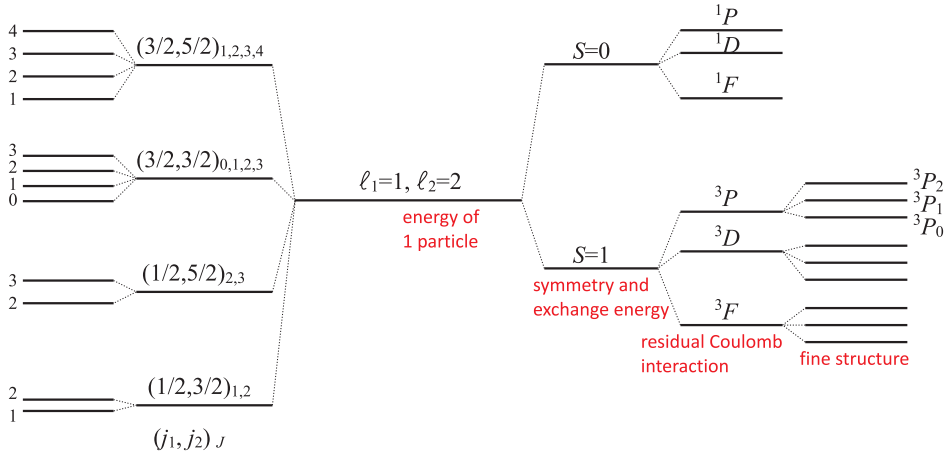


Figure 10.7: Hierarchy of coupling energies at the example of two electrons out of closed shells,  $(2p)(3d)$ , under the presumption of perfect  $jj$ -coupling (left) or  $LS$ -coupling (right).

Pure  $jj$ -coupling only exists for very heavy nuclei. Normally, we have a so-called *intermediate coupling*, which is a mixture of  $LS$  and  $jj$ -coupling. This can considerably relax the intercombination prohibition. When the coupling is pure, we have the following dipolar selection rules:

$LS$ -coupling:  $\Delta S = 0, \Delta L = \pm 1, \Delta \ell = \pm 1$

$jj$ -coupling:  $\Delta j = 0, \pm 1$  for one  $e^-$ ,  $\Delta j = 0$  for all others

In addition we have for the two couplings:  $\Delta J = 0, \pm 1$ , but  $J, J' = 0$  is forbidden,  $\Delta m_J = 0, \pm 1$  when  $\Delta J = 0$  but  $m_J, m_{J'} = 0$  is forbidden.

### 10.4.3 Summary of contributions to the atomic energy levels

The total Hamiltonian of a single atom is composed of the kinetic energy of the nucleus and the electrons, of various interaction potentials between the nucleus and the electrons, and of interactions with various types of external electromagnetic fields.

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla_R^2 + \sum_{i=1}^N \left( -\frac{\hbar^2}{2m} \nabla_{r_i}^2 \right) + V(\mathbf{r}_1, \mathbf{s}_1, \dots, \mathbf{r}_N, \mathbf{s}_N) + V_{ext} . \quad (10.83)$$

Of course, with the presence of other atoms, other interactions may generate other relevant contributions to the Hamiltonian.

The following interactions contribute to the potential  $V$ : The Coulomb interactions,

$$V_{ncl-ele} = -\sum_{i=1}^Z \frac{Ze^2}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}_i|} \quad \text{and} \quad V_{ele-ele} = \sum_{i < j=1}^Z \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} , \quad (10.84)$$

the antisymmetry of the wavefunction, that is, exchange integrals,

$$V_{sym} , \quad (10.85)$$

the energies of spin-orbit couplings,

$$V_{ls} = - \sum_{i=1}^Z \frac{1}{e2m^2c^2} \frac{1}{|\mathbf{r} - \mathbf{r}_i|} \frac{dV_{cl}}{dr_i} (\mathbf{l}_i \cdot \mathbf{s}_i) , \quad (10.86)$$

the energies of spin-spin couplings,

$$V_{ss} = \sum_{i \neq j=1}^Z \frac{e^2}{m^2} \left[ \frac{\sigma_i \cdot \sigma_j}{|r_i - r_j|^3} - 3 \frac{[\sigma_i \cdot (\mathbf{r}_i - \mathbf{r}_j)][\sigma_j \cdot (\mathbf{r}_i - \mathbf{r}_j)]}{(\mathbf{r}_i - \mathbf{r}_j)^5} \right] , \quad (10.87)$$

the energies of orbit-orbit couplings,

$$V_{ll} = \sum_{i \neq j=1}^Z c_{ij} (\mathbf{l}_i \cdot \mathbf{l}_j) , \quad (10.88)$$

interactions between the spin of the electrons and the nuclear spin and between the orbital angular momentum of the electrons and the nuclear spin,

$$V_{hfs} = \frac{A}{\hbar^2} \mathbf{J} \cdot \mathbf{I} , \quad (10.89)$$

and relativistic corrections.

$$V_{rel} , \quad (10.90)$$

In addition, static external fields may displace energy levels and can influence the internal coupling of angular momenta and spins,

$$V_{ext} = -\mathbf{d} \cdot \vec{\mathcal{E}} , \quad -\vec{\mu} \cdot \vec{\mathcal{B}} . \quad (10.91)$$

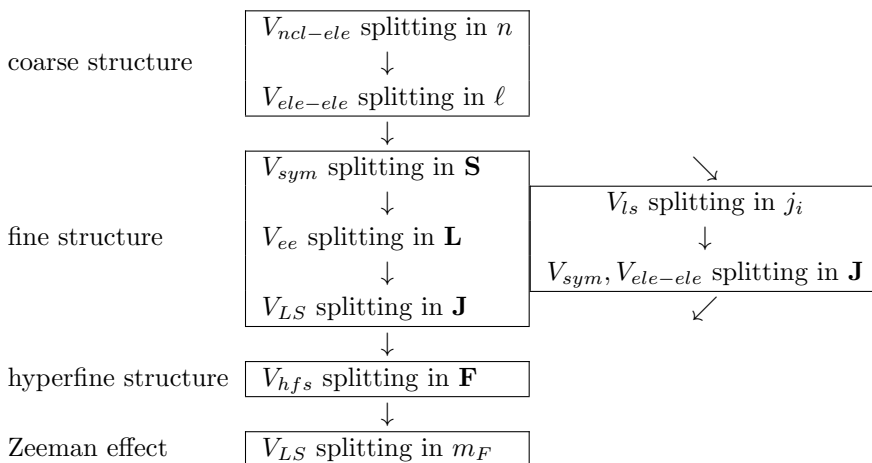
What quantum numbers are good depends on the relative amplitudes of intra-atomic interactions:

Case 1: fine structure with  $\mathbf{L} \cdot \mathbf{S}$ -coupling plus Zeeman splitting of hyperfine structure:  $V_{ncl-ele}, V_{ele-ele}^r \gg V_{ele-ele}^a, V_{sym} \gg V_{ls} \gg V_{hfs} \gg V_B$  the quantum number are  $|n_i, \ell_i, \mathbf{L}, \mathbf{S}, \mathbf{J}, \mathbf{F}, m_F\rangle$ .

Case 2: fine structure with  $\mathbf{j} \cdot \mathbf{j}$ -coupling plus Zeeman splitting of hyperfine structure:  $V_{ncl-ele}, V_{ele-ele}^r \gg V_{ls} \gg V_{ele-ele}^a, V_{sym} \gg V_{hfs} \gg V_B$  the quantum number are  $|n_i, \ell_i, j_i, \mathbf{J}, \mathbf{F}, m_F\rangle$ .

Case 3: fine structure with  $\mathbf{L} \cdot \mathbf{S}$ -coupling plus hyperfine structure of Zeeman splitting:  $V_{ncl-ele}, V_{ele-ele}^r \gg V_{ele-ele}^a, V_{sym} \gg V_{ls} \gg V_B \gg V_{hfs}$  the quantum number are  $|n_i, \ell_i, \mathbf{L}, \mathbf{S}, \mathbf{J}, m_J, m_I\rangle$ .

Case 4: fine structure with  $\mathbf{L} \cdot \mathbf{S}$ -coupling plus Paschen-Back splitting of fine structure:  $V_{ncl-ele}, V_{ele-ele}^r \gg V_{ele-ele}^a, V_{sym} \gg V_B \gg V_{ls} \gg V_{hfs}$  the quantum number are  $|n_i, \ell_i, \mathbf{L}, \mathbf{S}, m_L, m_S, m_I\rangle$ .



## 10.4.4 Exercises

### 10.4.4.1 Ex: Filled electronic shells

Show at the example of hydrogen that completely filled electronic layer are isotropic.

### 10.4.4.2 Ex: Electronic excitation levels of alkaline

Explain why

- state [Li]  $(2s)^2S_{1/2}$  has lower energy than [H]  $(2s)^2S_{1/2}$ ;
- state [Li]  $(2s)^2S_{1/2}$  has lower energy than [Li]  $(2p)^2P_J$ ;
- state [Na]  $(4s)^2S_{1/2}$  has lower energy than [Na]  $(3d)^2D_J$ .

## 10.5 Further reading

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# Chapter 11

## Molecular dimers

In systems of many particles (gases, fluids, or solids) interatomic interactions must be considered. These interactions usually have electrostatic origins, but generally can not be given in the form of closed expressions. For example, the collision of two atoms  $i$  and  $j$  can occur in a multitude of channels, that is, interaction potentials  $V(\mathbf{r}_i - \mathbf{r}_j)$ . Interatomic forces do not only govern collisions, but can sustain molecular bound states. This introduces new degrees of freedom in the systems of many particles through possible excitations of vibration or rotation movements.

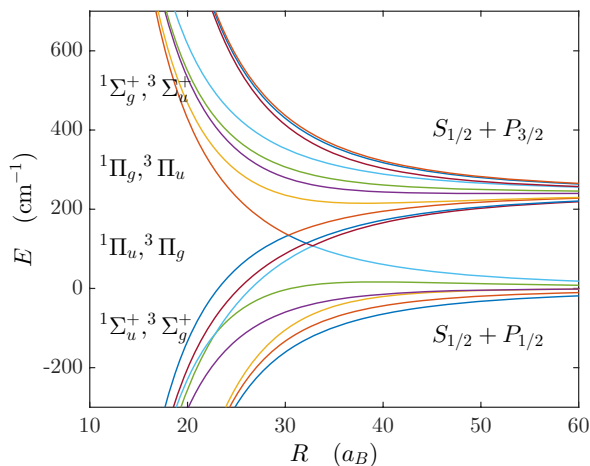


Figure 11.1: (code) Example of an interatomic potential spaghetti: The lowest states of the molecule  $^{85}\text{Rb}_2$ .

In this course, we will not go beyond homo- or heteronuclear dimers, that is, molecules consisting of two identical or different atoms.

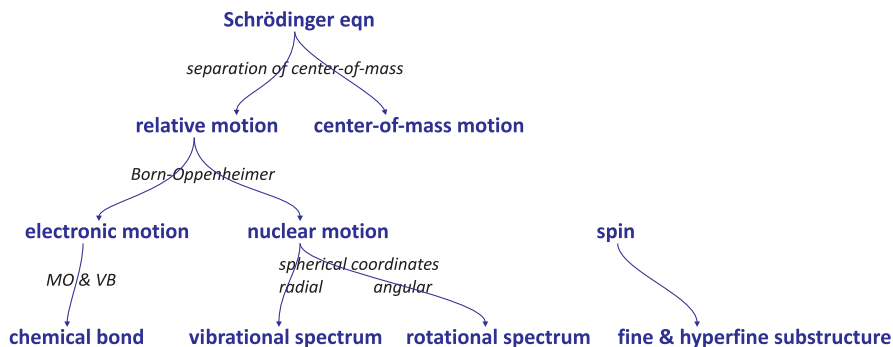


Figure 11.2: Approximations made in the molecular physics.

## 11.1 Molecular binding

### 11.1.1 Ionic and covalent binding

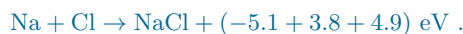
There are two fundamental ways of binding two atoms together, the ionic bond and the covalent bond<sup>1</sup>. The *ionic bond* is ruled by the quantities *electroaffinity* (EA), *electronegativity* (EN), and *ionization energy* (IE):

- **Ionization energy:** This energy is needed for the release of an electron by a neutral atom, e.g.  $\text{Na} + 5.1 \text{ eV} \rightarrow \text{Na}^+ + e^-$ .
- **Electroaffinity:** This energy is released by the capture of an electron by a neutral atom, e.g.  $\text{Cl} + e^- \rightarrow \text{Cl}^- + 3.8 \text{ eV}$ .
- **Electronegativity:** This quantity measures the stability of a valence orbital, e.g. that of fluorine (3.98) is more stable than that of cesium (0.79), such that fluorine holds its electrons tighter than cesium.

At short distances, the exchange of an electron between atoms can decrease energy. The so-called *ionic bond* is then sustained by the Coulombian attraction between two ions, and the binding energy can be estimated through electrostatic interaction.

**Example 51 (Ionic binding in NaCl):** For example, a sodium and a chlorine atom gain energy by forming a molecule,

(11.1)



<sup>1</sup>We are not considering metallic bonds nor hydrogen bridge bonds, here.

The molecules are polar and, therefore, have a permanent electric dipole moment. The bond has no preferential direction, since each atom is perfectly isotropic. Therefore, this type is well suited for the construction of crystalline lattices.

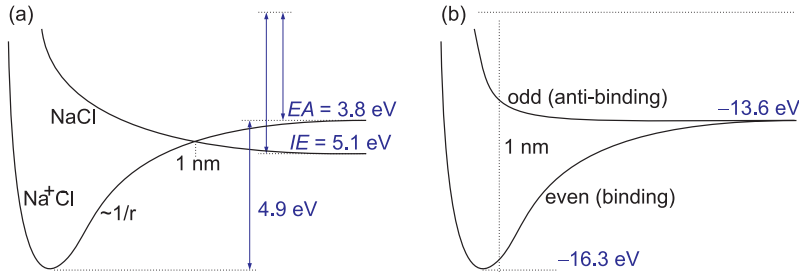


Figure 11.3: Scheme for (a) ionic binding of NaCl and (b) covalent binding of  $\text{H}_2$ .

To understand *covalent bond*, we consider the example  $\text{H}_2^+$  and estimate the interaction energy for each distance  $R$  between the nuclei. In this case, in contrast to atoms, the spherical symmetry is broken, and therefore the energy degeneracy with respect to parity is abolished, that is, for wavefunctions  $\psi(-x) = \pm\psi(x)$  the energies vary differently with  $R$ . The even wavefunction, which has an increased probability of the electron of being between the nuclei, is binding, which means that the interaction potential exhibits a minimum at a certain distance. The odd wavefunction, which disappears between the nuclei, is anti-binding, which means that the interaction potential is repulsive at all distances. In fact, an electron located at the center between two positive charges can overcome the Coulomb repulsion between the nuclei, whose mutual distance is twice. Obviously, the energy can not fall below that of the fundamental state of  $\text{He}^+$ , being approximately  $-4 \times 13.6$  eV. With two electrons, as in the case of the neutral molecule  $\text{H}_2$ , the anti-parallel orientation of the spins,  $\uparrow\downarrow$ , allows us to place the two electrons in the same orbital, while for parallel orientation,  $\uparrow\uparrow$ , we expect anti-binding. Each electron without a partner in an orbital can form a covalent bond, for example, phosphorus  $[\text{P}] = [\text{Ne}]3s^23p^{\uparrow\uparrow}$  has three available orbitals corresponding to different magnetic quantum numbers. The covalent bond is directional ( $sp^1$ ,  $sp^2$ , or  $sp^3$  hybridization), which is essential for the molecular structure such as in  $\text{CH}_4$ . Do the Exc. 11.1.6.1.

### 11.1.2 Born-Oppenheimer approximation and the $\text{H}_2^+$ molecule

The *Born-Oppenheimer approximation* in molecular physics consists in considering, at first, the positions of the nuclei as being fixed in space. This allows us to study the stationary states of the electrons subject to the potential created by the nuclei for a given internuclear distance  $R$ . Varying  $R$ , the electronic energies (computed for a fixed  $R$ ) remain the same, because the electronic wavefunctions adjust instantaneously due to their mass being much lower than that of the nuclei. The non-varying electronic energies play the role of interaction potential energies between the nuclei [28].

### 11.1.2.1 Separation of the center-of-mass

Let us consider two heavy masses,  $M_{a,b} = M$  separated by a distance  $R$  and interacting through a potential  $V_{nn}(R)$ . Furthermore, there is a light-weighted mass  $m_e$  interacting with the other masses through  $V_{ne}(r)$ . The Hamiltonian is,

$$\hat{H} = \frac{-\hbar^2}{2M} \nabla_a^2 + \frac{-\hbar^2}{2M} \nabla_b^2 + \frac{-\hbar^2}{2m_e} \nabla_e^2 + V_{nn}(|\mathbf{R}_a - \mathbf{R}_b|) + V_{ne}(|\mathbf{R}_a - \mathbf{R}_e|) + V_{ne}(|\mathbf{R}_b - \mathbf{R}_e|). \quad (11.2)$$

We transform to the center-of-mass system of the two heavy masses anchored at

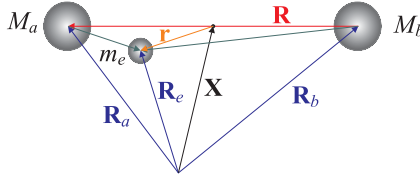


Figure 11.4: System with two heavy and one light mass.

$\mathbf{X} \equiv \frac{M_a \mathbf{R}_a + M_b \mathbf{R}_b}{M} = \frac{1}{2}(\mathbf{R}_a + \mathbf{R}_b)$ . The distance of the *heavies* is  $\mathbf{R} \equiv \mathbf{R}_a - \mathbf{R}_b$ , and the coordinate of the light mass counting from the center-of-mass is  $\mathbf{r} = \mathbf{R}_a - \frac{1}{2}\mathbf{R} - \mathbf{R}_e$ . Introducing the reduced mass of the *heavies*  $M_r = \frac{M}{2}$ ,

$$\left[ \frac{-\hbar^2}{2M} \nabla_X^2 + \frac{-\hbar^2}{2M_r} \nabla_R^2 + V_{nn}(R) + \frac{-\hbar^2}{2m_e} \nabla_r^2 + V_{ne}(|\mathbf{r} + \frac{\mathbf{R}}{2}|) + V_{ne}(|\mathbf{r} - \frac{\mathbf{R}}{2}|) \right] \Theta(\mathbf{X}) \Psi(\mathbf{R}, \mathbf{R}_e) = E_{tot} \Theta(\mathbf{X}) \Psi(\mathbf{R}, \mathbf{R}_e), \quad (11.3)$$

Here, we made the ansatz for the total wavefunction  $\Psi = \Theta(\mathbf{X}) \Psi(\mathbf{R}, \mathbf{R}_e)$ , assuming that the center-of-mass is only determined by the heavy masses,

$$\frac{-\hbar^2}{2M} \nabla_X^2 \Theta(\mathbf{X}) = E_{cm} \Theta(\mathbf{X}) \quad (11.4)$$

$$\left[ \frac{-\hbar^2}{2M_r} \nabla_R^2 + V_{nn}(R) + \frac{-\hbar^2}{2m_e} \nabla_r^2 + V_{ne}(|\mathbf{r} + \frac{1}{2}\mathbf{R}|) + V_{ne}(|\mathbf{r} - \frac{1}{2}\mathbf{R}|) \right] \Psi(\mathbf{R}, \mathbf{R}_e) = E \Psi(\mathbf{R}, \mathbf{R}_e),$$

where  $E_{tot} = E_{cm} + E$ .

### 11.1.2.2 Adiabatic approximation

The Born-Oppenheimer approximation now consists in assuming that the movement of the *heavies* is independent of the position of  $m_e$ , which allows us to separate the corresponding wavefunction  $\phi$  via the ansatz  $\Psi(\mathbf{R}, \mathbf{R}_e) = \psi(\mathbf{R}, \mathbf{r}) \phi(\mathbf{R})$ . On the other hand, the orbital  $\psi$  of the light mass  $m_e$  does not change much, when we vary the distance of the *heavies*,  $\nabla_R \psi(\mathbf{R}, \mathbf{r}) \simeq 0$ . This is only valid, as long as the *heavies* are inert on the time scale of the movement of  $m_e$ . Therefore, we can approximate the second derivative,

$$\begin{aligned} \nabla_R^2 [\psi(\mathbf{R}, \mathbf{r}) \phi(\mathbf{R})] &= \phi(\mathbf{R}) \nabla_R^2 \psi(\mathbf{R}, \mathbf{r}) + 2[\nabla_R \phi(\mathbf{R})] \cdot [\nabla_R \psi(\mathbf{R}, \mathbf{r})] + \psi(\mathbf{R}, \mathbf{r}) \nabla_R^2 \phi(\mathbf{R}) \\ &\simeq \psi(\mathbf{R}, \mathbf{r}) \nabla_R^2 \phi(\mathbf{R}), \end{aligned} \quad (11.5)$$

postulating that the first two terms are negligible compared to the third. We can now separate the second equation (11.4) in two parts, the first being,

$$\left[ \frac{-\hbar^2}{2m_e} \nabla_{\mathbf{r}}^2 + V_{ne}(|\mathbf{r} + \frac{1}{2}\mathbf{R}|) + V_{ne}(|\mathbf{r} - \frac{1}{2}\mathbf{R}|) \right] \psi(\mathbf{r}, \mathbf{R}) = \varepsilon(R) \psi(\mathbf{r}, \mathbf{R}) . \quad (11.6)$$

We solve this equation for the electronic degree of freedom  $\mathbf{r}$  by choosing a fixed internuclear distance  $\mathbf{R}$ , and we substitute in the second expression (11.4), which gives,

$$\left[ \frac{-\hbar^2}{2M_r} \nabla_R^2 + V_{nn}(R) + \varepsilon(R) \right] \phi(\mathbf{R}) = E \phi(\mathbf{R}) . \quad (11.7)$$

Treating the interatomic distance  $R$  as a fixed parameter, the solution of Eq. (11.6) provides the electronic orbitals and their energies  $\varepsilon(R)$ . The *Born-Oppenheimer potential* is composed of the electrostatic repulsive potential of the nuclei and the kinetic energy of the electron,  $V_{nn}(R) + \varepsilon(R)$ . In other words, the presence of the electrons generates an additional interaction energy between the nuclei. By inserting this complete interatomic potential into Eq. (11.7), we can determine its vibrational structure  $\phi_{vib}(\mathbf{R})$ .

Fig. 11.5 shows an example of binary effective nuclear potentials, as a function of the distance  $R$  between the two nuclei. Each curve corresponds to a different solution of the electronic equation, that is, to a different electronic state. In many cases, such nuclear potentials have a stable equilibrium region. The bound states located in these regions are *molecular* bound states of two atoms.

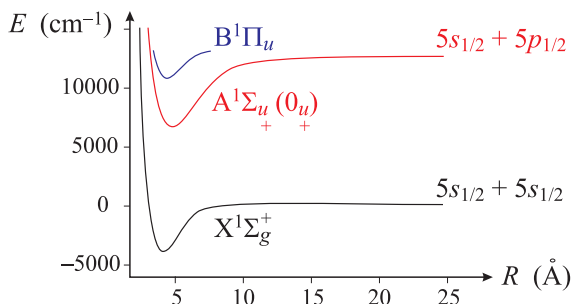


Figure 11.5: Effective nuclear potentials for the interaction between two rubidium atoms ( $\text{Rb}_2$ ).

In practice, the calculation of adiabatic Born-Oppenheimer potentials is difficult and makes it the subject of sophisticated theories, such as the *molecular orbital model* or the *valence bond model*<sup>2</sup>. We study in Exc. 11.1.6.2 a generalization of the Born-Oppenheimer approximation.

<sup>2</sup>Note that the Born-Oppenheimer approximation is no longer good in the presence of relativistic or spin-orbit coupling effects.

### 11.1.3 Linear combination of orbitals and the H<sub>2</sub> molecule

In the following we will discuss the electronic structure of the simplest neutral molecule: H<sub>2</sub>. For the low electron states of this molecule, the Born-Oppenheimer approximation is totally satisfactory, that is, we want to solve a Schrödinger type equation (11.6), but with two electrons. We are, therefore, interested in the electronic Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m_e}(\nabla_1^2 + \nabla_2^2) + \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{R_{ab}} - \frac{1}{|\mathbf{r}_1 - \mathbf{R}_a|} - \frac{1}{|\mathbf{r}_1 - \mathbf{R}_b|} - \frac{1}{|\mathbf{r}_2 - \mathbf{R}_a|} - \frac{1}{|\mathbf{r}_2 - \mathbf{R}_b|} + \frac{1}{r_{12}} \right), \quad (11.8)$$

where '1' and '2' denote the two electrons and 'a' and 'b' the nuclei.

This problem can not be solved analytically. The standard procedure begins with choosing a suitable basis, i.e. a very compact basis which does not depend on the configuration of the molecule. That is, we want the basis to be composed of functions that do not depend on the distance between the two nuclei,  $R_{ab}$ , to avoid calculations for different bond lengths.

The most natural basis functions are the available atomic orbitals of the individual hydrogen atoms. When the bond length is too large, the system approaches the limit of two non-interacting hydrogen atoms. In this case, the electron wavefunction can be approximated by the product of *atomic orbitals* (AO) of atom 'a' and atom 'b'. Therefore, the smallest basis that gives us a realistic picture of the fundamental state of the H<sub>2</sub> molecule must comprise two functions:  $|1s_a\rangle$  and  $|1s_b\rangle$ . For finite bond lengths, it is advisable to allow the AOs to polarize and deform in response to the presence of the other electron (and the other nucleus). However, the  $|1s_a\rangle$  and  $|1s_b\rangle$  functions do not have to be exactly the hydrogenic eigenfunctions. It is sufficient to require them to be similar to the 1s orbitals and be centered on them. Since the actual shape of the orbitals is not yet fixed, we will give all the expressions in abstract matrix form, leaving the spatial integration for once the shape of the orbitals has been specified. This is the method of *linear combination of atomic orbitals* (LCAO).

### 11.1.4 Molecular orbital theory

We are now in a position to discuss the basic principles of the *molecular orbital method* (MO), which is the basis of the theory of the electronic structure of real molecules. The first step in any MO approach is to separate the Hamiltonian into two parts, one part describing the electrons '1' and '2' separately and one part counting for the interaction between them:

$$\hat{H} = \hat{h}(1) + \hat{h}(2) + \hat{V}_{12} + \frac{e^2}{4\pi\epsilon_0} \frac{1}{R_{ab}} \quad \text{with} \quad (11.9)$$

$$\hat{h}(i) = -\frac{\hbar^2\nabla_i^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{|\mathbf{r}_i - \mathbf{R}_a|} + \frac{1}{|\mathbf{r}_i - \mathbf{R}_b|} \right) \quad \text{and} \quad \hat{V}_{12} = \frac{e^2}{4\pi\epsilon_0} \frac{1}{r_{12}},$$

where  $i = 1, 2$ . We must remember that, within the BO approximation,  $R_{ab}$  is just a number. We choose the Hamiltonian  $\hat{h}(i)$  as the one-electron part of the complete Hamiltonian in matrix representation on the minimum basis:

$$\begin{pmatrix} \langle 1s_a | \hat{h} | 1s_a \rangle & \langle 1s_a | \hat{h} | 1s_b \rangle \\ \langle 1s_b | \hat{h} | 1s_a \rangle & \langle 1s_b | \hat{h} | 1s_b \rangle \end{pmatrix} \equiv \begin{pmatrix} \epsilon & h_{ab} \\ h_{ab} & \epsilon \end{pmatrix}, \quad (11.10)$$

defining the average one-electron energy  $\epsilon \equiv \langle 1s_a | \hat{h} | 1s_a \rangle$  and the non-diagonal coupling (often called *resonance integral*)  $h_{ab} \equiv \langle 1s_a | \hat{h} | 1s_b \rangle = \langle 1s_a | \hat{h} | 1s_b \rangle$ . We can immediately diagonalize this matrix, the eigenvalues and the eigenvalues being:

$$\epsilon_{\pm} = \epsilon \pm h_{ab} \quad \text{and} \quad |\phi_{\pm}\rangle \propto \frac{1}{2}(|1s_a\rangle \pm |1s_b\rangle). \quad (11.11)$$

The one-electron effective Hamiltonian eigenstates are called *molecular orbital* (MO). They are one-electron wavefunctions delocalized over the spatial regions of the molecule.

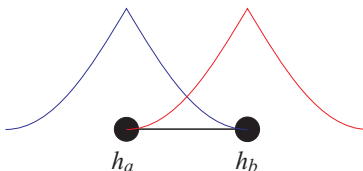


Figure 11.6: Illustration of the atomic orbitals.

We need to first normalize the MOs, which is more complicated than it might seem, because the AOs are not orthogonal. For example, when the atoms approach each other, their AOs may have the shape shown in Fig. 11.6. However, by defining the overlap integral by  $S \equiv \langle 1s_a | 1s_b \rangle$ , we can normalize as follows:

$$|\phi_{\pm}\rangle = \frac{1}{\sqrt{2(1 \pm S)}}(|1s_a\rangle \pm |1s_b\rangle), \quad (11.12)$$

since,

$$\langle \phi_{\pm} | \phi_{\pm} \rangle = \frac{1}{2(1 \pm S)} (\langle 1s_a | 1s_a \rangle \pm \langle 1s_a | 1s_b \rangle \pm \langle 1s_b | 1s_a \rangle + \langle 1s_b | 1s_b \rangle) = 1. \quad (11.13)$$

These eigenfunctions merely show the symmetry of the molecule. The two hydrogen atoms are equivalent and, therefore, the eigenorbital must give equal weight to each  $1s$  orbital. Thus, our choice of the one-electron Hamiltonian does not really matter that much, because every one-electron Hamiltonian exhibiting the symmetry of the molecule would give the same molecular orbitals. For historical reasons,  $|\phi_{+}\rangle$  is denoted by  $|\sigma\rangle$  and  $|\phi_{-}\rangle$  by  $|\sigma^*\rangle$ .

The second step in MO theory consists of constructing the determinant from the MOs corresponding to the wanted states. For illustration we will look at the lowest singlet state constructed from molecular orbitals. We note that  $h_{ab} < 0$ , such that  $|\sigma\rangle$  has an energy inferior to  $|\sigma^*\rangle$ . Neglecting the interaction, the lowest singlet state,

$$|\Phi_{MO}\rangle = |\sigma\rangle|\sigma^*\rangle, \quad (11.14)$$

is the molecular ground state of  $H_2$ . To estimate the validity of the approximation, we calculate the expectation value of the energy,  $\left| \langle \sigma | \langle \sigma^* | \hat{H} | \sigma \rangle | \sigma^* \rangle \right|$ , decomposing the wavefunction into spin and spatial parts, noting that the spin part is normalized:

$$\begin{aligned} \left| \langle \sigma | \langle \sigma^* | \hat{H} | \sigma \rangle | \sigma^* \rangle \right| &= \langle \sigma(1) | \langle \sigma(2) | \hat{H} | \sigma(1) \rangle | \sigma(2) \rangle \langle \Phi_{spin} | \Phi_{spin} \rangle \\ &= \langle \sigma(1) | \langle \sigma(2) | \hat{H} | \sigma(1) \rangle | \sigma(2) \rangle. \end{aligned} \quad (11.15)$$



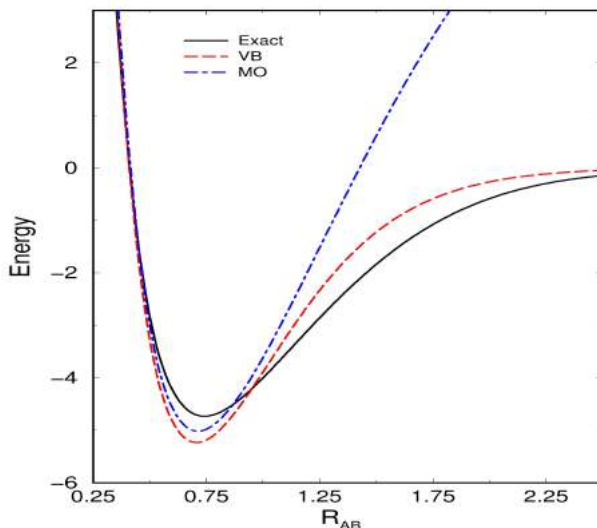


Figure 11.7: Total energy as a function of interatomic distance.

Hence, with (11.10) we get,

$$\begin{aligned}
 \langle \sigma(1) | \langle \sigma(2) | \hat{h}(2) | \sigma(2) \rangle | \sigma(1) \rangle | \sigma(2) \rangle &= \langle \sigma(1) | \sigma(1) \rangle \langle \sigma(2) | h(2) | \sigma(2) \rangle = \langle \sigma(2) | h(2) | \sigma(2) \rangle \equiv \epsilon_\sigma \\
 \langle \sigma(1) | \langle \sigma(2) | \hat{h}(1) | \sigma(1) \rangle | \sigma(2) \rangle &= \langle \sigma(1) | h(1) | \sigma(1) \rangle \langle \sigma(2) | \sigma(2) \rangle = \langle \sigma(1) | h(1) | \sigma(1) \rangle \equiv \epsilon_\sigma \\
 \langle \sigma(1) | \langle \sigma(2) | \hat{V}_{12} | \sigma(1) \rangle | \sigma(2) \rangle &\equiv J_{\sigma\sigma} .
 \end{aligned} \tag{11.16}$$

Putting these facts together, we can write,

$$\begin{aligned}
 \langle \Phi_{MO} | \hat{H} | \Phi_{MO} \rangle &= \langle \Phi_{MO} | \hat{h}_1 | \Phi_{MO} \rangle + \langle \Phi_{MO} | \hat{h}_2 | \Phi_{MO} \rangle + \langle \Phi_{MO} | \hat{V}_{12} | \Phi_{MO} \rangle + \frac{e^2}{4\pi\epsilon_0 R_{ab}} \\
 &= 2\epsilon_\sigma + J_{\sigma\sigma} + \frac{e^2}{4\pi\epsilon_0 R_{ab}} .
 \end{aligned} \tag{11.17}$$

Each of the first two terms represents the energy of a single electron (either 1 or 2) in the field produced by both the nuclei ( $\hat{h}$ ), while the third is the average repulsion between the two electrons. Note that the first and second term are both positive, such that the bond must come from the one-electron part. This is the MO energy for the ground state of the  $\text{H}_2$ . We can try a more reasonable ansatz for the  $1s$ -type basis functions <sup>3</sup> by determining the unknown quantities from above ( $\epsilon_\sigma$  and  $J_{\sigma\sigma}$ ) numerically and plot the total energy as a function of  $R_{ab}$  (blue dotted curve in Fig. 11.7). The exact adiabatic energy function determined from experimental data (solid black curve) agrees well at low energies. Summarizing the results with some key numbers, we note that MO theory predicts a bond distance of 0.072 nm in reasonable agreement with the exact value of 0.074 nm. We can also compare the

<sup>3</sup>It turns out that it is more convenient to adjust the exponential decomposition of the hydrogenic orbitals to a sum of Gaussians.

binding energies,

$$D_e = E_{H_2}(R_{equil}) - 2E_H . \quad (11.18)$$

MOs theory predicts a binding energy of 5.0 eV compared to the experimental value of 4.75 eV. In view of the simplicity of the wavefunction and the absence of adjustable parameters the agreement is not so bad. Unfortunately, far away from the equilibrium distance, we have an unpleasant surprise: the molecule does not dissociate into two hydrogen atoms!

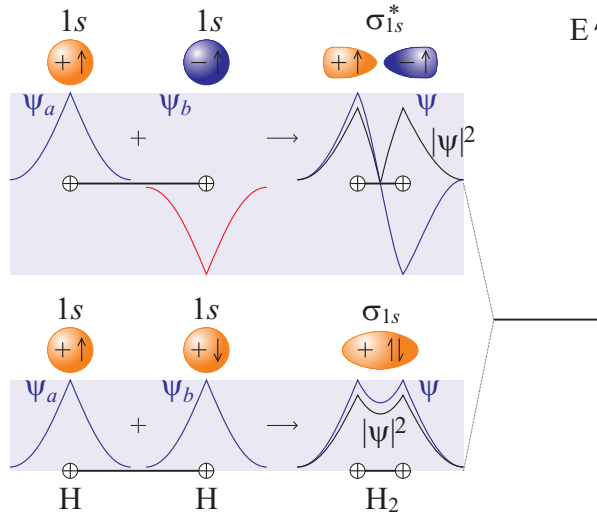


Figure 11.8: Illustration of MO theory for a dimer of two equal atoms, each one with a valence electron in the atomic 1s orbital: When the atoms approach, the atomic orbitals form new molecular binding and anti-biding orbitals.

To get an idea of what is happening near dissociation, we expand the fundamental MO state in terms of AO configurations:

$$\begin{aligned} |\Phi_{MO}\rangle &\propto |\sigma(1)\rangle|\sigma(2)\rangle|\Phi_{spin}\rangle \\ &= \frac{1}{2(1+S)}(|1s_a(1)\rangle + |1s_b(1)\rangle)(|1s_a(2)\rangle + |1s_b(2)\rangle)|\Phi_{spin}\rangle \\ &= \frac{1}{2(1+S)}(|1s_a(1)\rangle|1s_a(2)\rangle + |1s_a(1)\rangle|1s_b(2)\rangle + |1s_b(1)\rangle|1s_a(2)\rangle + |1s_b(1)\rangle|1s_b(2)\rangle)|\Phi_{spin}\rangle . \end{aligned} \quad (11.19)$$

The two terms in the middle of the last line, called *covalent configurations*, are exactly what we expect near dissociation: one electron in each hydrogen atom. However, the first and last term (which are called *ionic configurations*) correspond to having two electrons in one atom and none in the other, which gives us  $H^+$  and  $H^-$  at dissociation! Since the weight of these terms is fixed, it is obvious that we got the wrong wavefunction (and therefore the wrong energy) when dissociating the molecule. Near the equilibrium point, the ionic terms contribute significantly to the true wavefunction, such that the MO theory is good at this point. But it is always terrible at dissociation.

### 11.1.5 Valence binding

An alternative to MO theory represents the *valence bond* theory (VB). Here, we use significantly more physical intuition and discard the ionic configurations from the MO wavefunction. Thus, the VB ground state wavefunction is:

$$\begin{aligned}
 |\Psi\rangle &\propto \frac{|1s_a(1)\rangle|1s_a(2)\rangle + |1s_b(1)\rangle|1s_a(2)\rangle}{\sqrt{2}} \frac{|\uparrow(1)\rangle|\downarrow(2)\rangle + |\downarrow(1)\rangle|\uparrow(2)\rangle}{\sqrt{2}} \\
 &\equiv |\Psi_{space}\rangle|\Psi_{spin}\rangle .
 \end{aligned} \tag{11.20}$$

VB theory assumes that this wavefunction is a good approximation to the true wavefunction at *all* binding distances and not only at large distances  $R_{ab}$ . To verify this approximation, we can calculate the average energy for this VB state. First, we normalize the VB wavefunction,

$$\begin{aligned}
 \langle\Psi|\Psi\rangle &= \langle\Psi_{space}|\langle\Psi_{spin}|\Psi_{space}\rangle|\Psi_{spin}\rangle = \langle\Psi_{space}|\Psi_{space}\rangle \\
 &= \frac{1}{2} (\langle 1s_a(1)|\langle 1s_b(2)| + \langle 1s_b(1)|\langle 1s_a(2)|) (|1s_a(1)\rangle|1s_a(2)\rangle + |1s_b(1)\rangle|1s_a(2)\rangle) \\
 &= \frac{1}{2} (\langle 1s_a(1)|1s_b(2)|1s_a(1)\rangle|1s_b(2)\rangle + \langle 1s_a(1)|1s_b(2)|1s_b(1)\rangle|1s_a(2)\rangle \\
 &\quad + \langle 1s_b(1)|1s_a(2)|1s_a(1)\rangle|1s_b(2)\rangle + \langle 1s_b(1)|1s_a(2)|1s_b(1)\rangle|1s_a(2)\rangle) \\
 &= \frac{1}{2}(1 + S^2 + S^2 + 1) = 1 + S^2 .
 \end{aligned} \tag{11.21}$$

Therefore, the correctly normalized VB wavefunction is:

$$|\Psi_{VB}\rangle = \frac{1}{2\sqrt{1+S^2}} (|1s_a(1)\rangle|1s_a(2)\rangle + |1s_b(1)\rangle|1s_a(2)\rangle) (|\uparrow(1)\rangle|\downarrow(2)\rangle - |\downarrow(1)\rangle|\uparrow(2)\rangle) . \tag{11.22}$$

Now we want to calculate  $\langle\hat{H}_{el}\rangle$  for this state. We note that the spin part does not matter, since the Hamiltonian is independent of spin:

$$\begin{aligned}
 \langle\Psi_{VB}|\hat{H}|\Psi_{VB}\rangle &= \langle\Psi_{spin}|\langle\Psi_{space}|\hat{H}|\Psi_{space}\rangle|\Psi_{spin}\rangle \\
 &= \langle\Psi_{space}|\hat{H}|\Psi_{space}\rangle\langle\Psi_{spin}|\Psi_{spin}\rangle = \langle\Psi_{space}|\hat{H}|\Psi_{space}\rangle .
 \end{aligned} \tag{11.23}$$

The only remnant of the spin state is the fact that the spatial wavefunction is symmetric, which is only possible when the spin part is antisymmetric. Treating each term in  $\langle\hat{H}\rangle$  separately,

$$\begin{aligned}
 \langle\Psi|\hat{h}_1|\Psi\rangle &= \frac{1}{2} (\langle 1s_a(1)|\langle 1s_b(2)| + \langle 1s_b(1)|\langle 1s_a(2)|) \hat{h}_1 (|1s_a(1)\rangle|1s_a(2)\rangle + |1s_b(1)\rangle|1s_a(2)\rangle) \\
 &= \frac{1}{2} \left( \langle 1s_a(1)|1s_b(2)|\hat{h}_1|1s_a(1)\rangle|1s_b(2)\rangle + \langle 1s_a(1)|1s_b(2)|\hat{h}_1|1s_b(1)\rangle|1s_a(2)\rangle \right. \\
 &\quad \left. + \langle 1s_b(1)|1s_a(2)|\hat{h}_1|1s_a(1)\rangle|1s_b(2)\rangle + \langle 1s_b(1)|1s_a(2)|\hat{h}_1|1s_b(1)\rangle|1s_a(2)\rangle \right) \\
 &= \frac{1}{2}(\epsilon + Sh_{ab} + \epsilon + Sh_{ab}) ,
 \end{aligned} \tag{11.24}$$

or,

$$\boxed{\langle\Psi_{VB}|\hat{h}_1|\Psi_{VB}\rangle = \frac{\epsilon + Sh_{ab}}{1 + S^2}} . \tag{11.25}$$

Since the two electrons are identical, the elements of the  $\hat{h}_2$  are the same as those of  $\hat{h}_1$ . The only remaining term is the average value of the interaction:

$$\begin{aligned} \langle \Psi | \hat{V}_{12} | \Psi \rangle &= \frac{1}{2} (\langle 1s_a(1) | 1s_b(2) \rangle + \langle 1s_b(1) | 1s_a(2) \rangle) \hat{V}_{12} (|1s_a(1)\rangle |1s_a(2)\rangle + |1s_b(1)\rangle |1s_a(2)\rangle) \\ &= \frac{1}{2} \left( \langle 1s_a(1) | 1s_b(2) \rangle \langle \hat{V}_{12} | 1s_a(1)\rangle |1s_b(2)\rangle + \langle 1s_a(1) | 1s_b(2) \rangle \langle \hat{V}_{12} | 1s_b(1)\rangle |1s_a(2)\rangle \right. \\ &\quad \left. + \langle 1s_b(1) | 1s_a(2) \rangle \langle \hat{V}_{12} | 1s_a(1)\rangle |1s_b(2)\rangle + \langle 1s_b(1) | 1s_a(2) \rangle \langle \hat{V}_{12} | 1s_b(1)\rangle |1s_a(2)\rangle \right). \end{aligned} \quad (11.26)$$

The second and third terms are the same. They are called *exchange integrals*, because the 'bra' orbitals have switched order as compared to the 'kets':

$$K = \langle 1s_a(1) | 1s_b(2) \rangle \langle \hat{V}_{12} | 1s_b(1)\rangle |1s_a(2)\rangle = \langle 1s_b(1) | 1s_a(2) \rangle \langle \hat{V}_{12} | 1s_a(1)\rangle |1s_b(2)\rangle. \quad (11.27)$$

The first and fourth terms are also the same. They are called *Coulomb integrals*, because they seem to be due to the Coulomb interaction between two charge densities:

$$J = \langle 1s_b(1) | 1s_a(2) \rangle \langle \hat{V}_{12} | 1s_a(1)\rangle |1s_b(2)\rangle = \langle 1s_a(1) | 1s_b(2) \rangle \langle \hat{V}_{12} | 1s_b(1)\rangle |1s_a(2)\rangle. \quad (11.28)$$

Therefore, we have the result,

$$\boxed{\langle \Psi_{VB} | \hat{V}_{12} | \Psi_{VB} \rangle = \frac{J + K}{1 + S^2}}. \quad (11.29)$$

Adding all terms, we get:

$$\begin{aligned} \langle \Psi_{VB} | \hat{H} | \Psi_{VB} \rangle &= \langle \Psi_{VB} | \hat{h}_1 | \Psi_{VB} \rangle + \langle \Psi_{VB} | \hat{h}_2 | \Psi_{VB} \rangle + \langle \Psi_{VB} | \hat{V}_{12} | \Psi_{VB} \rangle + \frac{1}{R_{ab}} \\ &= 2 \frac{\epsilon + S h_{ab}}{1 + S^2} + \frac{J + K}{1 + S^2} + \frac{1}{R_{ab}}. \end{aligned} \quad (11.30)$$

The Coulomb and exchange terms are positive. Nuclear repulsion is clearly positive. Thus, the only terms that lead to binding in this picture are the average energy of an electron  $\epsilon$  and the resonance integral  $h_{ab}$ . If the first term is dominant, the bond is due to *electronic delocalization*, since an electron located near one of the atoms would only contribute the atomic value to  $\epsilon$ , which does not imply a bound state. If  $h_{ab}$  is large, the bond involves some resonance character, which can be related to the familiar concept of resonance between different Lewis point structures.

A numerical evaluation of all integrals gives the potential curve presented in Fig. 11.7 for VB theory. As expected, this simple VB wavefunction gives the correct dissociation threshold, where MO theory fails. In addition, the accuracy of the simple VB result is surprisingly good even near the equilibrium distance: The VB predicts a bond distance of 0.071 nm (compared to the correct value of 0.074 nm) and  $D_e = 5.2$  eV (compared to 4.75 eV). Thus, the VB wavefunction also gives a good agreement without adjustable parameters. But more importantly, it indicates a way of improving the wavefunction whenever we encounter an obvious error: in this case, we saw that the description of the dissociation was weak, and we constructed a VB ansatz curing the problem. This approach to VB is often generalized as follows

when dealing with polyatomic molecules. We write the wavefunction as a product of a spatial part and a spin:

$$|\Psi\rangle = |\Psi_{space}\rangle |\Psi_{spin}\rangle . \quad (11.31)$$

The main assumption in VB theory is that the spatial part can be well represented by a product of atomic-like functions. For example, for water, we would immediately write a spatial part as:

$$|\Psi_{space}\rangle \simeq |1s_{H_a}\rangle |1s_{H_b}\rangle |1s_O\rangle |1s_O\rangle |2s_O\rangle |2s_O\rangle |2p_{xO}\rangle |2p_{xO}\rangle |2p_{yO}\rangle |2p_{yO}\rangle . \quad (11.32)$$

However, there are two things wrong with this wavefunction. First, we know that atomic orbitals hybridize in a molecule. Therefore, we need to make appropriate linear combinations of AOs (in this case  $sp^3$  hybrids) to obtain the hybridized AOs. In this case, the four  $sp^3$  hybrids can be written symbolically as:

$$|sp^3\rangle = c_{s,i}|2s\rangle + c_{x,i}|2p_x\rangle + c_{y,i}|2p_y\rangle + c_{z,i}|2p_z\rangle . \quad (11.33)$$

and therefore, a more appropriate spatial configuration is:

$$|\Psi_{space}\rangle \simeq |1s_{H_a}\rangle |1s_{H_b}\rangle |1s_O\rangle |1s_O\rangle |sp_{1O}^3\rangle |sp_{1O}^3\rangle |sp_{2O}^3\rangle |sp_{2O}^3\rangle |sp_{3O}^3\rangle |sp_{4O}^3\rangle . \quad (11.34)$$

The other problem with this state is that it lacks the adequate symmetry to describe fermions; the general state must be antisymmetric. In the case of two electrons this concept is easy to apply - singlets have symmetric space parts and triplets antisymmetric ones. However, in the case of many electrons, the rules are not so simple; in fact, the time of numerical computation grows exponentially with the number of electrons.

Formally, we will leave the derivation at this point to defining an operator  $\mathcal{A}$  which 'antisymmetrizes' the wavefunction. In this case,

$$|\Psi_{space}\rangle \simeq \mathcal{A} [ |1s_{H_a}\rangle |1s_{H_b}\rangle |1s_O\rangle |1s_O\rangle |sp_{1O}^3\rangle |sp_{1O}^3\rangle |sp_{2O}^3\rangle |sp_{2O}^3\rangle |sp_{3O}^3\rangle |sp_{4O}^3\rangle ] . \quad (11.35)$$

In general, the results of VB theory are very accurate for small systems, where it can be applied. The predicted bond lengths are rather short, and the binding energies tend to be too small, but the results are nevertheless qualitatively excellent. In addition, the correct hybridized atomic orbitals fall directly off the calculation, giving a good qualitative insight. Also, note that the atomic configurations should not change (or very little) when the geometry of the molecule changes (since the orbitals depend on the atom and not on the molecular structure). Therefore, these VB wavefunctions have a strong connection to the diabatic states discussed above. However, the exponential amount of time that one must invest to perform these calculations makes them impractical for most molecules of interest.

## 11.1.6 Exercises

### 11.1.6.1 Ex: Classical model of the covalent binding

Consider the molecule  $H_2^+$  with the two nuclei separated by 1 nm and an electron located in the middle between the nuclei. Calculate the electrostatic force acting on the nuclei.

**11.1.6.2 Ex: Beyond the Born-Oppenheimer approximation for molecules**

For molecules, the Born-Oppenheimer approximation may fail in some situations. Therefore, it is common to use another approach known as Born-Huang. To illustrate this approach, we consider a diatomic molecule in the laboratory frame.

- Write down the many-body Hamiltonian of the molecule in atomic units.
- If we change the coordinate system to the position of the center-of-mass of the nuclei of the molecule, we eliminate the dependency on the global translation of the molecule. The Hamiltonian is now given by,

$$-\frac{\nabla_R^2}{2\mu_{AB}} - \sum_{i,j} \frac{1}{2M} \nabla_i \nabla_j - \sum_i \frac{\nabla_i^2}{2} + V$$

where that the Coulombian interactions are included in the fifth term. Write down the time-independent Schrödinger equation for this molecule.

- The Born-Huang approximation consists in assuming that the total wavefunction can be expanded on a basis of wavefunctions of the nuclei and the electrons, that is,

$$\Psi(\mathbf{r}, \mathbf{R}) = \sum_k |\chi_k(\mathbf{R})\rangle |\phi_k(\mathbf{r}, \mathbf{R})\rangle ,$$

where  $\chi$  and  $\phi$  are the wavefunctions of the nuclei and the electrons, respectively. For the Schrödinger equation calculated in the previous item, use the Born-Huang approximation and obtain the set of coupled equations

$$\left\{ \sum_k \left[ -\frac{1}{2\mu_{AB}} (\nabla_R^2 + \langle \phi_k | \nabla_R^2 | \phi_k \rangle + 2\langle \phi_k | \nabla_R | \phi_k \rangle \cdot \nabla_R) \right] - \sum_k \left[ \frac{1}{2M} \left( \sum_{i,j} \langle \phi_i | \nabla_i \cdot \nabla_j | \phi_k \rangle \right) + \frac{1}{2} \sum_i \langle \phi_i | \nabla_i^2 | \phi_k \rangle - \langle \phi_i | V | \phi_k \rangle \right] \right\} |\chi_k\rangle = E \sum_k |\chi_k\rangle$$

which includes, although approximately, the kinetic energy of nuclei and electrons.

**Help:** Use  $\nabla^2(\alpha\beta) = \alpha\nabla^2\beta + \beta\nabla^2\alpha + 2\nabla\alpha \cdot \nabla\beta$ .

- Make a brief comparison between the Born-Huang approximation (and the coupled equations obtained in the previous equation) and the Born-Oppenheimer approximation.

**11.1.6.3 Ex: Classical model of the covalent bond**

Calculate the energies of the ground state and the last bound state of the potential  $V_n = -\frac{C}{r^n}$  for any  $n$ .

**11.1.6.4 Ex: Homonuclear collision**

We consider the example of homonuclear collisions of  $^{85}\text{Rb}$  atoms. For ground state collisions in the channel  $^3\Sigma_+$ ,  $|f=2, m_f=-2\rangle$ , the long-range part of the potential is fixed by  $C_6 = 4550$ ,  $C_8 = 550600$ , and  $C_{10} = 7.67 \times 10^7$  [155, 585], where  $R_m = 9.8a_B$ ,  $D_m = 0.13$ , and  $B_m = 1/2.5a_B$ . The potentials can be merged at a given distance  $R_t = 27.6a_B$ . Prepare a plot of potential.

## 11.2 Rovibrational structure of molecular potentials

The separation of the motion of the nuclei from the electronic dynamics made in the Born-Oppenheimer approximation led to equations (11.6) and (11.7). In a preceding section we analyzed in detail the equation (11.6) with the objective of understanding the phenomenon of molecular binding.

In the following section we will analyze the equation (11.7), which determines the motion of the nuclei. By separating the radii and angular parts of the motion, we will discover vibrational and rotational states.

### 11.2.1 The radial and angular equations

The interaction between two identical atoms is described by the following Hamiltonian, where  $M_r = (M_a^{-1} + M_b^{-1})^{-1} = M/2$  is the *reduced mass* of the nuclei,

$$\hat{H} = \frac{\mathbf{P}^2}{2M_r} + V_{mol}(R) \quad \text{with} \quad V_{mol}(R) = \frac{e^2}{4\pi\epsilon_0 R} + V_{BO}(R). \quad (11.36)$$

The interaction potential  $V_{mol}$  is composed of a repulsive internuclear Coulomb force and a Born-Oppenheimer adiabatic potential due to the interaction of the electrons with each other and with the two nuclei<sup>4</sup>. The kinetic energy is that of the relative motion (the center-of-mass motion has already been separated in Sec. 11.1.2, such that this inertial system is free of translational kinetic energy). In spherical coordinates,

$$\frac{\mathbf{P}^2}{2M_r} \phi(\mathbf{R}) = -\frac{\hbar^2}{2M_r} \left[ \frac{1}{R} \frac{\partial^2}{\partial R^2} [R\phi(\mathbf{R})] + \frac{1}{R^2} \frac{\hat{\mathbf{L}}^2}{\hbar^2} \phi(\mathbf{R}) \right]. \quad (11.37)$$

The wavefunction can be separated into an angular part and a radial part,  $\phi(\mathbf{R}) = \mathcal{R}_v(R) Y_{\ell m}(\theta, \phi)$ . The angular part, which was discussed in Sec. 4.1.3, describes a *rigid rotation* of the homonuclear atoms around their center-of-mass with the rotation energy,

$$V_\ell(R) = \frac{\mathbf{L}^2}{2M_r R^2} = \frac{\hbar^2 \ell(\ell+1)}{2M_r R^2}, \quad (11.38)$$

also called *centrifugal barrier*. The radial part is ruled by,

$$\left[ -\frac{\hbar^2}{2M_r} \frac{\partial^2}{\partial R^2} + V_\ell(R) + V_{BO}(R) \right] u_v(R) = E u_v(R), \quad (11.39)$$

where  $u_v(R) = r\mathcal{R}_v(R)$  is the radial wavefunction of nuclear motion. The interatomic potential causes a motion of *vibration*. The vibrational states of the adiabatic potential are quantized and characterized by a well-defined vibrational energy. We will discuss the ro-vibrational structure in the following sections.

<sup>4</sup>We note here that at great distances other forces called *van der Waals forces* dominate the interatomic interaction. These will be discussed in Sec. 11.3.

### 11.2.1.1 Rotational and vibrational bands

Molecules have much more degrees of freedom than atoms. For example, the atoms of a molecular dimer may vibrate inside the mutual interaction potential. In the center-of-mass system we can imagine these vibrations as oscillations of an atom with reduced mass and quantized energy. The molecule can rotate and have a momentum of inertia. These degrees of freedom contribute energies to the molecule's Hamiltonian, either directly or through interactions with other degrees of freedom. Therefore, molecular spectra are characterized by a much greater complexity.

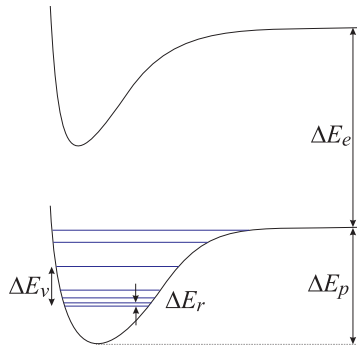


Figure 11.9: Molecular energy scales.

However, the energy regimes of the strongest excitations are quite different. A typical range for binding energies (depth of the interatomic potential) is  $\Delta E_p \simeq 20..200$  THz (0.1..1 eV)<sup>5</sup>. Electronic excitations occur in the regime  $\Delta E_e \simeq 100..1000$  THz (1..10 eV). The spacing between vibrational excitations typically is  $E_{v+1} - E_v \simeq$  THz (0.01 eV). Finally, the rotational excitations are on the scale of  $E_{\ell+1} - E_\ell \simeq 100$  MHz ( $10^{-6}$  eV). Since at room temperature (a gas of molecules in thermal equilibrium at  $T = 300$  K) the energy is on a scale of  $2.5 \times 10^{-2}$  eV, the degree of freedom of the electronic excitation is frozen, while a wide distribution of vibrational and rotational states can be excited (e.g. by intermolecular collisions). The large difference of scales facilitates their separation and, therefore, the identification of the origin of the observed states in experimental measurements.

## 11.2.2 Vibrational molecular states

The potential energy of a molecule grows when the nuclei are displaced from their equilibrium positions. When the displacement,  $x \equiv R - R_e$  is small, we can expand the potential energy,

$$V_{mol}(x) = V_{mol}(0) + \frac{dV_{mol}(0)}{dx}x + \frac{1}{2} \frac{d^2V_{mol}(0)}{dx^2}x^2 + \dots \quad (11.40)$$

<sup>5</sup>Electronically excited states (that is, one of the valence electrons moves to an excited orbital) are more weakly bound, because the electrons are not in the most binding orbital.



The equilibrium energy is not of interest here, and the first derivative disappears in equilibrium. Therefore,

$$V_{mol}(x) \simeq \frac{1}{2}k^2x^2 \quad \text{with} \quad k \equiv \frac{d^2V_{mol}(0)}{dx^2}. \quad (11.41)$$

Using the effective mass we can write the Hamiltonian,

$$\hat{H}_{mol} = -\frac{\hbar^2}{2m_1} \frac{d^2}{dx_1^2} - \frac{\hbar^2}{2m_2} \frac{d^2}{dx_2^2} + \frac{1}{2}kx^2 = -\frac{\hbar^2}{2M_r} \frac{d^2}{dx^2} + \frac{1}{2}kx^2. \quad (11.42)$$

The energy spectrum of this degree of freedom, therefore, is

$$E_v = \hbar\omega\left(v + \frac{1}{2}\right). \quad (11.43)$$

with  $\omega = \sqrt{k/M_r}$ . That is, at the bottom of deep potentials, the energy levels are equidistant.

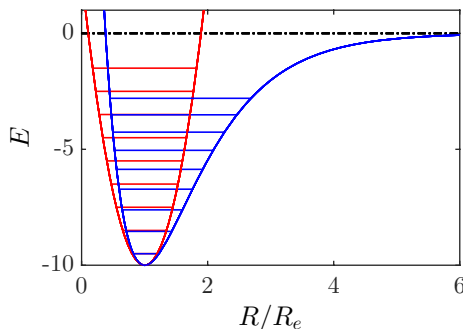


Figure 11.10: (code) Many potentials are approximately harmonic at the center such as, for instance, the Morse potential (blue). The red curve shows the approximate harmonic potential.

### 11.2.2.1 Anharmonic vibrations in the Morse potential

For larger displacements we can no longer despise the anharmonic terms in the Taylor expansion. A better approximation is the *Morse potential*. This potential (blue in Fig. 11.10), unlike the harmonic potential (red in Fig. 11.10), is characterized by an asymptote for large interatomic distances. Therefore, it is often used as an analytical approximation to molecular potentials,

$$V_{morse} = D_e(1 - e^{-a(R-R_e)})^2, \quad (11.44)$$

where  $r$  is the interatomic distance,  $r_e$  the equilibrium bond distance,  $D_e$  the depth of the potential measuring from the *dissociation limit*, and  $a$  a parameter controlling the range of the potential. At the bottom of the potential we can make the harmonic

approximation,  $V_{\text{morse}}(R) \simeq \frac{k}{2}(R - R_e)^2$  with  $k = 2a^2D_e$ . Rewriting the potential in the form,

$$\tilde{V}(R) \equiv V(R) - D_e = D_e(e^{-2a(R-R_e)} - 2e^{-a(R-R_e)}) , \quad (11.45)$$

we see, that it is a combination of a short-range repulsive potential and long-range attractive potential (similar to the Lennard-Jones's potential).

The calculation of the energy spectrum of this potential is more difficult [164],

$$E_v = \hbar\omega(v + 1/2) - \hbar\omega\chi_e(v + 1/2)^2 - D_e, \quad (11.46)$$

with  $\omega\chi_e \equiv \frac{\hbar a^2}{2M_r}$  and  $\omega \equiv \sqrt{k/M_r}$ , but the availability of an analytical expression is interesting for the calibration of numerical methods. The second term of the expression (11.46), which is proportional to the anharmonicity constant  $\chi_e$ , becomes dominant at high excitations. The potential is finite with a dissociation energy of,

$$D_0 = D_e - E_0 . \quad (11.47)$$

The number of vibrational states is limited  $v = 0, 1, \dots, v_{\text{max}}$ . With  $E < 0$ , we find,

$$v_{\text{max}} < \frac{1}{x_e} - \frac{1}{2} . \quad (11.48)$$

**Example 52 (Morse potential):** To solve the Schrödinger equation

$$\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial R^2} + V(R) \right) \Psi(v) = E_v \Psi(v) ,$$

it is convenient to introduce new variables,

$$x \equiv aR \quad , \quad \lambda \equiv \frac{\sqrt{2mD_e}}{a\hbar} \quad , \quad \varepsilon_v \equiv \frac{2m}{a^2\hbar^2} E_v ,$$

such that,

$$\left( -\frac{\partial^2}{\partial x^2} + V(x) \right) \Psi_n(x) = \varepsilon_n \Psi_n(x) \quad \text{with} \quad V(x) = \lambda^2 \left( e^{-2(x-x_e)} - 2e^{-(x-x_e)} \right) .$$

The eigenvalues and eigenfunctions are [164]:

$$\varepsilon_n = 1 - \frac{1}{\lambda^2} \left( \lambda - n - \frac{1}{2} \right)^2 = \frac{2}{\lambda} \left( n + \frac{1}{2} \right)^2 - \frac{1}{\lambda^2} \left( n + \frac{1}{2} \right)^2 \quad \text{and} \quad \Psi_n(z) = N_n z^{\lambda-n-\frac{1}{2}} e^{-\frac{1}{2}z} L_n^{(2\lambda-2n-1)}(z) ,$$

where  $z = 2\lambda e^{-(x-x_e)}$  e  $N_n = \left[ \frac{n!(2\lambda-2n-1)}{\Gamma(2\lambda-n)} \right]^{\frac{1}{2}}$  and,

$$L_n^{(\alpha)}(z) = \frac{z^{-\alpha} e^z}{n!} \frac{d^n}{dz^n} (z^{n+\alpha} e^{-z}) = \frac{\Gamma(\alpha+n+1)/\Gamma(\alpha+1)}{\Gamma(n+1)} {}_1F_1(-n, \alpha+1, z) ,$$

is the generalized Laguerre polynomial. The matrix elements of the spatial operator  $\hat{x}$  are (assuming  $m > n$  and  $N = \lambda - \frac{1}{2}$ ),

$$\langle \Psi_m | x | \Psi_n \rangle = \frac{2(-1)^{m-n+1}}{(m-n)(2N-n-m)} \sqrt{\frac{(N-n)(N-m)\Gamma(2N-m+1)m!}{\Gamma(2N-n+1)n!}} .$$

In the original variables the eigenenergies are:

$$E_v = \hbar\omega(v + 1/2) - \frac{[\hbar\omega(v + 1/2)]^2}{4D_e} ,$$

where  $v$  is the vibrational quantum number and  $\omega = a\sqrt{\frac{2D_e}{m}}$ . The energy difference between adjacent levels decreases with  $v$ ,

$$E_{v+1} - E_v = \hbar\omega - (\hbar\omega)^2 \frac{v+1}{2D_e}.$$

This fact describes well the vibrational structure of non-rotating molecules. However, the equation fails above some value of  $v > v_{max}$ , where  $E_{v_{max}+1} - E_{v_{max}}$  is zero or negative,

$$v_{max} = \frac{2D_e - \hbar\omega}{\hbar\omega}.$$

This failure is due to the finite number  $v_{max}$  of bound states in the Morse potential. For energies above  $v_{max}$  all energies are possible, and the equation for  $E_v$  is no longer valid.

### 11.2.2.2 Vibrational selection rules

Electromagnetic fields of the type  $E1$ , e.g., black body radiation, can induce transitions between vibrational states and redistribute their populations such as to establish a thermal equilibrium. However, as the stronger transitions are induced by dipole migrations of charges, we need to analyze in more detail the selection rules imposed on the dipole moment  $\langle f|\mathbf{d}|i\rangle$ .

The states which are relevant for vibrational transitions are specified by  $|\epsilon, v\rangle$ , where  $\epsilon$  denotes the electronic state of the molecule, since the vibrational spectrum depends on the electronic structure. The *Born-Oppenheimer approximation* allows us to consider the slow vibrations separately from the dynamics of the electrons. The time scale for electronic transitions is  $1/\Delta E_e = 10^{-16}$  s $^{-1}$ , and for a nuclear vibration it is  $1/\Delta E_v = 10^{-13}$  s $^{-1}$ . For each internuclear distance the electrons form an adapted stationary state, minimizing their energy for that distance. This is equivalent to the formation of an adiabatic interaction potential between the nuclei on which the nuclei can vibrate. To find out which vibrational transitions are possible, we need to calculate the matrix,

$$\langle \epsilon', v' | \hat{\mathbf{d}} | \epsilon, v \rangle = \langle v' | \hat{\mathbf{d}}_\epsilon | v \rangle. \quad (11.49)$$

The dipole moment,  $\mathbf{d}_\epsilon = \langle \epsilon | \hat{\mathbf{d}} | \epsilon \rangle$ , of the molecule depends on the distance of the nuclei, since the electronic orbitals  $|\epsilon\rangle$  depend on distance. Therefore, we can expand,

$$\hat{\mathbf{d}} = \hat{\mathbf{d}}_0 + \frac{d\hat{\mathbf{d}}_0}{dx} \hat{x} + \frac{1}{2} \frac{d^2\hat{\mathbf{d}}_0}{dx^2} \hat{x}^2 + \dots \quad (11.50)$$

Therefore, the transition matrix is,

$$\langle \epsilon', v' | \hat{\mathbf{d}} | \epsilon, v \rangle = \hat{\mathbf{d}}_0 \delta_{v,v'} + \frac{d\hat{\mathbf{d}}_0}{dx} \langle v' | \hat{x} | v \rangle + \frac{d^2\hat{\mathbf{d}}_0}{dx^2} \langle v' | \hat{x}^2 | v \rangle + \dots \quad (11.51)$$

The first term disappears, that is, transitions can only occur, when the dipole moment varies with the distance. Therefore, *homonuclear dimers do not undergo vibrational transitions*.

For heteronuclear molecules with electronic charges that do not depend on the interatomic distance, the dipole moment varies linearly with small displacements. In this case, we only need the second term of the expansion. Within the harmonic approximation, the position operator can be expressed by,  $\hat{x} \propto \hat{a} + \hat{a}^\dagger$ . Therefore, only transitions  $\Delta v = \pm 1$  are possible. However, due to anharmonicities, higher order terms,  $\hat{x}^n \propto (\hat{a} + \hat{a}^\dagger)^n$  become influential, and transitions with  $\Delta v = \pm 2, \pm 3, ..$  become possible.

Thus, in anharmonic potentials, the vibrational selection rules are replaced by the concept the overlapping wavefunctions called *Franck-Condon factor*.

Raman spectroscopy is a very useful tool to analyze ro-vibrational spectra. In this method, inelastic Raman scattering gives rise to Stokes and anti-Stokes lines in the spectrum at frequencies corresponding to  $\Delta v = \pm 1, \pm 2$ . The ground state spectrum is asymmetric, because of the absence of the lower state. In homonuclear dimers, the nuclear spins have a major impact on the Raman spectra. Parity considerations show that there can only be odd or even lines.

### 11.2.3 The Franck-Condon principle

The intensity of molecular transitions are, qualitatively, described by the *Franck-Condon principle*, whose *classical* formulation goes as follows:

*The jump of an electron in a molecular transition occurs during a very small time compared to the time scale of the nuclear motion, so that immediately after the jump, the nuclei remain practically at the same positions and at the same velocities as before the jump [330].*

For this reason, the transitions are drawn vertically in the scheme of potentials shown in Fig. 11.11(right). To yield considerable rates, transitions must occur when the nuclear velocities in the two coupled states are similar, which is the case at the classical turning points. At these points, the wavefunctions are maximal<sup>6</sup>.

With this Franck-Condon principle, we can determine which are the strongest transitions between vibrational levels of a molecule, as represented in Fig. 11.11(left). In particular, we are interested in transitions between vibrational levels of different electronic states.

The exact transition probabilities are calculated via the square module of the *transition dipole moment* (TDM). The TDM is an out-of-diagonal matrix element of the electric dipole operator  $\mathbf{M}$ , given by:

$$\mathbf{M}_{AB} = \langle \Psi^{(A)} | \hat{\mathbf{M}} | \Psi^{(B)} \rangle, \quad (11.52)$$

being  $|\Psi^{(A)}\rangle$  and  $|\Psi^{(B)}\rangle$  two molecular states.

Still within the Born-Oppenheimer approximation, we can split the dipole moment operator into two terms, a nuclear and an electronic term, according to:

$$\hat{\mathbf{M}}(\mathbf{r}, \mathbf{R}) = \hat{\mathbf{M}}_e(\mathbf{r}, \mathbf{R}) + \hat{\mathbf{M}}_n(\mathbf{R}). \quad (11.53)$$

<sup>6</sup>Note that the presence of a hyperfine structure can modify the selection rules.

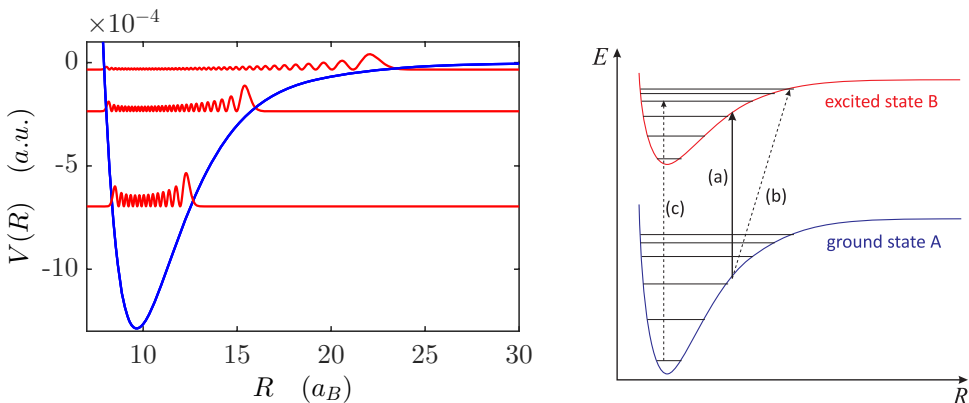


Figure 11.11: (Left, code) Molecular wavefunctions in a potential for three different vibrational states. (Right) Pictorial representation of the classical statement of the Franck-Condon principle. Transition (a) has high intensity (or probability), because here both, the position and the relative velocity of the nuclei do not change. Transitions (b) and (c) are unlikely, because they necessitate either a change in the position of the nuclei (case b) or in velocity (case c).

Thus, the TDM is:

$$\begin{aligned} \mathbf{M}_{AB} &= \int \Psi^{(A)*} \hat{\mathbf{M}} \Psi^{(B)} dR dr & (11.54) \\ &= \int \hat{\mathbf{M}}_e \psi_e^{(A)*} \psi_e^{(B)} \psi_n^{(A)*} \psi_n^{(B)} dR dr + \int \hat{\mathbf{M}}_n \psi_n^{(A)*} \psi_n^{(B)} \int \psi_e^{(A)*} \psi_e^{(B)} dr dR . \end{aligned}$$

Since the electronic wavefunctions of different states are orthogonal, it follows that  $\int \psi_e^{(A)*} \psi_e^{(B)} dr = 0$ , canceling the second term.

Looking at the first term, we note that the electronic dipole moment  $\hat{\mathbf{M}}_e(\mathbf{r}, \mathbf{R})$  also depends on the nuclear coordinates as a parameter. The quantum formulation of the Franck-Condon principle consists in stating that, in a *molecular state*, the *electronic dipole moment varies little with the nuclear coordinates*. Thus, along with the condition of the Born-Oppenheimer approximation, we can split the first TDM term into electronic and nuclear integrals:

$$\mathbf{M}_{AB} = \int \hat{\mathbf{M}}_e \psi_e^{(A)*} \psi_e^{(B)} dr \int \psi_n^{(A)*} \psi_n^{(B)} dR . \quad (11.55)$$

Thus, we have a comparative expression for the transition probability given by:

$$P_{AB} \propto |\mathbf{M}_{AB}|^2 = \left| \int \hat{\mathbf{M}}_e \psi_e^{(A)*} \psi_e^{(B)} dr \right|^2 \left| \int \psi_n^{(A)*} \psi_n^{(B)} dR \right|^2 . \quad (11.56)$$

The second factor in equation (11.56) is called *Franck-Condon factor*. When we study the transitions between two electronic states, this factor compares the intensities of the transitions between distinct pairs of vibrational levels.

**Example 53 (Ultracold molecules):** Ultracold molecules have been proposed for a variety of applications, such as ultra high resolution spectroscopy [470], test of fundamental laws of physics [185, 615], quantum computation [184] and others [123]. Most of these applications, however, require that the molecular sample be in a single quantum state. This is an experimental challenge, since molecules have more degrees of freedom than atoms, such as rotation and vibration.

To create a sample of molecules trapped in the ground state of vibration, a possible method is to first produce the molecules from ultracold atoms using a process called *photo association*, and then pump these molecules to the vibrational ground state.

Photoassociation consists in the excitation of a pair of free atoms to the bound state of an excited electronic potential by the absorption of a photon. The pair then decays by spontaneous emission either back to the state of two free atoms (which is not desirable), or to a bound state of the fundamental electronic potential. For  $\text{Rb}_2$  molecules, photoassociation is efficient at certain frequencies [475], with the  $A^1\Sigma_u^+$  potential as the excited state (see Fig. 11.12).

Soon after being formed, the molecules are usually in levels of high vibrational energy (around  $\nu \approx 80$ ), because these levels connect best (high Franck-Condon overlap) to the excited state. The transfer of population to the fundamental state of vibration is done by 'optical pumping'.

Vibrational cooling via optical pumping can be done by irradiating a broad frequency band of light that excites transitions to vibrational levels of the excited nuclear potential. These excited states are chosen such that their Franck-Condon overlap with the ground states of lower vibrational energy is larger. As a consequence, a molecule sent to an excited state returns with higher probability to a level of lower vibrational energy. The absorption and emission cycles are repeated, until the molecules reach the fundamental vibrational state.

### 11.2.4 Rotational progression

Until now we neglected the centrifugal energy (11.38),

$$V_\ell(R) = \frac{\mathbf{L}^2}{2M_r R^2} = \frac{\hbar^2 \ell(\ell + 1)}{2M_r R^2}. \quad (11.57)$$

As we shall now see, this energy creates a substructure of the vibrational levels.

The moments of inertia in the three axes of space are,

$$I_{qq} = \sum_i m_i r_i^2(q). \quad (11.58)$$

The kinetic energy of the rotation is,

$$E_{rot} = \frac{1}{2} \sum_{q=1,2,3} m_q \mathbf{v}_q^2 = \frac{1}{2} \sum_{q=1,2,3} I_{qq} \omega_q^2 = \frac{L_x^2}{2I_{xx}} + \frac{L_y^2}{2I_{yy}} + \frac{L_z^2}{2I_{zz}}, \quad (11.59)$$

with the angular momentum  $L_q = I_{qq} \omega_q$ .

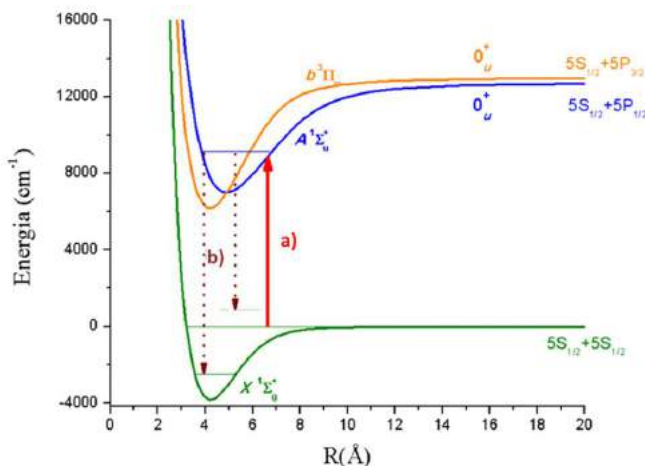


Figure 11.12: Photoassociation scheme to form  $\text{Rb}_2$  molecules. In process (a), a pair of free atoms absorbs a photon of the incident radiation, forming a bound state in the excited potential. Then, in (b), the newly formed molecule decays by spontaneous emission to a bound state of the fundamental potential, or it can return to a state of two free atoms.

Many molecules have a symmetry axis, such that there are two different moments of inertia,  $I_{\perp} \equiv I_{xx} = I_{yy}$  and  $I_{\parallel} \equiv I_{zz}$ . Interpreting angular momenta as quantum operators,

$$\hat{H} = \frac{\hat{\mathbf{L}}^2}{2I_{\perp}} + \left( \frac{1}{2I_{\parallel}} - \frac{1}{2I_{\perp}} \right) \hat{L}_z^2. \quad (11.60)$$

We must first consider the rotation of the molecule relative to the symmetry axis of the molecule. Forgetting external fields we calculate the energy of the molecule associated with the observables  $\hat{\mathbf{L}}^2$  with the quantum number  $\ell$  and  $\hat{\mathbf{L}}_z$  with the quantum number  $K$ . We find the eigenvalues,

$$E(\ell, K, M_{\ell}) = \frac{\hbar^2 \ell(\ell + 1)}{2I_{\perp}} + \left( \frac{1}{2I_{\parallel}} - \frac{1}{2I_{\perp}} \right) \hbar^2 K^2 = B\ell(\ell + 1) + (A - B)K^2, \quad (11.61)$$

with  $\ell = 0, 1, \dots$ ,  $K = -\ell, \dots, \ell$ , and  $M_{\ell} = -\ell, \dots, \ell$  and introducing the *rotational constants*,  $A \equiv \hbar^2/2I_{\parallel}$  and  $B \equiv \hbar^2/2I_{\perp}$ . We then analyze this equation in the context of applying an external field that defines both, the direction  $\hat{\mathbf{e}}'_z$  in the laboratory as well as the projection of the angular motion  $\hat{\mathbf{L}}^2$  on this direction,  $m_{\ell}$ . That is, we have two axes, the internuclear axis  $\hat{\mathbf{e}}_z$  and the rotation axis of the molecule  $\hat{\mathbf{e}}'_z$ .

Each level  $|\ell, m_{\ell}\rangle$  is  $2(2\ell + 1)$  times degenerate, because  $K = -\ell, \dots, \ell$  and  $K$  can be positive or negative. Each level  $\ell$  contains  $2\ell + 1$  states. Note that for spherical molecules,  $A = B$ , and the degree of freedom  $K$  disappears. In Exc. 11.2.6.2 we calculate the rotational spectrum of a homonuclear diatomic molecule.

The rotational constant can be approximated by,

$$E_{rot} = \frac{\hbar^2 \ell(\ell + 1)}{2M_r \langle R^2 \rangle}, \quad (11.62)$$

where  $\sqrt{\langle R^2 \rangle}$  is the expectation value for the outer turning point of the vibrational level. As an example, the rotational constant for the vibrational state of  $^{87}\text{Rb}_2$  which is  $5.9 \text{ cm}^{-1}$  below the dissociation limit is  $B_v = \nu_{rot}^{\ell=1} - \nu_{rot}^{\ell=0} = 81 \text{ MHz}$ . To be more precise, we would need to calculate  $\langle R^2 \rangle_v = \langle \psi_v | R^2 | \psi_v \rangle$ .

Transitions between vibrational levels occur together with rotational transitions  $\Delta\ell = \pm 1$ . Therefore, the frequencies of transitions depend on the rotational constant  $B_v$ , which depends on the vibrational state. The energies of the molecule are,

$$E_{v,\ell} = \hbar\omega(v+1/2) - \hbar\omega x_e(v+1/2)^2 + \dots + hcB_v\ell(\ell+1) - hcD_v\ell^2(\ell+1)^2 + \dots \quad (11.63)$$

Under the influence of a rapid rotation, the atoms of the molecule are subjected to centrifugal force and, hence, are further away from each other <sup>7</sup>.

Since at ambient temperatures many rotational levels are populated, we experimentally observe many lines known as *P*-branch, when  $\Delta\ell = -1$ , as *Q*-branch, when  $\Delta\ell = 0$ , and as *R*-branch, when  $\Delta\ell = 1$ . See Exc. 11.2.6.3.

### 11.2.4.1 Rotational selection rules

For transitions between electronic states, the selection rules are  $\Delta r = 0, \pm 1$ . Rotational transitions can occur between levels  $\Delta r = \pm 1$ .  $\Delta r = 0$  is not allowed, because it violates the conservation of parity. Note also that the nuclear isotope influences the ro-vibrational levels via the reduced mass.

We consider a linear molecule in the state  $|\epsilon, \ell, M_\ell\rangle$ , where  $\epsilon$  denotes the electronic and vibrational state of the molecule. To find out which transitions are possible, we need to calculate the matrix,

$$\langle \epsilon', \ell', M'_\ell | \mathbf{d} | \epsilon, \ell, M_\ell \rangle = \langle \ell', M'_\ell | \mathbf{d}_\epsilon | \ell, M_\ell \rangle, \quad (11.64)$$

with  $\mathbf{d}_\epsilon = \langle \epsilon | \mathbf{d} | \epsilon \rangle$ . Here, we apply the *Born-Oppenheimer approximation*, which allows us to separate the dynamics of the electrons and also the vibrations of the molecule, because these movements are so fast, that they are always in a steady state, adiabatically following the slow movement of the rotation.

The selection rules can now be derived from the *Wigner-Eckart theorem*,

$$\frac{\langle \ell', M'_\ell | \mathbf{d}_\epsilon | \ell, M_\ell \rangle^2}{|\langle \ell' || \mathbf{d}_\epsilon || \ell, M_\ell \rangle|^2} = \frac{1}{2\ell' + 1} \begin{pmatrix} \ell & 1 & \ell' \\ m_\ell & \kappa & -m'_\ell \end{pmatrix}. \quad (11.65)$$

We find  $\Delta\ell = 1$  e  $\Delta M_\ell = 0, \pm 1$ . See Exc. 11.2.6.4.

## 11.2.5 Computation of vibrational states

### 11.2.5.1 Localization energy

One consequence of Heisenberg's uncertainty relation is that a certain *localization energy* is always required to localize a particle. As an example, we consider the attractive potential,

$$V = -\frac{C}{R^z\alpha}. \quad (11.66)$$

---

<sup>7</sup>See [28], p.326



The space available for the particle is limited between the classical turning point, which for a given energy is  $r_t = \left(\frac{C}{|E|}\right)^{1/\alpha}$ . The momentum corresponding to this energy is  $k_t = \left(\frac{2m|E|}{\hbar^2}\right)^{1/2}$ . Heisenberg's uncertainty relation requires  $k_t r_t > 2$ , that is, at least half of the wavelength must fit within the potential (between 0 and  $r_t$ ) at the height of the bound state. Therefore,

$$|E|^{1-2/\alpha} > \frac{2\hbar^2}{mC^{2/\alpha}}. \quad (11.67)$$

For a Coulomb potential, with  $\alpha = 1$  and  $C = e^2/4\pi\epsilon_0$ , we obtain the energy of the ground state of the hydrogen atom,

$$E > E_1 = -\frac{e^2}{4\pi\epsilon_0 2a_B}, \quad (11.68)$$

but there is no state higher than all others. That is, all energies  $E_n = E_1/n^2$  exist.

For  $\alpha = 2$ , we do not get a condition for the energy. For the Casimir-Polder potential,  $\alpha = 3$ , we obtain,

$$E < -\frac{8\hbar^6}{m^3 C^2}. \quad (11.69)$$

This means that, in contrast to the Coulomb potential, the *binding energy* must be *lower* than a certain limit.

### 11.2.5.2 The LeRoy-Bernstein method

The *LeRoy-Bernstein method* allows us to estimate the highest bound levels. It only applies near the dissociation limit, where the semi-classical formula of quantization is valid,

$$v + \frac{1}{2} = \sqrt{\frac{8M_r}{\hbar^2}} \int_0^{R_1} dR \sqrt{E(v) - V(R)}. \quad (11.70)$$

Inserting the potential

$$V(R) = D_e - \frac{C}{R^n}, \quad (11.71)$$

we get

$$E(v^*) = D_e - \left( \frac{(n-2)\Gamma\left(1 + \frac{1}{n}\right)}{2\Gamma\left(\frac{1}{2} + \frac{1}{n}\right)} (v^* + v_D) \right)^{\frac{2n}{n-2}} \left( \frac{\hbar^{2n}}{(2\pi M_r)^n C^2} \right)^{\frac{1}{n-2}}, \quad (11.72)$$

where  $v^*$  is a number counting the vibrational levels from the top to the bottom starting at the dissociation limit.

### 11.2.5.3 Open channels

For a given interatomic potential  $V(R)$ , neglecting the spin structure [377], the relative wavefunction of a two-atom system satisfies the Schrödinger equation,

$$\left[ -\frac{1}{2\mu} \Delta + V(R) \right] \psi(\mathbf{R}) = E\psi(\mathbf{R}). \quad (11.73)$$

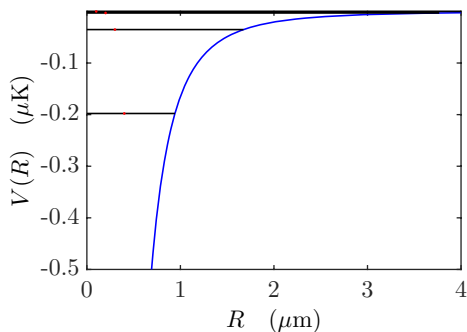


Figure 11.13: (code) Highest vibrational states obtained by the LeRoy-Bernstein method.

Separating the radial and angular contributions,  $\psi(\mathbf{R}) \equiv Y(\vartheta, \varphi)f(R)/R$ , we obtain,

$$\left[ -\frac{1}{2\mu} \frac{\partial^2}{\partial R^2} + V(R) + \frac{l(l+1)}{2\mu R^2} \right] f(R) = E f(R) . \quad (11.74)$$

Now, we introduce the local wavevector,  $k(R) = \sqrt{2\mu[E - V(R)] - l(l+1)/R^2}$  and write,

$$f'' = -k^2 f . \quad (11.75)$$

This differential equation can be solved numerically [see Fig. 11.14(a)].

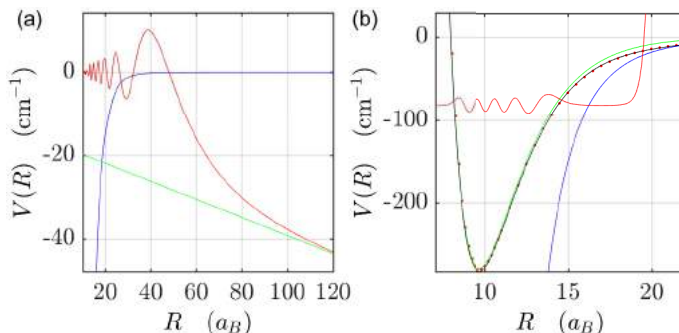


Figure 11.14: (code) (a) Numerical computation of the relative wavefunction for a low energy collision,  $E \gtrsim 0$  and  $\ell = 0$ . The blue curve shows the interatomic Li-Rb potential  $(a)^3\Sigma$ , the red curve illustrates the relative Broglie wavefunction of the molecule. The asymptote of this extrapolated wavefunction (green curve) cuts the abscissa at  $a_s = -120a_B$ , which is just the scattering length for collisions in this channel. (b) Numerical computation of the wavefunction for a vibrational state. The potential is an interpolation (black) between a short-range Morse potential (green), and a long range potential (blue). The red curve illustrates the relative wavefunction for the ninth vibrational state (counting from ground state).

### 11.2.5.4 Bound states

For bound states, we must simultaneously satisfy the eigenvalue problem. We can, for example, guess an eigenvalue  $E$ , calculate the associated wavefunction  $f(R)$ , check whether it diverges for  $R \rightarrow \infty$ , and vary  $E$  until  $f(R)$  no longer diverges. Fig. 11.14(b) shows the wavefunction of a vibrational state obtained by solving the Schrödinger equation and adjusting the energy until the function stops diverging in the classically forbidden range.

### 11.2.5.5 The Fourier grid method

Another, extremely rapid, numerical method for determining the spectrum of vibrational states of a potential, is the *Fourier grid method*. It is based on the discretization of the Hamiltonian along the interatomic potential. We write the Hamiltonian as,

$$H\psi(R) = [T(R) + V(R)]\psi(R) = E\psi(R) , \quad (11.76)$$

and put it in a matrix form using the set of functions of the basis  $\phi_i(R_j) = \delta(R_i - R_j)$  with  $i = 1, \dots, N$ , where  $R_i = R_0 + i(R_N - R_0)/N$ . This problem has  $N$  eigenvalues  $E_i$ . The Fourier grid method now evaluates the kinetic energy at each point in the grid. We insert the local terms  $H_{ii} = H(R_i)$  and the non-local terms  $H_{ij} = H(R_i, R_j)$  into the Hamiltonian, as well as the potential energies  $V_{ij} = V(R_i)\delta_{ij}$ . The kinetic energy is the inverse Fourier transform from momentum space of  $T_{rs} = T(k_r)\delta_{rs} = (k_r^2/2\mu)\delta_{rs}$  and becomes [479, 456, 215],

$$H_{ij} = \frac{\pi^2}{4\mu(R_N - R_1)^2} (-1)^{i-j} \left( \frac{1}{\sin^2 \frac{\pi(i-j)}{2N}} - \frac{1}{\sin^2 \frac{\pi(i+j)}{2N}} \right) \quad \text{for } i \neq j \quad (11.77)$$

$$H_{ij} = \frac{\pi^2}{4\mu(R_N - R_1)^2} \left( \frac{2N^2 + 1}{3} - \frac{1}{\sin^2 \frac{\pi i}{2N}} \right) + V(R_i) \quad \text{for } i = j .$$

To improve the wavefunction, we can interpolate,

$$\psi(q) = \sum_{j=1}^n \psi(q_j) \operatorname{sinc} \frac{\pi(q - q_j)}{\Delta q} . \quad (11.78)$$

The method can be extended to coupled channels  $\sigma = A, B$  via,

$$H_{\{i\sigma\}\{j\tau\}} = T_{ij}\delta_{\sigma\tau} + V_{\sigma\tau}(R_i)\delta_{ij} . \quad (11.79)$$

The Hamiltonian has the general form,

$$H = \begin{pmatrix} T & 0 \\ 0 & T \end{pmatrix} + \begin{pmatrix} V_A & 0 \\ 0 & V_B \end{pmatrix} + \begin{pmatrix} W_{AA} & W_{AB} \\ W_{AB} & W_{BB} \end{pmatrix} , \quad (11.80)$$

where all matrices  $V_k$  and  $W_k$  are diagonal <sup>8</sup>.

<sup>8</sup>Note that the Fourier grid method can be improved by using a grid with spacings adjusted to the potential gradient [404, 684, 436].

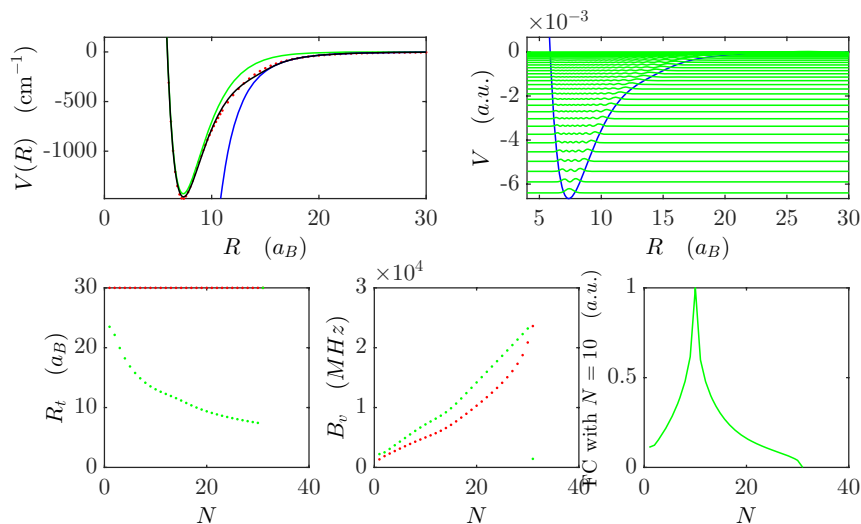


Figure 11.15: (code) Numerical computation of the wavefunction using the Fourier grid method at example of the interatomic potential Li-Rb  $(1)^1\Pi$ . (a) Short range Morse potential (green), long range (blue), interpolation (black) and [406]. (b) Vibrational wavefunctions, (c) external turning point (red) and center of mass (green), (d) rotational progression, and (e) Franck-Condon overlap with the tenth vibrational state.

## 11.2.6 Exercises

### 11.2.6.1 Ex: Transitions between vibrational states

Calculate the dipole moment between two arbitrary vibrational states of (a) a harmonic potential and (b) a Morse potential.

### 11.2.6.2 Ex: Rotational spectrum of diatomic molecules

Calculate the rotational spectrum for a diatomic molecule from the result (11.59).

### 11.2.6.3 Ex: Ro-vibrational spectrum

Determine the frequency spectra of ro-vibrational transitions for the branches  $P$ ,  $Q$ , and  $R$ .

### 11.2.6.4 Ex: Rotational spectrum

Determine the rules and the spectrum of rotational transitions for a spherical molecule.

## 11.3 Van der Waals forces and spin coupling

The individual atoms have a complex substructure due to the angular momenta of the electronic motion, its spins and the nuclear spin. All of these angular momenta can

interact, couple and generate new energy terms, which need to be taken into account when calculating the various potentials of interatomic interaction,

$$\hat{H} = \frac{\mathbf{P}^2}{2M_r} + V_{coulomb}(R) + \sum_{k=1,2} \left( V_{hfs}^{(k)} + V_{zeeman}^{(k)} \right) + V_{dipole,spin-spin}(R) + V_{dipole,spin-orbit}(R). \quad (11.81)$$

The Coulomb interaction for interacting alkaline gases can be expressed as:

$$V_{coulomb}(R) = V_{coulomb}^{S=0} \mathcal{P}_{S=0} + V_{coulomb}^{S=1} \mathcal{P}_{S=1}. \quad (11.82)$$

The projectors  $\mathcal{P}_{S=0,1}$  will be required to expand the Hilbert space for the degrees of freedom of the spins.

The *van der Waals forces* include all intermolecular forces. These are long-range forces that occur between permanent and induced atomic dipoles  $\sim 1/r^6$ <sup>9</sup>

### 11.3.1 Analytical models for short and long-range potentials

In general, the potentials are estimated by ab initio Hartree-Fock calculations. A short-range potential, or *Morse potential*, can be approximated by,

$$V_{morse} = D_m \left( \left[ 1 - e^{-B_m(R-R_m)} \right]^2 - 1 \right). \quad (11.83)$$

Here,  $B_m$  is the width of the minimum,  $R_m$  the position of the minimum,  $D_m$  the length. A long-range potential can be written,

$$V_{vdw}(R) = D_e - \frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}}. \quad (11.84)$$

$D_e$  is the energy of dissociation. The *van der Waals coefficients*  $C_k$ , which determine the potential shape at large distances, can be calculated using other methods with higher precision. To obtain a closed formula, the short and long range parts can be joined by,

$$V = V_{morse}F + V_{vdw}(1 - F), \quad (11.85)$$

where  $F \equiv e^{-(R/R_t)^{10}}$ .

The situation is different for collisions of identical atoms in excited states, which has a much larger range because of the resonant interaction between dipoles. In this case, an additional *Movre-Pichler potential* dominated by a coefficient  $C_3$  arises,

$$V_{vdw}^e = V_{movre}^e + V_{dispersion}^e. \quad (11.86)$$

In contrast, excited state collisions of different species are purely short ranged.

<sup>9</sup>They also occur, in a pure form, in optical resonators such as in the *Casimir effect*. Since the lowest frequency in a cavity is  $\omega = \sqrt{2\pi c/L}$ , the zero point energies inside and outside the cavity are different. This causes an attractive force between the cavity mirrors  $\sim 1/r^3, 1/r^4$ .

### 11.3.2 Spin coupling in dimers, molecular quantum numbers

We consider two interacting alkaline atoms, each being described by a set of quantum numbers of internal angular momenta, they couple their spins:

$$\begin{aligned}
 \mathbf{l}_i & \text{ angular momentum of the individual atom} & (11.87) \\
 \mathbf{s}_i & \text{ electronic spin} \\
 \mathbf{i}_i & \text{ nuclear spin} \\
 \mathbf{l}_i + \mathbf{s}_i = \mathbf{j}_i & \text{ total electronic angular momentum} \\
 \mathbf{j}_i + \mathbf{i}_i = \mathbf{f}_i & \text{ total angular momentum .}
 \end{aligned}$$

When the atoms approach each other, at intermediate distances, they couple their spins:

$$\begin{aligned}
 \ell \perp \hat{\mathbf{e}}_z & \text{ molecular rotation} & (11.88) \\
 \Lambda \equiv |M_L| \hat{\mathbf{e}}_z & \text{ projection of } \mathbf{L} \text{ onto the interatomic } \hat{\mathbf{e}}_z \\
 \Sigma \equiv M_S \hat{\mathbf{e}}_z & \text{ projection of } \mathbf{S} \text{ onto the interatomic } \hat{\mathbf{e}}_z \\
 \Omega \equiv \Lambda + \Sigma & \text{ projection of } \mathbf{L} + \mathbf{S} \text{ onto the interatomic } \hat{\mathbf{e}}_z .
 \end{aligned}$$

At short distances, they form a molecular dimer described by the quantum numbers:

$$\begin{aligned}
 \mathbf{L} = \mathbf{l}_1 + \mathbf{l}_2 & \text{ total electronic angular momentum} & (11.89) \\
 \mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2 & \text{ electronic spin} \\
 \mathbf{I} = \mathbf{i}_1 + \mathbf{i}_2 & \text{ nuclear spin} \\
 \mathbf{f} = \mathbf{f}_1 + \mathbf{f}_2 & \text{ total angular momentum or } (\mathbf{L}, \mathbf{S})\mathbf{k} + \mathbf{I} \\
 \mathbf{J} = \Omega + \ell & \\
 \mathbf{F} = \mathbf{f} + \ell & .
 \end{aligned}$$

The quantum numbers couple like,

$$\begin{array}{rccccccc}
 \mathbf{l}_1 & + & \mathbf{l}_2 & = & \mathbf{L} & \xrightarrow{\hat{\mathbf{e}}_z} & \Lambda \\
 + & & + & & + & & + \\
 \mathbf{s}_1 & + & \mathbf{s}_2 & = & \mathbf{S} & \xrightarrow{\hat{\mathbf{e}}_z} & \Sigma \\
 = & & = & & = & & = \\
 \mathbf{j}_1 & + & \mathbf{j}_2 & = & \mathbf{j} & \xrightarrow{\hat{\mathbf{e}}_z} & \Omega + \ell = \mathbf{J} \\
 + & & + & & + & & + \\
 \mathbf{i}_1 & + & \mathbf{i}_2 & = & \mathbf{I} & & \mathbf{I} \\
 = & & = & & = & & = \\
 \mathbf{f}_1 & + & \mathbf{f}_2 & = & \mathbf{f} & + \ell = & \mathbf{F}
 \end{array} \quad (11.90)$$

Obviously, the atomic angular momentum is no longer a conserved quantity, but its projection onto the interatomic molecular axis is. The various possibilities how  $\mathbf{L}$ ,  $\mathbf{S}$ , and  $\mathbf{j}$  are projected onto the internuclear axis or directly couple to the rotational angular momentum  $\ell$  are handled by Hund's cases (a) to (e). The spin coupling is described by  $\{9j\}$ -symbols, as discussed below.

### 11.3.3 Hund's coupling cases

The coupling force between atomic spins depends on the distance between the atoms. Due to the variety of spins appearing in atoms, there are many possibilities how they can couple. These were classified by Hund into five cases.

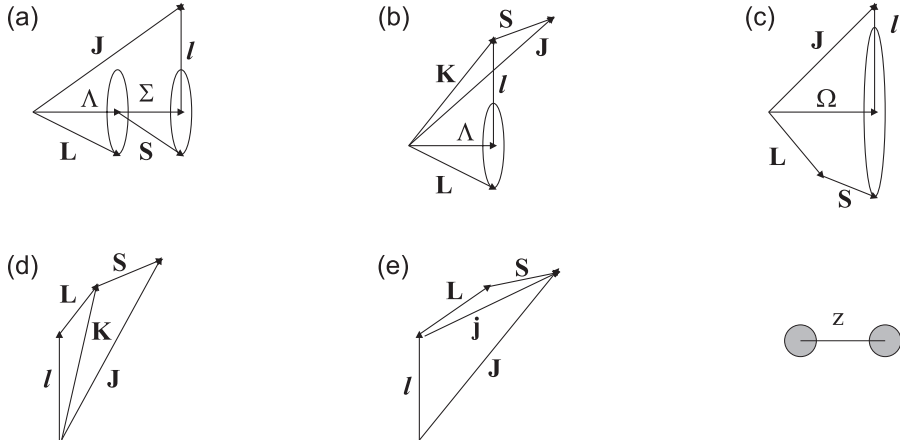


Figure 11.16: Hund's coupling cases.

#### 11.3.3.1 Hund's case (a)

The molecular interaction is so strong that  $\mathbf{L}$  and  $\mathbf{S}$  couple to the  $z$ -axis instead of coupling to each other. This case is analogous to the Paschen-Back effect,

$$\mathbf{L} \rightarrow \mathbf{\Lambda} \quad \text{and} \quad \mathbf{S} \rightarrow \mathbf{\Sigma} \quad (11.91)$$

$$((\mathbf{\Lambda}, \mathbf{\Sigma})\mathbf{\Omega}, \ell)\mathbf{J} .$$

A common notation is to label the states  $\mathbf{\Lambda} = \mathbf{\Sigma}, \mathbf{\Pi}, \mathbf{\Delta}, \dots$ . That is, in the symbol  $X^{(2S+1)\Lambda_{\Omega}}_{\sigma}$ , where  $\sigma = g, u$  is the inversion symmetry,  $X, A, B, \dots$  and  $a, b, \dots$  are the singlet and triplet series starting from the lowest energy levels. An alternative notation is to assign labels ordered by energy  $X = (1), (2), \dots$ . Finally,  $\pm$  is the symmetry upon reflection. For example,  $X^1\Sigma_g^+$ .

#### 11.3.3.2 Hund's case (b)

$\mathbf{L}$  is projected onto the  $z$ -axis before coupling to  $\ell$ . The resulting angular momentum afterward directly couples to  $\mathbf{S}$ .

$$\mathbf{L} \rightarrow \mathbf{\Lambda} \quad (11.92)$$

$$((\mathbf{L}, \ell)\mathbf{k}, \mathbf{S})\mathbf{J} .$$

### 11.3.3.3 Hund's case (c)

$\mathbf{L}$  and  $\mathbf{S}$  couple together instead of projecting themselves onto the  $z$ -axis. This case is analogous to the Zeeman effect,

$$\begin{aligned} (\mathbf{L}, \mathbf{S})\mathbf{j} &\rightarrow \boldsymbol{\Omega} \\ &(\boldsymbol{\Omega}, \ell)\mathbf{J} . \end{aligned} \quad (11.93)$$

A common notation is to label the states by  $\boldsymbol{\Omega} = 0, 1, 2, \dots$ . That is, in the symbol  $X(\boldsymbol{\Omega})_s^\pm$ , the letter  $X = 1, 2, \dots$  is a label ordered by energy. For example  $2(0_g^-)$ .

### 11.3.3.4 Hund's case (d)

$\mathbf{L}$  is not projected on the  $z$ -axis, but directly couples to the rotational angular momentum. The resulting angular momentum afterward only couples to the  $\mathbf{S}$

$$((\mathbf{L}, \ell)\mathbf{k}, )\mathbf{J} . \quad (11.94)$$

### 11.3.3.5 Hund's case (e)

$\mathbf{L}$  and  $\mathbf{S}$  mutually couple as in the case (c), but are not projected on the  $z$ -axis, but couple directly with  $\ell$ , which is quantized,

$$((\mathbf{L}, \mathbf{S})\mathbf{j}, \ell)\mathbf{J} . \quad (11.95)$$

## 11.3.4 Molecular hyperfine structure

The scattering length in specific channels can be expressed via singlet and triplet scattering lengths,

$$a_{|f_1, m_{f_1}\rangle + |f_2, m_{f_2}\rangle} = P_{S=0}a_s + P_{S=1}a_t . \quad (11.96)$$

The projectors are  $P_S = |\langle S | (f_1 f_2) f \rangle|$ . According to [111]<sub>DOI</sub> or [481]<sub>DOI</sub> the recoupling from the uncoupled hyperfine representation into the short range representation is given by,

$$\begin{aligned} \langle S m_S \ I m_I \ \ell' m_{\ell'} | f_1 m_{f_1} \ f_2 m_{f_2} \ \ell m_{\ell} \rangle &= \delta_{\ell \ell'} \delta_{m_{\ell} m_{\ell'}} \sum_{f, m_f} \langle S m_S \ I m_I | f m_f \rangle \langle f_1 m_{f_1} \ f_2 m_{f_2} | f m_f \rangle \times \\ &\times \begin{Bmatrix} s_1 & s_2 & S \\ i_1 & i_2 & I \\ f_1 & f_2 & f \end{Bmatrix} \sqrt{\hat{S} \hat{I} \hat{f}_1 \hat{f}_2} \left( \frac{1 - (1 - \delta_{f_1 f_2})(-1)^{S+I+\ell}}{\sqrt{2 - \delta_{f_1 f_2}}} \right) . \end{aligned} \quad (11.97)$$

The last bracket is dropped for unsymmetrized recoupling. We will study examples of spin recoupling in the ground state channels in Exc. 11.3.5.1, 11.3.5.2, and 11.3.5.3.

## 11.3.5 Exercises

### 11.3.5.1 Ex: Spin recoupling of identical $^{87}\text{Rb}$ ground state channels

- Unravel the molecular hyperfine structure of identical  $^{87}\text{Rb}$  ground state channels.
- Project the collisional channels  $|f_1 m_{f_1} \ f_2 m_{f_2}\rangle = |1 - 1 \ 1 - 1\rangle$  and  $|22 \ 22\rangle$  on the singlet and triplet potentials,  $S = 0, 1$ .



**11.3.5.2 Ex: Spin recoupling of  ${}^6\text{Li}{}^{87}\text{Rb}$  ground state channels**

- a. Unravel the molecular hyperfine structure of  ${}^6\text{Li}{}^{87}\text{Rb}$  ground state channels.
- b. Project the collisional channels on short range potentials.

**11.3.5.3 Ex: Hyperfine structure of  ${}^6\text{Li}{}^{23}\text{Na}$  and  ${}^6\text{Li}{}^{87}\text{Rb}$** 

- a. Unravel the molecular hyperfine structure of  ${}^6\text{Li}{}^{23}\text{Na}$  and  ${}^6\text{Li}{}^{87}\text{Rb}$  bound state.
- b. How about the open channels?

**11.4 Further reading**

et al., [\[DOI\]](#)

# Chapter 12

## Collisions

Until now, we mostly restricted our studies to individual atoms or molecules. In practice, however, we investigate atomic or molecular gases by spectroscopic methods. The constituents of thermal gases are constantly in motion. They are subject to Doppler-shifts of their spectral lines and they collide with each other. Colliding atoms often get so close, that the electronic orbitals affect each other, which leads to distortions of the interaction potentials, spectral lineshifts and modifications of the interatomic forces. These are the topics to be addressed in the present chapter.

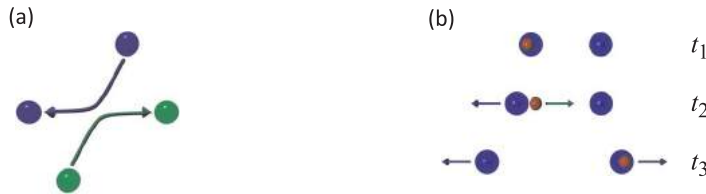


Figure 12.1: Atoms may interact via exchange of (a) virtual photons or (b) real photons.

### 12.1 Motion of interacting neutral atoms

The following sections, devoted to the relative motion of two neutral atoms, are adapted from J. Walraven's excellent lectures on *Quantum Gases* available at [708]. The atoms are presumed to move slowly, typically at large separation, and to interact pair wise through a potential of the Van der Waals type. The term slowly refers to,

$$k_{therm}r_0 \ll 1 \quad \text{where} \quad \lambda_{therm} = \frac{2\pi}{k_{therm}} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}} \quad (12.1)$$

is the *thermal de Broglie wavelength* and  $r_0$  the range of the interaction potential. As the Van der Waals interaction gives rise to elastic collisions, the total energy of the relative motion is conserved in time. As the potential energy vanishes at large interatomic separation the total energy is usually expressed in the form  $E = \hbar^2 k^2 / 2m_r$ . This implies that also the wavenumbers for the relative motion before and after the collision must be the same and shows that, far from the potential center, the collision can only affect the phase of the wavefunction - not its wavelength. Apparently, the appearance of a shift in phase relative to the free atomic motion

provides the key to the quantum mechanical description of elastic collisions. This being said, we postpone the discussion of the actual collisional behavior to Sec. 12.2. First we prepare ourselves for this discussion by analyzing the stationary states for the motion in the presence of an interaction potential.

An important simplifying factor in the description of ultracold collisions is the emergence of universal behavior in the relative motion of the atoms. The latter applies to low-energy collisional states as well as to weakly bound states. Universal means in this context that, asymptotically (for  $r \gg r_0$ ), the wavefunctions become independent of the details of the interaction potential but can be characterized in terms of a few parameters, each representing some characteristic length scale of the collisional system. In other words, very different short-range physics can give rise to the same scattering behavior. From a theory point of view this universality has the enormous advantage that the essential features of ultracold collisions can be described with the aid of simple model potentials for which analytical solutions can be obtained.

In our analysis of the collisional motion three characteristic length scales will appear, the interaction range  $r_0$  the scattering length  $a$  and the effective range  $r_e$ , each expressing a different aspect of the interaction. The range  $r_0$  is the distance beyond which the interaction may be neglected even for  $k \rightarrow 0$ . The second characteristic length, the  $s$ -wave scattering length  $a$ , acts as an effective hard-sphere diameter. It is a measure for the interaction strength and determines the collision cross section in the limit  $k \rightarrow 0$  as will be elaborated on in Sec. 12.2. The third characteristic length, the effective range  $r_e$  expresses how the potential affects the energy dependence of the cross section and determines when the  $k \rightarrow 0$  limit is reached.

The  $s$ -wave scattering length is the central parameter for the theoretical description of bosonic quantum gases. It determines both the thermodynamic and the collisional properties of these gases. In single-component fermionic gases the  $s$ -wave scattering length plays no role because the wavefunction for the relative motion of the atoms has to be antisymmetric. In two-component fermionic gases this restriction is absent for collisions between atoms of different components. As a consequence, in these systems the inter-component  $s$ -wave scattering length determines the collision related properties - for instance the thermalization rate.

In Sec. 12.1.1 we show how the phase shift appears as a result of interatomic interaction in the wavefunction for the relative motion of two atoms. For free particles the phase shift is zero. An integral expression for the phase shift is derived. In Sec. 12.1.2 and beyond we specialize to the case of low-energy collisions ( $kr_0 \ll 1$ ). The basic phenomenology is introduced and analyzed for simple model potentials like the hard-sphere (Sec. 12.1.2) and the spherical well (Sec. 12.1.3), where the existence of a short range is manifest. For the discussion of arbitrarily shaped potentials, we refer to the script [708].

### 12.1.1 The collisional phase shift

12.1.1.1 Schrödinger equation

The starting point for the description of the relative motion of two atoms at energy  $E$  is the Schrödinger equation (4.33),

$$\left[ \frac{1}{2m_r} \left( p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + V(r) \right] \psi(r, \vartheta, \varphi) = E\psi(r, \vartheta, \varphi) . \quad (12.2)$$

Here  $m_r$  is the reduced mass of the atom pair and  $V(r)$  the interaction potential. As discussed in Sec. 4.1.3 the eigenfunctions  $\psi(r, \vartheta, \varphi)$  can be separated in a radial and a angular part,  $\psi = R_\ell(r)Y_{\ell m}(\vartheta, \varphi)$ , where the functions  $Y_{\ell m}$  are spherical harmonics and the functions  $R_\ell(r)$  satisfy the radial wave equation,

$$\left[ \frac{\hbar^2}{2m_r} \left( -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{\ell(\ell+1)}{r^2} \right) + V(r) \right] R_\ell(r) = ER_\ell(r) . \quad (12.3)$$

By the separation procedure the angular momentum term is replaced by a repulsive effective potential,

$$V_{rot}(r) = \frac{\hbar^2 \ell(\ell+1)}{2m_r r^2} , \quad (12.4)$$

representing the rotational energy of the atom pair at a given distance and for a given rotational quantum number  $\ell$ . In combination with an attractive interaction it gives rise to a centrifugal barrier for the radial motion of the atoms. This is illustrated in Fig. 12.2 for the example of hydrogen.

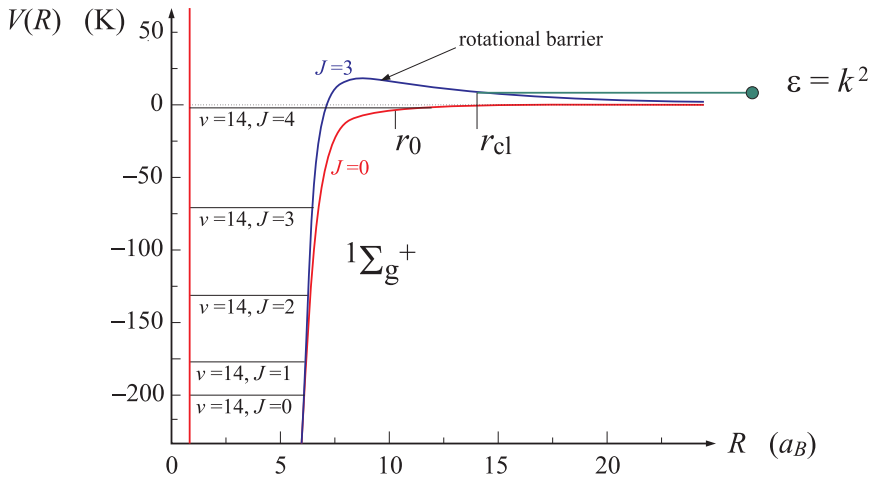


Figure 12.2: Example showing the high-lying bound states near the continuum of the singlet potential  $1\Sigma_g^+$  (the bonding potential) of the hydrogen molecule;  $v$  and  $J$  are the vibrational and rotational quantum numbers, respectively. The dashed line shows the effect of the  $J = 3$  centrifugal barrier. The presence of a rotational barrier gives rise to an exponential suppression of the radial wavefunction for  $r < r_{tp}$  and is negligible at distances where the interaction becomes noticeable  $r \ll r_0$ .

To analyze the radial wave equation we introduce reduced energies,

$$\varepsilon = \frac{2m_r E}{\hbar^2} = \begin{cases} k^2 & \text{for } k > 0 \\ -\kappa^2 & \text{for } k < 0 \end{cases} \quad \text{and} \quad \tilde{V}(r) = \frac{2m_r V(r)}{\hbar^2}, \quad (12.5)$$

choosing  $k$  and  $\kappa$  as real positive number. This puts Eq. (12.3) in the form,

$$\boxed{R_\ell'' + \frac{2}{r}R_\ell' + \left[ \varepsilon - \tilde{V}(r) - \frac{\ell(\ell+1)}{r^2} \right] R_\ell = 0}. \quad (12.6)$$

With the substitution  $u_\ell(r) = rR_\ell(r)$  it reduces to a 1D Schrödinger equation,

$$\boxed{u_\ell'' + \left[ \varepsilon - \tilde{V}(r) - \frac{\ell(\ell+1)}{r^2} \right] u_\ell = 0}. \quad (12.7)$$

### 12.1.1.2 Low-energy limit: the $s$ -wave regime

For two atoms with relative angular momentum  $\ell > 0$  there exists a distance  $r_{tp}$ , called the classical turning point, below which the rotational energy exceeds the total energy  $E$ ,

$$k^2 = \frac{\ell(\ell+1)}{r_{tp}^2}. \quad (12.8)$$

This is illustrated in Fig. 12.2. In the classically inaccessible region of space ( $r < r_{tp}$ ) the radial wavefunction is exponentially suppressed<sup>1</sup>. Combining Eq. (12.8) with the condition (12.1) we obtain the inequality,

$$kr_0 = \sqrt{\ell(\ell+1)} \frac{r_0}{r_{tp}} \ll 1, \quad (12.9)$$

which implies that, for  $\ell \neq 0$ , the classical turning point is found at a distance much larger than the range  $r_0$  of the interaction. As the range  $r_0$  defines the distance beyond which the potential can be neglected, this inequality shows that the radial motion is not affected by the presence of the potential  $V(r)$  in the radial wave equation. The notable exception is the case  $\ell = 0$ , where the barrier is absent and the potential gives rise to a substantial distortion of the radial waves. In other words, for  $kr_0 \ll 1$  phase shifts (i.e. scattering) can *only arise from collisions with zero angular momentum*. The range of collision energies where the inequalities (12.9) are valid is called the  $s$ -wave regime.

### 12.1.1.3 Free particle motion

We first have a look at the case of free particles or particles in a homogeneous potential,  $V(r) = V_0$ . By introducing the dimensionless variable  $\varrho = kr$ , where  $k \equiv \sqrt{2m(E - V_0)}/\hbar$ , the radial wave equation (12.6) can be rewritten in the form of the spherical Bessel differential equation,

$$R_\ell'' + \frac{2}{\varrho}R_\ell' + \left[ 1 - \frac{\ell(\ell+1)}{\varrho^2} \right] R_\ell = 0. \quad (12.10)$$

<sup>1</sup>At this point we exclude tunneling through the barrier and the occurrence of shape resonances.

Here, the derivatives are with respect to the new variable.

The general solution of Eq. (12.10) for angular momentum  $\ell$  is a linear combination of two particular solutions, one regular with amplitude  $A_\ell$ , the spherical Bessel function  $j_\ell(\varrho)$ , and one irregular with amplitude  $B_\ell$ , the spherical Neumann function  $n_\ell(\varrho)$ :

$$\boxed{R_\ell(\varrho) = A_\ell j_\ell(\varrho) + B_\ell n_\ell(\varrho) = c_\ell [\cos \eta_\ell j_\ell(\varrho) + \sin \eta_\ell n_\ell(\varrho)]}, \quad (12.11)$$

where the new parameters  $c_\ell$  and  $\eta_\ell$ , defined by

$$A_\ell \equiv c_\ell \cos \eta_\ell \quad \text{and} \quad B_\ell \equiv c_\ell \sin \eta_\ell, \quad (12.12)$$

represent the amplitude  $c_\ell$  and the asymptotic phase  $\eta_\ell$  of the wavefunction. Note that this equation is singular in the origin except for the case of vanishing phase shifts. Therefore, in the case of free particles we require  $\eta_\ell = 0$  for all angular momentum values  $\ell$ . This implies that the general solution reduces to the regular one,

$$R_\ell(\varrho) = c_\ell \cos \eta_\ell j_\ell(\varrho). \quad (12.13)$$

#### 12.1.1.4 Significance of the phase shifts

To investigate the effect of a short-range interaction potential  $V(r)$  we return to the radial wave equation (12.6). As the potential is of short range it may be neglected for  $r \gg r_0$  and the general solutions coincide with those of the spherical Bessel equation,

$$R_\ell(k, r) \xrightarrow{r \gg r_0} c_\ell [\cos \eta_\ell j_\ell(kr) + \sin \eta_\ell n_\ell(kr)]. \quad (12.14)$$

For  $r \gg 1/k$  the spherical Bessel and Neumann functions assume their asymptotic form and we find,

$$\begin{aligned} R_\ell(k, r) &\xrightarrow{kr \rightarrow \infty} \frac{c_\ell}{kr} [\cos \eta_\ell \sin(kr - \frac{1}{2}\ell\pi) + \sin \eta_\ell \cos(kr - \frac{1}{2}\ell\pi)] \\ &= \frac{c_\ell}{kr} \sin(kr + \eta_\ell - \frac{1}{2}\ell\pi). \end{aligned} \quad (12.15)$$

where we introduced a the constant  $\eta_\ell$  representing the asymptotic phase shift. For a given value of  $k$  this phase shift fixes the general solution of the radial wavefunction  $R_\ell(k, r)$  up to an  $\ell$  dependent normalization constant  $c_\ell$ . Note that in view of the  $k$  dependence of the phase shift,  $R_\ell$  is a function of  $k$  and  $r$  rather than a function of the product  $kr$ . Whereas in the case of free particles the phase shifts must all vanish, in the presence of the interaction they provide the proper asymptotic form of the distorted waves. The non-zero asymptotic phase shift is the signature of the interaction at short distance; the motion becomes free-particle like (undistorted) only at large distance from the scattering center. In elastic scattering the relative energy  $\hbar^2 k^2 / 2m$  is conserved; hence, asymptotically also  $k$  and the de Broglie wavelength. This leaves only the asymptotic phase of the wave to be affected.

**Example 54 (Scattering matrix):** Rewriting Eq. (12.15) in complex notation,

$$R_\ell(k, r) \underset{r \rightarrow \infty}{\simeq} \frac{c_\ell}{2k} i \left[ e^{-i\eta_\ell} \frac{e^{-i(kr - \frac{1}{2}\ell\pi)}}{r} - e^{i\eta_\ell} \frac{e^{i(kr - \frac{1}{2}\ell\pi)}}{r} \right], \quad (12.16)$$

we see that for  $r \rightarrow \infty$  the stationary solution  $R_\ell(k, r)$  can be regarded as an 'incoming' spherical wave interfering with an 'outgoing' spherical wave. It is convention to choose the phase of the normalization constant such that the phase of the incoming wave is zero,

$$R_\ell(k, r) \underset{r \rightarrow \infty}{\simeq} \frac{c'_\ell}{2k} i \left[ \frac{e^{-ikr}}{r} - e^{-i\ell\pi} e^{2i\eta_\ell} \frac{e^{ikr}}{r} \right], \quad (12.17)$$

Apart from the sign, the ratio of the phase factors of the outgoing over the incoming wave is,

$$\mathcal{S}_\ell = e^{2i\eta_\ell}. \quad (12.18)$$

This quantity is called the scattering matrix ( $\mathcal{S}$  matrix) or, better, the  $l$ -wave contribution to the  $\mathcal{S}$  matrix. Being unitary it does not suffer from the divergences of the ratio  $B_\ell/A_\ell = \tan \eta_\ell$ . In the present context the name scattering matrix is a bit heavy because we only have a single matrix element ( $1 \times 1$  matrix). The term matrix finds its origin in the description of scattering of particles with an internal degree of freedom (like spin), for which the phase factor is replaced by a unitary matrix.

### 12.1.2 Hard-sphere potentials

We now turn to analytical solutions for model potentials in the limit of low energy. We first consider the case of two hard spheres of equal size. These can approach each other to a minimum distance equal to their diameter  $a$ . For  $r \leq a$  the radial wave function vanishes,  $R_\ell(r) = 0$ : Outside the hard sphere we have free atoms,  $V(r) = 0$ , with relative wave number  $k = [2m_r E/\hbar^2]^{1/2}$ . Thus, for  $r \leq a$  the general solution for the radial wave functions of angular momentum  $\ell$  is given by the free atom expression (12.11), which asymptotically this takes the form (12.15) of a phase-shifted spherical Bessel function,

$$R_\ell(k, r) = c_\ell [\cos \eta_\ell j_\ell(kr) + \sin \eta_\ell n_\ell(kr)] \underset{r \rightarrow 0}{\simeq} \frac{c_\ell}{kr} \sin(kr + \eta_\ell - \frac{1}{2}\ell\pi). \quad (12.19)$$

To determine the phase shift we require as a boundary condition that  $R_\ell(k, r)$  vanishes at the surface of the hard sphere (see Fig. 12.3),

$$\cos \eta_\ell j_\ell(ka) + \sin \eta_\ell n_\ell(ka) = 0. \quad (12.20)$$

Hence, the phase shift follows from the expression,

$$\tan \eta_\ell = \frac{j_\ell(ka)}{n_\ell(ka)}. \quad (12.21)$$

This expression allows to derive asymptotic expressions (for  $ka \ll 1$  and for  $ka \gg 1$ ) for the radial wave function (12.19), as will be shown in Exc. 12.1.5.1.

#### 12.1.2.1 $s$ -wave phase shifts for hard spheres

For the case  $\ell = 0$ , inserting the analytical expressions for the Bessel and von Neumann function, (12.19) becomes without approximation,

$$R_0(k, r) = \frac{c_0}{kr} (\cos \eta_0 \sin kr + \sin \eta_0 \cos kr) = \frac{c_0}{kr} \sin(kr + \eta_0). \quad (12.22)$$

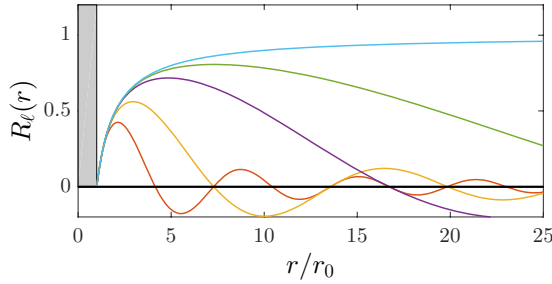


Figure 12.3: (code) Radial wavefunctions ( $\ell = 0$ ) for various values of  $k$  (down to the  $k \rightarrow 0$  limit) in the case of a hard sphere potential. The boundary condition is fixed by the requirement that the wavefunction vanishes at the edge of the hard sphere,  $R_0(ka) = 0$ .

The phase shift follows from the boundary condition  $R_0(k, a) = 0$ , which can be written in the form,

$$\cos \eta_0 \sin ka + \sin \eta_0 \cos ka = 0 . \quad (12.23)$$

Hence, the phase shift is

$$\eta_0 = -ka . \quad (12.24)$$

With this expression Eq. (12.22) reduces to

$$R_0(k, r) = \frac{c_0}{kr} \sin[k(r - a)] . \quad (12.25)$$

This expression is exact for any value of  $k$ , as announced above. The linear  $k$  dependence of  $\eta_0$  simply expresses its definition in which the shift of the wave (by  $a$ ) is compared to the de Broglie wavelength  $\lambda_{dB}$ ,  $\eta_0 = -2\pi a/\lambda_{dB}$ . As a consequence the phase shift vanishes for  $k \rightarrow 0$ ,

$$\lim_{k \rightarrow 0} \eta_0(k) = 0 . \quad (12.26)$$

This result is obvious when comparing the finite shift  $a$  to the diverging wavelength  $\lambda_{therm}$ . Interestingly, in the limit  $k \rightarrow 0$  the expression (12.25) becomes  $k$  independent,

$$R_0(r) \underset{k \rightarrow 0}{\sim} 1 - \frac{a}{r} \quad \text{for} \quad a \leq r \ll 1/k . \quad (12.27)$$

This important result is illustrated in Fig. 12.3. In the limit  $k \rightarrow 0$  the wavefunction is essentially constant throughout space (up to a distance  $1/k \rightarrow \infty$  at which it starts to oscillate), except for a small region of radius  $a$  around the potential center.

### 12.1.3 Spherical wells with a flat bottom

The second model potential to consider is the spherical well of range  $r_0$  sketched in Fig. 12.4,

$$\tilde{V}(r) = \begin{cases} 2m_r V_0/\hbar^2 = \tilde{V}_0 = -\kappa_0^2 & \text{for } r \leq r_0 \\ 0 & \text{for } r > r_0 \end{cases} . \quad (12.28)$$



Here  $|U_0| = \kappa_0^2$  is called the well depth ( $\kappa_0$  is chosen to be real and positive,  $\kappa_0 > 0$ ). The energy of the continuum states is given by  $\varepsilon = k^2$ . In analogy, the energy of the bound states is written as,

$$\varepsilon_b = -\kappa^2. \quad (12.29)$$

We now have to solve the radial wave equation (12.6) with the spherical well potential (12.28). Since the potential is constant inside the well ( $r \leq r_0$ ) the wavefunction has to be free-particle like with the wave number given by,

$$K_+ = \sqrt{2m_r(E - V_0)/\hbar^2} = \sqrt{\kappa_0^2 + k^2}. \quad (12.30)$$

As the wavefunction has to be regular in the origin, inside the well it is given by,

$$R_\ell(r) = C_\ell j_\ell(K_+ r) \quad \text{for } r \leq r_0, \quad (12.31)$$

where  $C_\ell$  is a normalization constant. This expression holds for  $E > V_0$  (both  $E > 0$  and  $E \leq 0$ ).

Outside the well ( $r > r_0$ ) we have for  $E > 0$  free atoms,  $\tilde{V}(r) = 0$ , with relative wavevector  $k = [2m_r E/\hbar^2]^{1/2}$ . Thus, for  $r > r_0$  the general solution for the radial wave functions of angular momentum  $\ell$  is given by the free atom expression (12.11),

$$R_\ell(k, r) = c_\ell [\cos \eta_\ell j_\ell(kr) + \sin \eta_\ell n_\ell(kr)] \quad \text{for } r > r_0. \quad (12.32)$$

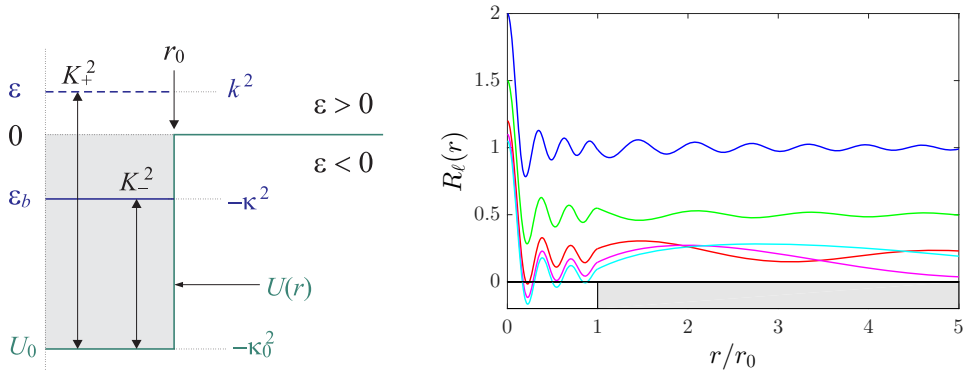


Figure 12.4: (code) (Left) Scheme of the flat bottom potential. (Right) (a) Radial wavefunctions for square wells: (a) continuum state ( $\varepsilon = k^2 > 0$ ); (b) Zero energy state ( $\varepsilon = k^2 = 0$ ) in the presence of an asymptotically bound level ( $\varepsilon = -\kappa^2 = 0$ ); (c) bound state ( $\varepsilon = -\kappa^2 < 0$ ). Note the continuity of  $R_0(r)$  and  $R'_0(r)$  at  $r = r_0$ . The wavefunctions are not normalized and are shifted relative to each other only for reasons of visibility.

The full solution [see Fig. 12.4(a)] is obtained by the continuity conditions for  $R_\ell(r)$  and  $R'_\ell(r)$  at the boundary  $r = r_0$ . These imply continuity of the logarithmic derivative with respect to  $r$ ,

$$K_+ \frac{j'_\ell(\varrho_i)}{j_\ell(\varrho_i)} = \frac{R'_\ell(r)}{R_\ell(r)} \Big|_{r=r_0} = k \frac{\cos \eta_\ell j'_\ell(\varrho_e) + \sin \eta_\ell n'_\ell(\varrho_e)}{\cos \eta_\ell j_\ell(\varrho_e) + \sin \eta_\ell n_\ell(\varrho_e)}, \quad (12.33)$$

where we defined the abbreviations  $\varrho_i \equiv K_+ r_0$  and  $\varrho_e \equiv k r_0$ . This ratio suffices to determine  $\eta_\ell$  independently of the normalization constants  $C_\ell$  and  $c_\ell$ . Once the phase shift is known, the relation between  $C_\ell$  and  $c_\ell$  follows from the continuity condition for  $R_\ell(r)$ . Furthermore, it shows that the asymptotic phase shift  $\eta_\ell$  can take any (real) value depending on the depth of the well. In view of the importance of the  $\mathcal{S}$  matrix in scattering theory Sec. 12.2, it is advantageous to determine  $e^{2i\eta_\ell}$  rather than  $\eta_\ell$  itself. Expressing  $\sin \eta_\ell$  and  $\cos \eta_\ell$  in terms of  $e^{i\eta_\ell}$  and  $e^{-i\eta_\ell}$  Eq. (12.33) becomes,

$$K_+ \partial_\varrho \ln j_\ell(\varrho_i) = k \frac{e^{2i\eta_\ell} h_\ell^{(2)'}(\varrho_e) + h_\ell^{(1)'}(\varrho_e)}{e^{2i\eta_\ell} h_\ell^{(2)}(\varrho_e) + h_\ell^{(1)}(\varrho_e)}, \quad (12.34)$$

with the definition of the Hankel functions of the first and second kind:  $h_\ell^{(1,2)} \equiv j_\ell \pm i n_\ell$ . Solving for  $e^{2i\eta_\ell}$  this leads to the following expression for the  $\ell$ -wave contribution to the  $\mathcal{S}$  matrix,

$$e^{2i\eta_\ell} = - \frac{h_\ell^{(1)}(\varrho_e) K_+ \partial_\varrho \ln j_\ell(\varrho_i) - k \partial_\varrho \ln h_\ell^{(1)}(\varrho_e)}{h_\ell^{(2)}(\varrho_e) K_+ \partial_\varrho \ln j_\ell(\varrho_i) - k \partial_\varrho \ln h_\ell^{(2)}(\varrho_e)}, \quad (12.35)$$

where the expression  $\partial_\varrho \ln$  stands for the logarithmic derivative. This expression may look a bit heavy, but is valuable as it represents the exact result for arbitrary  $\ell$ . In Exc. 12.1.5.2 we simplify this formula for  $\ell = 0$ . As the formula (12.35) lacks transparency from the physical point of view, we analyze in the coming sections the case  $\ell = 0$  directly discussing the radial wavefunctions  $u_\ell$ .

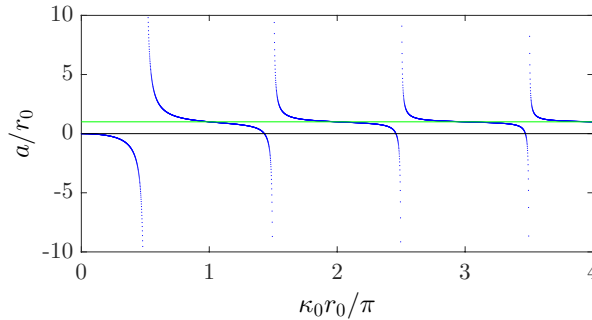


Figure 12.5: (code) The  $s$ -wave scattering length  $a$  normalized on  $r_0$  as a function of the depth of a spherical square potential well (blue curve). Note that, typically,  $a \simeq r_0$  (green line), except near the resonances at  $\kappa_0 r_0 = (n + \frac{1}{2})\pi$  being an integer.

### 12.1.3.1 $s$ -wave scattering ( $E > 0$ )

The analysis of spherical well potentials becomes particularly simple for the case  $\ell = 0$ . Let us first consider the case  $E > 0$ , for which the radial wave equation can be written as a 1D-Schrödinger equation (12.7) of the form,

$$u_0'' + [k^2 - \tilde{V}(r)]u_0 = 0. \quad (12.36)$$

The solution is,

$$u_0(kr) = \begin{cases} C_0 \sin(K_+ r) & \text{for } r \leq r_0 \\ c_0 \sin(kr + \eta_0) & \text{for } r > r_0 \end{cases} . \quad (12.37)$$

To determine  $\eta_0(k)$  it is sufficient to apply the boundary condition for continuity of the logarithmic derivative at the edge of the well,

$$\left. \frac{u'_0}{u_0} \right|_{r=r_0} = K_+ \cot K_+ r_0 = k \cot(kr_0 + \eta_0) . \quad (12.38)$$

Note that this expression coincides with the general result given by Eq. (12.33) for the case  $\ell = 0$ ; i.e. the boundary condition of continuity for  $u'_0/u_0$  coincides with that for  $R'_0/R_0$ , as we know from a calculation left to Exc. 12.1.5.3. Furthermore, for a vanishing potential ( $\kappa_0 \rightarrow 0$ ) we have  $K_+ \rightarrow k$  and the boundary condition properly yields a zero phase shift ( $\eta_0 = 0$ ).

At this point we introduce the effective hard-sphere diameter  $a(k)$  to describe, in analogy with Eq. (12.24), the behavior of the phase shift,

$$\eta_0(k) \equiv -ka(k) . \quad (12.39)$$

By this procedure we extract the linear  $k$  dependence as well as the negative sign from the phase shift. This is a good idea because the linear  $k$ -dependence does not arise from the potential but simply from the definition of the phase in which, as discussed earlier, the shift of the wave is compared to the de Broglie wavelength. In the limit  $k \rightarrow 0$ , we have  $K_+ r_0 \rightarrow \kappa_0 r_0$  and with the definition,

$$a \equiv \lim_{k \rightarrow 0} a(k) = - \lim_{k \rightarrow 0} \eta(k)/k \quad (12.40)$$

the boundary condition (12.38) becomes,

$$\left. \frac{u'_0}{u_0} \right|_{r=r_0} = \kappa_0 \cot \kappa r_0 = \frac{1}{r_0 - a} . \quad (12.41)$$

Solving for  $a$  we find,

$$a = r_0 \left( 1 - \frac{\tan \gamma}{\gamma} \right) , \quad (12.42)$$

where the dimensionless positive quantity,

$$\gamma \equiv \kappa_0 r_0 \quad (12.43)$$

is called the well parameter. As shown in Fig. 12.5, the value of  $a$  can be positive, negative or zero depending on the value of  $\gamma$ . Therefore, rather than using the pictorial term effective hard-sphere diameter the name scattering length is used for  $a$ . Next to the range, the scattering length represents the second characteristic length that can be associated with the interaction potential. As the name suggest, it is a measure for the scattering behavior of atoms, and we elaborate on this in Sec. 12.2. Also, in Sec. ?? we will show that  $a$  is also a measure for the effective strength of the interaction.

Fig. 12.5 and Eq. (12.42) show that  $a$  is typically a quantity of the size of  $r_0$ , although for  $\gamma = \tan \gamma$  it is zero and for  $\gamma = (\nu + \frac{1}{2})\pi$ , with  $\nu$  being an integer,

it diverges. The latter condition points to a resonance phenomenon occurring when (with increasing  $\gamma$ ) a new bound level enters the potential well. For the square well potential the scattering length is mostly positive; it is negative in the regions with  $\gamma < \tan \gamma$ , which become narrower for increasing  $\gamma$ . This unlikely occurrence of negative  $a$  is atypical for the general case; e.g. for Van der Waals potentials the probability to find a negative scattering length is 25% .

For  $r \geq r_0$  the radial wavefunction corresponding to Eq. (12.37) is of the form,

$$R_0(k, r) = \frac{c_0}{kr} \sin[kr - ka(k)] . \quad (12.44)$$

Recalling the definitions (12.39) and (12.40) we find that for  $k \rightarrow 0$  this radial wavefunction becomes  $k$ -independent,

$$R_0(r) \underset{k \rightarrow 0}{\sim} 1 - \frac{a}{r} \quad \text{for} \quad r_0 < r \ll \frac{1}{k} . \quad (12.45)$$

The latter two expressions for the radial wavefunction have the same formal appearance as the hard sphere results (12.25) and (12.27). However, whereas the diameter of the hard-sphere has a fixed value, the scattering length for the well depends on  $\gamma$ . As shown in Fig. 12.6, for positive scattering length the  $s$ -wave has a characteristic node at  $r = a$ ; for negative scattering length this becomes a virtual node.

Importantly, because Eq. (12.45) reaches the asymptotic value 1 only for distances  $r \gg a$ , the use of this equation in the modeling of dilute gases is only justified if  $a$  is much smaller than the interparticle spacing,

$$na^3 \ll 1 . \quad (12.46)$$

Otherwise, the interaction with neighboring atoms will distort the relative motion of the colliding pair. This violates the binary scattering approximation on which Eq. (12.45) is based. The dimensionless quantity  $na^3$  is called the gas parameter. When its value is small, the gas is called nearly ideal or weakly interacting<sup>2</sup>.

### 12.1.3.2 Bound $s$ -levels ( $E \leq 0$ )

Let us turn to the case  $E \leq 0$ . We shall show that the divergences of the scattering length obtained by analyzing the continuum states ( $E > 0$ ) result from the appearance of the next bound  $s$ -level when increasing the well parameter. The 1D Schrödinger equation takes the form,

$$u_0'' + [-\kappa^2 - \tilde{V}(r)]u_0(r) = 0 . \quad (12.47)$$

where  $\varepsilon = -\kappa^2$  is the discrete energy eigenvalue of a bound state with  $\ell = 0$ . The solutions are of the type (see Fig. 12.30),

$$u_0(k, r) = \begin{cases} C_0 \sin K_- r & \text{for } r \leq r_0 \\ c_0 e^{-\kappa r} & \text{for } r \leq r_0 \end{cases} \quad (12.48)$$

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<sup>2</sup>Note that weakly interacting does not mean that that the potential is 'shallow'. Any gas can be made weakly interacting by making the density sufficiently small.

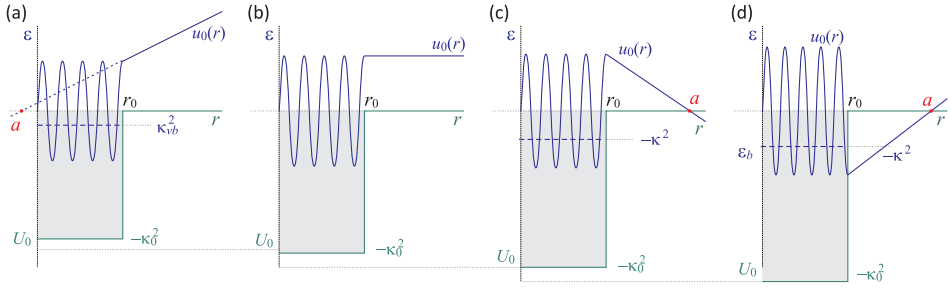


Figure 12.6: Reduced radial wavefunctions  $u_0(r)$  for continuum states ( $\varepsilon > 0$ ) in the  $k \rightarrow 0$  limit for increasing well depth near the threshold value  $\kappa_0 r_0 = (n + \frac{1}{2})\pi$ : (a) presence of an almost bound state ( $a < 0$ ); (b) presence of zero-energy resonance ( $\kappa_{vb} = 0$ ,  $a \rightarrow \pm\infty$ ); (c) presence of a weakly bound state ( $a > 0$ ); (d) deeper binding of the least bound state. For  $r > r_0$  the wavefunction is given by  $u_0(r) = c_0(r - a)$ ; hence, the value of  $a$  is given by the intercept with the horizontal axis. This gives rise to a characteristic node at  $r = a$ , which is *real* for  $a > 0$  (just as for hard spheres of diameter  $a$ ), but *virtual* for  $a < 0$ . The wavefunctions are not normalized.

where  $\kappa > 0$  because the bound state wavefunction has to be normalized. The bound state energy is obtained by requiring the continuity of the logarithmic derivative when connecting the inner part of the wavefunction to the outer part,

$$\left. \frac{u_0'(r)}{u_0(r)} \right|_{r=r_0} = K_- \cot K_- r_0 = -\kappa, \quad (12.49)$$

where  $\kappa > 0$  and

$$K_- = [2m_r(E - V_0)/\hbar^2]^{1/2} = (\kappa_0^2 - \kappa^2)^{1/2}. \quad (12.50)$$

With decreasing  $\gamma$ , the least bound level disappears in the limit  $\kappa \rightarrow 0$ ,  $K_- \rightarrow \kappa_0$ . In this limit Eq. (12.49) reduces to,

$$\left. \frac{u_0'(r)}{u_0(r)} \right|_{r=r_0} = \kappa_0 \cot \kappa_0 r_0 \underset{\kappa \rightarrow 0}{=} 0, \quad (12.51)$$

Increasing from zero the vibrational levels appear sequentially for

$$\gamma = (v + \frac{1}{2})\pi, \quad (12.52)$$

where  $v = 0, 1, \dots, r_{max}$  is the vibrational quantum number. This shows that a minimum well parameter ( $\gamma = \pi/2$ ) is required to bind the first state<sup>3</sup>. For the least-bound level,  $v_{max}$ , we have,

$$(v_{max} + \frac{1}{2})\pi = \text{Int} \left( \frac{\gamma}{\pi} - \frac{1}{2} \right) \quad (12.53)$$

and the total number of bound  $s$  levels follows with,

$$N_b = v_{max} + 1 = \text{Int} \left( \frac{\gamma}{\pi} + \frac{1}{2} \right). \quad (12.54)$$

<sup>3</sup>This conclusion cannot be extended to lower dimensions; in two dimensions bound states appear for arbitrarily shallow potentials.

The relation between  $\kappa$  and  $v$  for a given vibrational level depends on the ratio  $\kappa/K_-$  and is given by

$$\cot K_- r_0 = -\frac{\kappa}{K_-} . \quad (12.55)$$

Note that this relation corresponds to  $K_- r_0 \simeq (v_{max} + \frac{1}{2})\pi$  for the least-bound state

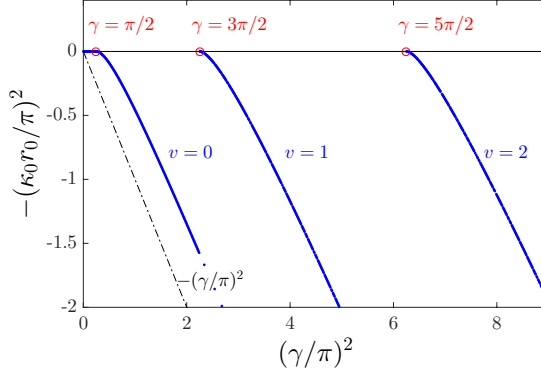


Figure 12.7: (code) Appearance and increase of binding of the first three bound levels for increasing well depth. The quadratic dependence near threshold is universal (i.e. independent of the well shape). The full crossover curve is obtained by numerical solution of Eq. (12.49) and corresponds to a  $\pi/2$  phase shift of  $K_+ r_0$  near threshold. The dashed line shows the increase in well depth.

( $\kappa/K_- \ll 1$ ) and to  $K_- r_0 \simeq (v_{max} + 1)\pi$  for deeply bound levels ( $K_-/\kappa \ll 1$ ), as is illustrated in Fig. 12.8(a).

### 12.1.3.3 Weakly bound $s$ -level: halo states

For weakly bound  $s$  levels ( $0 < \kappa r_0 \ll 1$ ) we have  $K_- \rightarrow \kappa_0$  and Eq. (12.49) may be approximated by

$$\left. \frac{u'_0(r)}{u_0(r)} \right|_{r=r_0} = \kappa_0 \cot \kappa_0 r_0 = -\kappa , \quad (12.56)$$

Furthermore, we recall that in the presence of a weakly bound  $s$ -level the scattering length is large and positive,  $a \gg r_0$ . From Eq. (12.41) we recall that for  $k \rightarrow 0$  the logarithmic derivative also satisfies the relation

$$\left. \frac{u'_0(r)}{u_0(r)} \right|_{r=r_0} = \kappa_0 \cot \kappa_0 r_0 = \frac{1}{r_0 - a} \simeq -\frac{1}{a} , \quad (12.57)$$

Interestingly, for  $a \gg r_0$  the logarithmic derivative of the continuum states becomes independent of  $r_0$  and  $\kappa_0$ ; i.e. it becomes independent of the shape of the potential well. As we shall see it only depends on the well parameter  $\gamma$  and not on the well shape. This points to a universal limiting shape of the wavefunction for large scattering length. As is sketched in Fig. 12.8(b), for decreasing  $\kappa$  the least-bound state turns into a halo state; i.e. for  $\kappa r_0 \ll 1$  most of the probability of the bound state is found in the classically inaccessible region outside the potential well, thus surrounding the

potential center like a halo. This behavior holds for arbitrary short-range potentials.

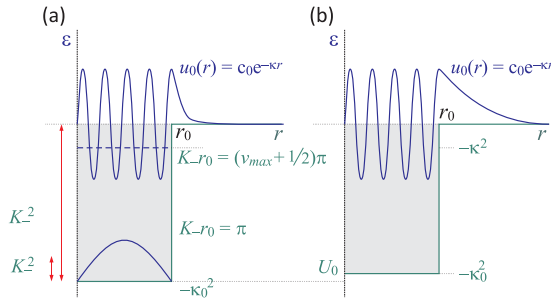


Figure 12.8: Bound states oscillate inside the well and decay exponentially outside the well: (a) the boundary condition depends on the ratio  $\kappa/K_-$ ; (b) a slight reduction of the well depth can turn the least bound state into a halo state.

With Eqs. (12.56) and (12.57) we have obtained two expressions for  $\kappa_0 \cot \kappa_0 r_0$  and arrive at the conclusion that in the presence of a weakly bound state the scattering length is given by,

$$a \underset{\kappa \rightarrow 0}{\simeq} 1/\kappa . \quad (12.58)$$

This expression reveals the tight relation between the binding energy of the least-bound state, given by Eq. (12.29), and the scattering length,

$$E_b = -\frac{\hbar^2 \kappa^2}{2m_r} \underset{\kappa \rightarrow 0}{\rightarrow} -\frac{\hbar^2}{2m_r a^2} . \quad (12.59)$$

#### 12.1.3.4 *s*-wave resonances in the continuum: The Breit-Wigner formula

To obtain the  $k$ -dependence of the phase shift for large but otherwise arbitrary well parameter ( $\gamma \gg 1$ ) we rewrite the boundary condition (12.38) in the form,

$$\eta_0(k) = -kr_0 + \arctan \frac{kr_0}{K_+ r_0 \cot K_+ r_0} \equiv \eta_{bg} + \eta_{res} . \quad (12.60)$$

The first term of (12.60) is called the *background contribution* to the phase shift and the second term the *s-wave resonance contribution*. Note that the background contribution shows the same phase development as we found in Sec. 12.1.2 for hard spheres. The phase development of the resonance contribution is shown in Fig. 12.9(a) for the case of a large well parameter slightly detuned from the threshold value (at  $\gamma = 31.5\pi \approx 98.960169$ ) such that the scattering length is negative ( $\Delta_\gamma = -0.5$ ). For potentials with  $\gamma \gg 1$  the argument of the arctangent is predominantly small,  $kr_0/|K_+ r_0 \cot K_+ r_0| \ll 1$ , because

$$K_+ r_0 = \kappa_0 r_0 (1 + k^2/\kappa_0^2)^{1/2} > \gamma \gg 1 . \quad (12.61)$$

However, the argument of the arctangent diverges when  $\cot K_+ r_0$  passes through zero; i.e. for

$$K_+ r_0 = (\tilde{\nu} + \frac{1}{2})\pi , \quad (12.62)$$

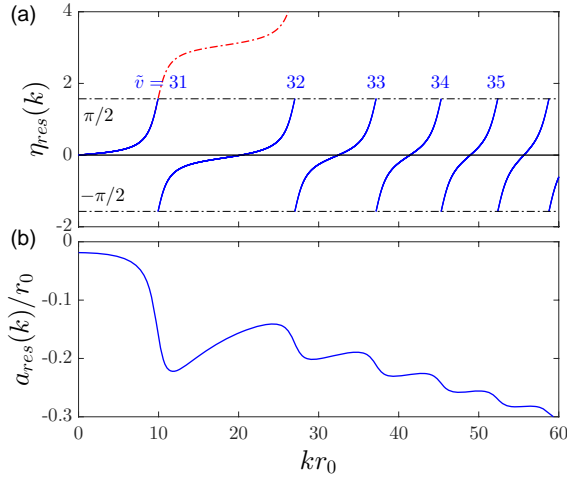


Figure 12.9: (code) (a) Resonance contribution to the  $s$ -wave phase shift  $\eta_0(k)$  for a large well parameter slightly detuned from the threshold value (at  $\gamma = 31.5\pi$ ), such that the scattering length is negative ( $\Delta\gamma = -0.5$ ): The linear shift of the background contribution is not included in the plot. Note that the  $\pi$  phase jumps arise from the modulo- $\pi$  representation of the arctangent and do not represent an observable phenomenon; the physical phase increases monotonically and equals  $\eta_{res} = \frac{1}{2}$  (modulo  $\pi$ ) at the center of the resonances; (b) contribution of the resonances to the effective hard sphere diameter  $a(k) = -\eta_0(k)/k$ . As (in this example) the lowest resonance is not close to threshold the resonant enhancement is small,  $|a_{res}(k)| = r_0 \ll 1$ .

where  $\tilde{v}$  is an integer called the resonance index. This divergence is observed as a small resonant enhancement of  $a(k)$ , as shown in Fig. 12.9(b). The physical phase is a continuous function of  $k$ , which changes by  $\pi$  when sweeping across the resonance. Because the arctangent remains finite for  $\cot K_+ r_0 = 0$  also the resonant phase shift remains finite, having the value  $\eta_{res}(k) = \frac{1}{2}\pi$  (modulo  $\pi$ ) at the center of each resonance.

In the remainder of this section we shall analyze the width and separation of the  $s$ -wave resonances for the case  $\gamma \gg 1$ . Since  $K_+ \geq \kappa_0 \geq K_-$ , we have,

$$\tilde{v} \geq \frac{\gamma}{\pi} - \frac{1}{2} \geq v_{max} , \quad (12.63)$$

which shows that for  $\gamma \gg 1$  the value of  $\tilde{v}$  is large ( $\tilde{v}_{min} \geq \tilde{v}_{max} \gg 1$ ). Hence, the resonance numbering starts where the numbering of bound states ends. To discuss the resonances we denote the wavevectors  $k$  and  $K_+$  at resonance by  $k_{res}$  and  $K_{res} \equiv \sqrt{\kappa_0^2 + k_{res}^2}$ , respectively. The resonance energies  $\varepsilon_{res} = k_{res}^2$  satisfy the condition,

$$\varepsilon_{res} = K_{res}^2 - \kappa_0^2 = (\tilde{v} + \frac{1}{2})\pi(\frac{\pi}{r_0})^2 - \kappa_0^2 \geq 0 . \quad (12.64)$$

The exceptional case for which the equal sign applies ( $\tilde{v} = v_{max}$ ) corresponds to a resonant bound state ( $\kappa = 0$ ) and the resonance is called a resonance at threshold or zero-energy resonance ( $k_{res} = 0$ ).

Let us first analyze  $s$ -wave resonances for large well parameters ( $\tilde{v} = v_{max}$ ) and far from threshold, ( $\kappa = 0$ ). The energy spacing between two subsequent resonances



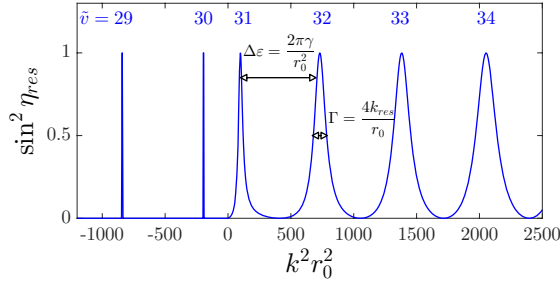


Figure 12.10: (code) (a) Transition from bound states to Breit-Wigner  $s$ -wave resonances plotted for  $\Delta\gamma = -0.5$  with respect to the threshold at  $\gamma = 31.5\pi$  (same conditions as Fig. 12.9). The bound states are indicated as zero-width spikes at energies  $\varepsilon = -\kappa^2$ , with  $\kappa$  following from Eq. (12.49). For  $\varepsilon > 0$  the plot is based on Eqs. (12.60). The width of the resonances increases with the square root of the energy. Note that the band of energies typical for the quantum gases ( $kr_0 \ll 1$ ) corresponds to a narrow zone, unresolved on the energy scale of the plot.

is,

$$\Delta\varepsilon_{res} = \varepsilon_{res}^{(\tilde{\nu}+1)} - \varepsilon_{res}^{(\tilde{\nu})} = 2(\tilde{\nu} + 1) \frac{\pi^2}{r_0^2} \simeq \frac{2\pi\gamma}{r_0^2}. \quad (12.65)$$

To analyze a given resonance we expand  $K_+ \cot K_+ r_0$  about the point of zero crossing. For this purpose we introduce the notation,

$$K_+ = \sqrt{\kappa_0^2 + (k_{res} + \delta k)^2} = K_{res} + \frac{\delta k k_{res}}{K_{res}}, \quad (12.66)$$

where  $\delta k = k - k_{res}$  is called the detuning from resonance. Thus, restricting ourselves to the low-energy (but not zero energy)  $s$ -wave resonances ( $1 < k_{res} r_0 \ll K_{res} r_0 \simeq \gamma$ ), we may approximate  $K_+ \cot K_+ r_0 \simeq K_{res} \cot K_+ r_0$ . Expanding  $\cot K_+ r_0$  about the zero crossing at  $K_+ r_0 = (\tilde{\nu} + 1/2)\pi$  and retaining only the linear term we obtain (see Problem 3.4),

$$K_{res} \cot K_+ r_0 = -\delta k k_{res} r_0. \quad (12.67)$$

Hence, the diverging argument of the arctangent becomes,

$$\tan \eta_{res} = \frac{k}{K_+ \cot K_+ r_0} \simeq -\frac{1}{\delta k r_0} = \frac{-(k + k_{res})}{(k^2 - k_{res}^2) r_0} \simeq \frac{-2k_{res}/r_0}{\varepsilon - \varepsilon_0}. \quad (12.68)$$

The expansion (12.66) is valid over the full range of the resonant change in phase provided the following condition holds,

$$\delta k r_0 \ll \frac{K_{res}}{k_{res}} \simeq \frac{\gamma}{k_{res} r_0}, \quad (12.69)$$

which is satisfied for the lowest resonances as long as the well parameter is sufficiently large ( $\gamma \gg k_{res} r_0$ ). As long as  $\delta k \ll k_{res}$  we may further approximate  $k \simeq k_{res}$ . With these approximations and after restoring the dimensions, Eq. (12.68) can be written as a function of the energy  $E = \hbar^2 2k^2 / 2m_r$ ,

$$\tan \eta_{res} = \frac{k}{K_+ \cot K_+ r_0} \simeq \frac{-\Gamma^2}{\varepsilon - \varepsilon_{res}}, \quad (12.70)$$

where

$$\Gamma/2 = 2k_{res}/r_0 \quad (12.71)$$

is called the spectral width of the resonance. Comparing the expressions for  $\Gamma$  and  $\Delta E_{res}$  we find that for given  $r_0$  the width  $\Gamma$  is independent of  $\gamma$ , whereas the resonance spacing is proportional to  $\gamma$ . Thus, only for sufficiently large well parameters ( $\gamma \gg 1$ ) the spectral width becomes smaller than the resonance spacing,

$$\Gamma \ll \Delta \varepsilon_{res} \iff k_{res} r_0 \ll \pi \gamma . \quad (12.72)$$

Knowing the tangent of  $\eta_{res}$ , we readily obtain the sine and Eq. (12.70) is replaced by the *Breit-Wigner formula*,

$$\sin^2 \eta_{res} = \frac{(\Gamma/2)^2}{(\varepsilon - \varepsilon_0)^2 + (\Gamma/2)^2} . \quad (12.73)$$

For optical resonances this energy dependence is known as the Lorentz lineshape. Note that  $\Gamma$  corresponds to the full-width-at-half-maximum (FWHM) of this line shape. The lowest energy resonances are plotted in Fig. 12.10 along with the highest-energy bound states.

The resonance near threshold (almost bound level) deserves special attention, as this type of resonance is the only one that can play an important role within the band of energies relevant for the quantum gases ( $kr_0 \ll 1$ ). Fig. 12.10 shows that near the threshold (at  $\gamma = 31.5\pi$ ) the resonance narrows down and becomes asymmetric, which means that the Breit-Wigner lineshape is lost. Using Eq. (12.54) we calculate  $\tilde{v} = 31$ . The narrow line is reminiscent of a bound level but the scattering length is negative (see Fig. 12.10). Under these conditions the wavefunction has a virtual node at  $r = -|a|$  (see Fig. 12.30). Accordingly, the level is called a virtual level and the wavefunction is said to represent a virtual bound state. In analogy with the bound states its energy is written as  $\varepsilon = \kappa_{res}^2$ , where  $\kappa$  is to be defined later.

## 12.1.4 Other types of potentials

### 12.1.4.1 Zero-range potentials

An important model potential is obtained by considering a spherical well in the zero-range limit  $r_0 \rightarrow 0$ . As illustrated in Fig. 12.11, it is possible to construct a zero-range well in such a way that the long-range properties of the wavefunction are unaffected; i.e. the scattering length  $a$  and the binding energy  $\varepsilon = -\kappa^2$  of the least-bound state remain unchanged.

For  $E < 0$  this can be demonstrated with the aid of the boundary condition (12.49),

$$-\kappa = K_- \cot K_- r_0 . \quad (12.74)$$

Reducing the radius  $r_0$  the value of the binding energy  $\varepsilon = -\kappa^2$ , can be conserved by increasing  $\kappa_0$ . In the limit  $r_0 \rightarrow 0$  the well depth should diverge in accordance with,

$$-\frac{\kappa}{K_-} = \cot K_- r_0 \rightarrow 0 . \quad (12.75)$$

This condition is satisfied for  $K_- r_0 \simeq \pi/2$ . To elucidate this point we consider the least-bound level with vibrational quantum number  $v = v_{max}$ , for which  $K_- r_0 =$

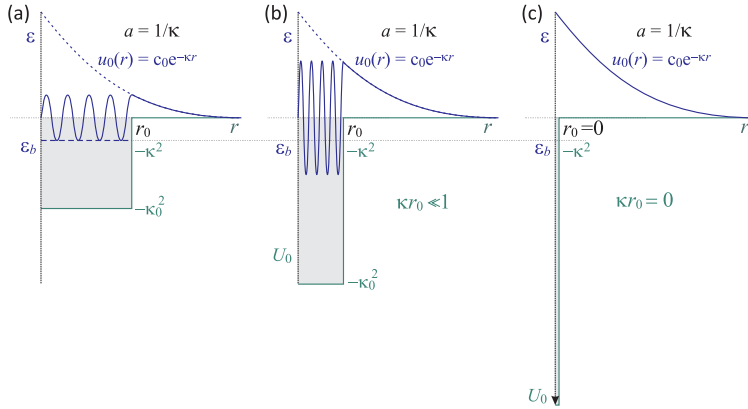


Figure 12.11: Wavefunctions corresponding to the same binding energy ( $\varepsilon = -\kappa^2$ ) plotted for three different values of  $r_0$ . Outside  $r_0$  the wavefunctions fall off exponentially, always with the same decay exponent  $\kappa$ ; this is the essence of the Bethe-Peierls boundary condition. The dashed lines show the extrapolation for  $r \rightarrow 0$ . (a) reference case; (b) for  $\kappa r_0 \ll 1$  most of the probability density of a bound state is found outside the well (halo state); (c) for zero-range potentials ( $\kappa r_0 = 0$ ) the oscillating part of the wavefunction is compressed into a delta function and only the decaying exponent remains (universal limit). Note that these wavefunctions do not share the same normalization.

$(v_{max} + 1/2)\pi$ . Reducing  $r_0$  by a factor of 2 the wavenumber  $K_-$  has to be doubled to conserve the number of nodes in the wavefunction (i.e. to conserve  $v_{max}$ ). This means that the kinetic energy inside the well has to increase by a factor 4. Since for the least-bound level we have  $K_- r_0 \simeq \gamma$ , it means that in this case the binding energy can be conserved at effectively constant well parameter. Obviously, the freedom to conserve (for decreasing  $r_0$ ) the binding energy of one of the levels can only be used once. It does not hold for the other levels because the level separation diverges with  $\kappa_0$ . In the zero range limit the potential only supports a single bound state and the wavefunction of that state is given by,

$$R_0(r) = c_0 \frac{e^{-\kappa r}}{r} \quad \text{for } r > 0, \quad (12.76)$$

and with  $\kappa > 0$ . Unit normalization,  $\int r^2 R_0^2(r) dr = 1$ , is obtained for  $c_0 = \sqrt{2\kappa}$ . For  $E > 0$  we can arrive at the same conclusion. The boundary condition for  $k \rightarrow 0$  and given value of  $r_0$  is given by Eq. (12.41), which we write in the form,

$$\frac{1}{r_0 - a} = \kappa_0 \cot \kappa_0 r_0. \quad (12.77)$$

Reducing the radius  $r_0$ , the scattering length  $a$  can be conserved by increasing  $\kappa_0$ . In the limit  $r_0 \rightarrow 0$  the well depth should diverge in accordance with,

$$-\frac{1}{\kappa_0 a} = \cot \kappa_0 r_0 \rightarrow 0. \quad (12.78)$$

This is again satisfied for  $\kappa_0 r_0 \simeq \pi/2$ . In the zero-range limit the radial wavefunction

for  $k \rightarrow 0$  is given by,

$$R_0(k, r) = \frac{1}{kr} \sin[k(r - a)] \quad \text{for } r > 0, \quad (12.79)$$

which implies  $R_0(k, r) \simeq 1 - a/r$  for  $0 < r \ll 1/k$ .

#### 12.1.4.2 Bethe-Peierls boundary condition

Note that Eq. (12.76) is the solution for  $E < 0$  of the 1D-Schrödinger equation in the zero-range approximation,

$$u_0'' - \kappa^2 u_0 \quad \text{for } r > 0, \quad (12.80)$$

under the boundary condition,

$$\left. \frac{u_0'}{u_0} \right|_{r \rightarrow 0} = -\kappa. \quad (12.81)$$

The latter relation is called the *Bethe-Peierls boundary condition* and was first used to describe the deuteron, the weakly bound state of a proton with a neutron [?]. It shows that for weakly bound states the wavefunction has the universal form of a halo state, which only depends on the binding energy,  $\varepsilon_0 = -\kappa^2$  (see Fig. 12.11).

For  $E > 0$  the 1D-Schrödinger equation in the zero-range approximation is given by,

$$u_0' + k^2 u_0 = 0 \quad \text{for } r > 0. \quad (12.82)$$

The general solution is  $u_0(k, r) = c_0 \sin[kr + \eta_0]$ . Using the Bethe-Peierls boundary condition we obtain,

$$k \cot \eta_0(k) = -\kappa, \quad (12.83)$$

which yields after substituting  $\eta_0(k \rightarrow 0) \simeq -ka$  the universal relation between the scattering length and the binding energy in the presence of a weakly bound  $s$ -level,  $\varepsilon_0 = -\kappa^2 = -1/a^2$ .

#### 12.1.4.3 Power-law potentials

The general results obtained in the previous sections presumed the existence of a finite range of interaction,  $r_0$ . Thus far this presumption was based only on the heuristic argument presented in Sec. ???. To derive a proper criterion for the existence of a finite range and to determine its value  $r_0$  we have to analyze the asymptotic behavior of the interatomic interaction [506]. For this purpose we consider potentials of the power-law type,

$$V(r) = -\frac{C_s}{r^s}, \quad (12.84)$$

where  $C_s = V_0 r_c^s$  is the power-law coefficient, with  $V_0 \equiv |V(r_c)| \equiv \hbar^2 \kappa_c^2 / 2m_r$  the well depth. These power-law potentials are important from the general physics point of view, because they capture major features of interparticle interactions.

For power-law potentials, the radial wave equation (12.6) takes the form,

$$R_\ell'' + \frac{2}{r} R_\ell' + \left[ k^2 + \frac{\kappa_c^2 r_c^s}{r^s} - \frac{\ell(\ell + 1)}{r^2} \right] = 0. \quad (12.85)$$

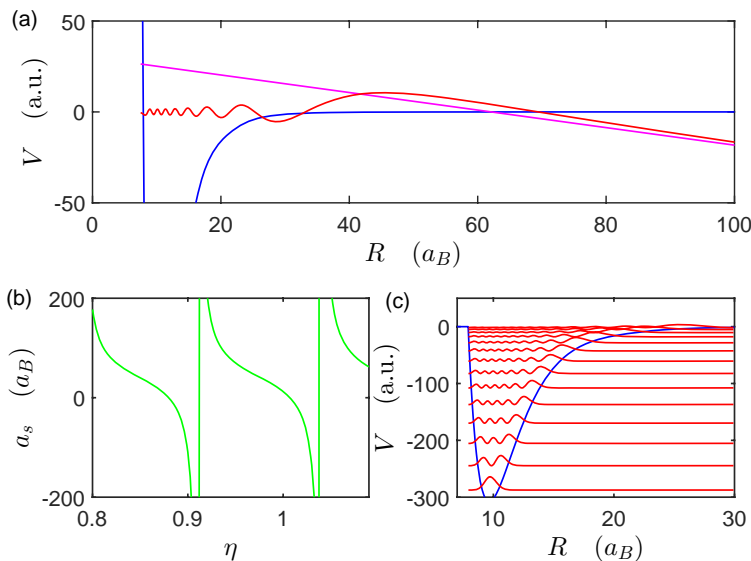


Figure 12.12: (code) Dependence of the scattering length on the potential depth.

Because this equation can be solved analytically in the limit  $k \rightarrow 0$  it is ideally suited to analyze the conditions under which the potential  $V(r)$  may be neglected and thus to determine  $r_0$ . To solve Eq. (12.85) we look for a clever substitution of the variable  $r$  and the function  $R_\ell(r)$  to optimally exploit the known  $r$  dependence of the potential in order to bring the differential equation in a well-known form. To leave exibility in the transformation we search for functions of the type,

$$G_\ell(x) = r^{-\nu} R_\ell(r) , \quad (12.86)$$

where the power  $\nu$  is to be selected in a later stage.

#### 12.1.4.4 Computation of the scattering length

The scattering length depends on the *binding energy*  $E_v$  of weakly bound states. If  $a$  is positive and much greater than the range of the potential, then [284, 247] (12.59),

$$E_v = -\frac{\hbar^2}{2m_r a^2} . \quad (12.87)$$

More precisely, for a potential behaving at long range as,

$$V = -\frac{C_6}{R^6} , \quad (12.88)$$

we get,

$$E_v = -[(v_D - v)H(m_r, C_6)]^{-1/3} , \quad (12.89)$$

where  $v_D$  is the vibrational quantum number at the dissociation limit and  $H$  a constant. Also,

$$a = \frac{\Gamma(3/4)}{2\sqrt{2}\Gamma(5/4)} \left( \frac{2\mu C_6}{\hbar^2} \right)^{1/4} \left[ 1 - \tan \pi(v_D + \frac{1}{2}) \right]. \quad (12.90)$$

#### 12.1.4.5 Second method

It yields for  $\gamma = \alpha, \beta$ ,

$$\frac{d^2}{dR^2} \varepsilon_\gamma(R) = 2m_r V(R) \varepsilon_\gamma(R). \quad (12.91)$$

Successive approaches start with  $\varepsilon_\alpha^{(0)} = R$  and  $\varepsilon_\beta^{(0)} = 1$  and get superior orders via,

$$\frac{d^2}{dR^2} \varepsilon_\gamma^{(k+1)}(R) = 2m_r V(R) \varepsilon_\gamma^{(k)}(R). \quad (12.92)$$

We define  $\delta_\gamma^{(k)} \equiv \varepsilon_\gamma^{(k)} - \varepsilon_\gamma^{(k-1)}$  starting with  $\delta_\gamma^{(0)} = \varepsilon_\gamma^{(0)}$ , such that,

$$\frac{d^2}{dR^2} \delta_\gamma^{(k+1)}(R) = 2m_r V(R) \delta_\gamma^{(k)}(R). \quad (12.93)$$

$\delta_\alpha(R \rightarrow \infty) = \delta_\beta(R \rightarrow \infty) = 0$ . Since  $\varepsilon_\alpha = \lim_{k \rightarrow \infty} \varepsilon_\alpha^{(k)}$ , the wavefunction is thus obtained from,

$$U(R) = \alpha(1 + \delta_\alpha^{(1)} + \delta_\alpha^{(2)} + \dots) + \beta(R + \delta_\beta^{(1)} + \delta_\beta^{(2)} + \dots). \quad (12.94)$$

This long-range expression must match the short-range value at a certain point  $R_0$ :

$$U(R_0) = \alpha \varepsilon_\alpha(R_0) + \beta \varepsilon_\beta(R_0). \quad (12.95)$$

$$U'(R_0) = \alpha \frac{d}{dR} \varepsilon_\alpha(R_0) + \beta \frac{d}{dR} \varepsilon_\beta(R_0)$$

and

$$a = -\frac{\beta}{\alpha} = \frac{U(R_0) \frac{d}{dR} \varepsilon_\alpha(R_0) - U'(R_0) \varepsilon_\alpha(R_0)}{U(R_0) \frac{d}{dR} \varepsilon_\beta(R_0) - U'(R_0) \varepsilon_\beta(R_0)} = \frac{\frac{d}{dR} \frac{\varepsilon_\alpha(R_0)}{U(R_0)}}{\frac{d}{dR} \frac{\varepsilon_\beta(R_0)}{U(R_0)}}. \quad (12.96)$$

Let us consider a specific potential,

$$V(R) = \frac{1}{2} B R^{m_r} e^{-\eta R} - \left( \frac{C_6}{R^6} + \frac{C_8}{R^8} + \frac{C_{10}}{R^{10}} \right) f_c(R) \quad (12.97)$$

$$f_c(R) = \theta(R_c - R) e^{-(R_c/R-1)^2} + \theta(R - R_c).$$

At very long range we have  $V(R) \simeq -\frac{C_6}{R^6}$ , such that,

$$\begin{aligned} \delta_\gamma^{(k+1)} &= \int_0^R 2m_r V \delta_\gamma^{(k+1)} dR = \delta_\gamma^{(k)}(\infty) - \int_R^\infty -\frac{2m_r C_6}{R^6} \delta_\gamma^{(k)} dR \\ &= 2m_r C_6 \int_R^\infty \frac{\delta_\gamma^{(k)}}{R^6} dR. \end{aligned} \quad (12.98)$$

In particular,

$$\begin{aligned} \delta_\alpha^{(1)} &= 2m_r C_6 \frac{-1}{4R^4}, & \delta_\alpha^{(2)} &= (2m_r C_6)^2 \frac{-1}{4 \cdot 9R^9} \\ \delta_\beta^{(1)} &= 2m_r C_6 \frac{1}{5R^5}, & \delta_\beta^{(2)} &= (2m_r C_6)^2 \frac{1}{5 \cdot 10R^{10}}. \end{aligned} \quad (12.99)$$

### 12.1.4.6 Third method

To estimate the scattering length for a particular interaction consult [455, ?, 532]. Following [455] we write the Schrödinger equation in atomic units as,

$$\frac{d^2U}{dR^2} = 2m_r V(R)U(R). \quad (12.100)$$

The ansatz  $U(R) = \alpha\varepsilon_\alpha(R) + \beta\varepsilon_\beta(R)$  with  $\varepsilon_\alpha(R \rightarrow \infty) = R$  and  $\varepsilon_\beta(R \rightarrow \infty) = 1$  shows that  $a = -\beta/\alpha$  is the desired scattering length.

### 12.1.4.7 Fourth method

The equation for the accumulated phase follows from the Schrödinger equation,

$$\begin{aligned} \phi(r_0) &\equiv \int_{\infty}^{r_0} k(r) dr & (12.101) \\ k^2(r) &= \frac{2m_r}{\hbar^2} \sqrt{E - V(r) - \frac{\hbar^2 l(l+1)}{2m_r r^2}}. \end{aligned}$$

According to [532] we start resolving,

$$\frac{d}{dR} \delta_{k,0}(R) = -k^{-1} V(R) \sin^2[kR + \delta_{k,0}(R)]. \quad (12.102)$$

### 12.1.4.8 Pseudo potentials

As in the low-energy limit ( $k \rightarrow 0$ ) the scattering properties only depend on the asymptotic phase shift it is a good idea to search for the simplest mathematical form that generates this asymptotic behavior. The situation is similar to the case of electrostatics, where a spherically symmetric charge distribution generates the same far field as a properly chosen point charge in its center. Not surprisingly, the suitable mathematical form is a point interaction. It is known as the pseudo potential and serves as an important theoretical Ansatz at the two-body level for the description of interacting many-body systems [234, 346]. The existence of such pseudo potentials is not surprising in view of the zero-range square well solutions discussed in Sec. 12.5.2.

As the pseudo potential cannot be obtained at the level of the radial wave equation, we return to the full 3D Schrödinger equation for a pair of free atoms,

$$(\nabla^2 + k^2)\psi_k(r) = 0, \quad (12.103)$$

where  $k = \sqrt{2m_r E/\hbar^2}$  is the wavenumber for the relative motion. Restricting ourselves to  $s$ -wave collisions we derived earlier the solution of this equation as being given by  $\psi_k(r) = \frac{c_0}{kr} \sin kr$ . However, we are now looking a solution of the type (12.37), which includes a phase shift  $\eta_0$ ,

$$\psi_k(r) = \frac{c_0}{kr} \sin(kr + \eta_0). \quad (12.104)$$

Inserting this expression into the wave equation (12.103) we encounter the problem that the solution is irregular in the origin when  $\eta_0 \neq 0$ . Apparently, we need to complement the wave equation by a (pseudo-)potential to remove this problem.

Our claim is now that the operator,

$$-\frac{4\pi}{k \cot \eta_0} \delta^3(\mathbf{r}) \frac{\partial}{\partial r} r \quad (12.105)$$

is the wanted *s*-wave *pseudo potential*  $\tilde{V}(r)$ . That is, the wave equation,

$$\left( \nabla^2 + k^2 + \frac{4\pi}{k \cot \eta_0} \delta^3(\mathbf{r}) \frac{\partial}{\partial r} r \right) \psi_k(r) = 0 \quad (12.106)$$

lets the phase-shifted wavefunction (12.104) be regular at the origin.

The presence of the delta function makes the pseudo-potential act as a boundary condition at  $r = 0$ ,

$$\begin{aligned} \frac{4\pi \delta^3(\mathbf{r})}{k \cot \eta_0} \left[ \frac{\partial}{\partial r} r \psi_k(r) \right]_{r=r_0} &= 4\pi \delta^3(\mathbf{r}) \frac{c_0}{k} \sin \eta_0 \\ &= -4\pi \delta^3(\mathbf{r}) \frac{c_0}{k} \sin(ka) \underset{k \rightarrow 0}{\simeq} -4\pi a c_0 \delta^3(\mathbf{r}), \end{aligned} \quad (12.107)$$

where we used the expression for the *s*-wave phase shift,  $\eta_0 = -ka$ . This is the alternative boundary condition we were looking for. Substituting this into Eq. (12.106) we obtain the inhomogeneous equation

$$(\nabla^2 + k^2) \psi_k(r) \underset{k \rightarrow 0}{\simeq} -4\pi a c_0 \delta^3(\mathbf{r}). \quad (12.108)$$

This inhomogeneous equation has the solution (12.104), as demonstrated in Exc. 12.1.5.4.

For functions  $f(\mathbf{r})$  with regular behavior in the origin we have <sup>4</sup>,

$$\left[ \frac{\partial}{\partial r} r f(\mathbf{r}) \right]_{r=0} = f(\mathbf{0}) + r \left[ \frac{\partial}{\partial r} f(\mathbf{r}) \right]_{r=0} = f(\mathbf{0}), \quad (12.109)$$

and the pseudo potential takes the form of a delta function potential <sup>5</sup>,

$$\tilde{V}(r) = -\frac{4\pi}{k \cot \eta_0} \delta^3(\mathbf{r}) \underset{k \rightarrow 0}{\simeq} 4\pi a \delta^3(\mathbf{r}), \quad (12.110)$$

or, equivalently, restoring the dimensions,

$$V(r) = \frac{g}{2} \delta^3(\mathbf{r}) \quad \text{with} \quad g = \frac{4\pi \hbar^2}{m_r}. \quad (12.111)$$

<sup>4</sup>Note that the wavefunction  $\psi_k$  is irregular,

$$\delta^3(\mathbf{r}) \frac{\partial}{\partial r} [r \psi_k(r)] = \delta^3(\mathbf{r}) \frac{\partial}{\partial r} \left( r \frac{c_0 \sin(kr + \eta_0)}{kr} \right) = \delta^3(\mathbf{r}) c_0 \cos[k(r - a)] \underset{k \rightarrow 0}{=} c_0 \delta^3(\mathbf{r}).$$

On the other hand,

$$\delta^3(\mathbf{r}) \frac{\partial}{\partial r} [r \psi_k(r)] = \delta^3(\mathbf{r}) \frac{c_0 \sin(kr + \eta_0)}{kr} = \delta^3(\mathbf{r}) \frac{c_0 \sin[k(r - a)]}{kr} \underset{k \rightarrow 0}{=} c_0 \delta^{(3)}(\mathbf{r}) \left[ 1 - \frac{a}{r} \right].$$

<sup>5</sup>Note that the dependence on the relative position vector  $\mathbf{r}$  rather than its modulus  $r$  is purely formal as the delta function restricts the integration to only zero-length vectors. This notation is used to indicate that normalization involves a 3-dimensional integration,  $\int \delta^3(\mathbf{r}) d^3r$ . Pseudo potentials do not carry physical significance but are mathematical constructions that can be chosen such that they provide wavefunctions with the proper phase shift.



This expression, for  $na^3 \ll 1$  valid in the zero energy limit, is convenient for calculating the interaction energy, as will be shown in Sec. ??.

### 12.1.4.9 Coupling of potentials

When molecular potentials cross and couple via collisions, via radiative coupling, or via a Feshbach resonance (cf. Sec. 12.4.2), new adiabatic potentials are formed. These are obtained as the  $r$ -dependent eigenvalues of the coupling Hamiltonian,

$$\hat{H}_{cpl} = \begin{pmatrix} V_1(R) & \Omega \\ \Omega & V_2(R) \end{pmatrix}. \quad (12.112)$$

Such calculations are known as *coupled channels* calculations.

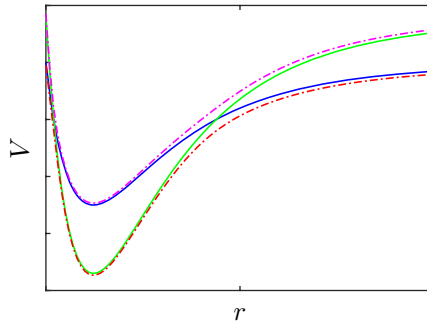


Figure 12.13: (code) The coupling of molecular potentials (solid lines) generates new adiabatic potentials (dash-dotted lines).

## 12.1.5 Exercises

### 12.1.5.1 Ex: Asymptotic radial function for hard-sphere potentials

Using asymptotic expressions for the Bessel and von Neumann functions derive the radial function  $R_\ell(k, r)$  for the two limiting cases  $ka \ll 1$  and  $ka \gg 1$ .

### 12.1.5.2 Ex: $s$ -wave collision on flat bottom potentials

Simplify the scattering matrix (12.35) for the collisional flat bottom potential for the case of  $s$ -wave collisions.

### 12.1.5.3 Ex: Equivalence of boundary conditions

Show that the radial wavefunction  $R_\ell$  and  $u_\ell$  satisfy equivalent boundary conditions at the surface of the spherical box potential.

### 12.1.5.4 Ex: Derivation of a linear expansion

Derive the linear expansion (12.67).

### 12.1.5.5 Ex: Pseudo-potential for $s$ -wave scattering

Verify the equation  $(\nabla^2 + k^2)\psi_k(r) = 4\pi\delta^3(\mathbf{r})\frac{1}{k}\sin\eta_0$  by direct substitution of the solution (12.104) setting  $c_0 = 1$ .

## 12.2 Scattering theory

In this chapter we discuss scattering by time independent potentials satisfying  $rV(r \rightarrow \infty) \rightarrow 0$ , that is short-range potentials. Such a potential may have attractive regions supporting bound states with energy  $E < 0$ . Here, however, we only consider states  $E > 0$ . Since the potential is supposed independent of time,  $\partial_t \hat{H} = 0$ , we will focus on time-independent problems,

$$\hat{H}\psi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{r}) , \quad (12.113)$$

with  $\hat{H} = p^2/2m + V(\mathbf{r})$  and  $E_{\mathbf{k}} = \hbar^2 k^2/2m$ . The boundary conditions are given by the scattering geometry in such a way that at long distances the wavefunction behaves as (see Fig. 12.14),

$$\psi_{\mathbf{k}}(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + f_k(\Omega)\frac{e^{ik_s r}}{r} . \quad (12.114)$$

For elastic scattering processes we have  $k_s = k$ . The *scattering amplitude*  $f_k(\Omega)$  depends on the energy  $E_k$  and on the scattering solid angle. Experimentally, we scatter individual particles described by wave packets. Since the scattering theory is linear, we can describe the packets by superpositions of stationary solutions  $\psi_{\mathbf{k}}$ <sup>6</sup>.

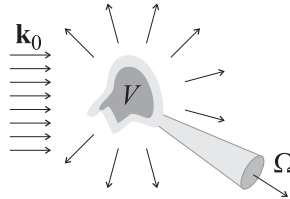


Figure 12.14: Scattering of incident light (wavevector  $\mathbf{k}_0$ ) by a potential  $V$ .

### 12.2.1 Lippmann-Schwinger equation

In order to consider the example of two particles involved in a collision we may go into the center-of-mass system (using reduced masses), fix the origin of the coordinate system on one of the particles, and analyze the trajectory of the second particle inside the interaction potential.

The scattering theory is based on *Green's method*, which we already know from electrostatics. So, let us start of a brief reminder of the use of the *Green's function* as a method to solve electrostatic problems.

<sup>6</sup>Note that  $\mathbf{k}$  is not a quantum number, since  $\psi_{\mathbf{k}}$  contains momentum components  $\neq \mathbf{k}$ .

**Example 55 (Green's method in electrostatics):** From Maxwell's third equation we obtain,

$$\nabla^2 \phi(\mathbf{r}) = -\varepsilon_0^{-1} \rho(\mathbf{r}) .$$

Being defined by,

$$\nabla^2 G(\mathbf{r}) = \delta^3(\mathbf{r}) ,$$

the Green function is,

$$G(\mathbf{r}) = \frac{-1}{4\pi} \frac{1}{|\mathbf{r}|} .$$

With this, we find the solution of the Maxwell equation,

$$\phi(\mathbf{r}) = (-G \star \varepsilon_0^{-1} \rho)(\mathbf{r}) = -\frac{1}{\varepsilon_0} \int_V \rho(\mathbf{r}_0) G(\mathbf{r}-\mathbf{r}_0) d^3 \mathbf{r}_0 = \frac{1}{4\pi \varepsilon_0} \int_V \frac{\rho(\mathbf{x})}{|\mathbf{r}-\mathbf{x}|} d^3 \mathbf{x} ,$$

known as *Poisson's law*.

### 12.2.1.1 Green's method in quantum mechanics

Green's method can be used to solve Schrödinger's equation with the boundary condition (12.114). We start from the reduced stationary Schrödinger equation (12.113) [678],

$$(\Delta + k^2) \psi_{\mathbf{k}}(\mathbf{r}) = \frac{2m}{\hbar^2} V(\mathbf{r}) \psi_{\mathbf{k}}(\mathbf{r}) . \quad (12.115)$$

This equation is not a common eigenvalue problem, since any energy  $E_k$  generates a solution. The equation (12.115) is a partial inhomogeneous differential equation with the left side describing free propagation and the right side describing a source that depends on the solution. Such differential equations are usually solved using Green's functions. We choose a point source and we solve,

$$(\Delta + k^2) G(\mathbf{r}, k) = \delta^3(\mathbf{r}) , \quad (12.116)$$

along with the boundary conditions. The solution takes the form [77],

$$G(\mathbf{r}, k) = -\frac{1}{4\pi} \frac{e^{ik|\mathbf{r}|}}{|\mathbf{r}|} , \quad (12.117)$$

such that,

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + (G \star \frac{2m}{\hbar^2} V \psi_{\mathbf{k}})(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{2m}{\hbar^2} \int_V d^3 \mathbf{r}' G(\mathbf{r}-\mathbf{r}', k) V(\mathbf{r}') \psi_{\mathbf{k}}(\mathbf{r}')} . \quad (12.118)$$

The equation (12.118) is called *Lippmann-Schwinger equation*. Of course, this equation does not solve, but only reformulate the problem taking into account the boundary conditions. It is more appropriate for an implementation of approximations. See Exc. 12.2.7.1 and 12.2.7.2.

Now let us consider the far field,  $r \rightarrow \infty$ , to verify the asymptotic behavior and find an expression for  $f_k(\Omega)$  as a function of  $V(\mathbf{r})$ . For  $r \rightarrow \infty$  we can approximate

$$k|\mathbf{r}-\mathbf{r}'| = kr \sqrt{(\hat{\mathbf{e}}_r - \mathbf{r}'/r)^2} = kr \sqrt{1 - 2\hat{\mathbf{e}}_r \cdot \mathbf{r}'/r + (r'/r)^2} \simeq kr - \mathbf{k}' \cdot \mathbf{r}' \simeq kr , \quad (12.119)$$

with  $\mathbf{k}' \equiv k\hat{\mathbf{e}}_r$ . With this the Lippmann-Schwinger equation (12.118) becomes,

$$\begin{aligned}\psi(\mathbf{r}) &\rightarrow e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{\hbar^2} \int_V \frac{1}{4\pi} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}')\psi(\mathbf{r}')d^3\mathbf{r}' \\ &= e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2} \frac{e^{ikr}}{kr} \int_V e^{-i\mathbf{k}'\cdot\mathbf{r}'} V(\mathbf{r}')\psi(\mathbf{r}')d^3\mathbf{r}' \equiv \psi_{in} + f_k(\Omega) \frac{e^{ikr}}{r},\end{aligned}\quad (12.120)$$

giving, in comparison with the expression (12.114), the *scattering amplitude*,

$$f_k(\Omega) = \frac{2m}{4\pi\hbar^2} \int_V e^{-i\mathbf{k}'\cdot\mathbf{r}'} V(\mathbf{r}')\psi(\mathbf{r}')d^3\mathbf{r}'. \quad (12.121)$$

Starting from the wavefunctions  $\psi_{in} \equiv e^{i\mathbf{k}\cdot\mathbf{r}}$  and  $\psi_s \equiv f_k(\Omega)e^{ikr}/r$  we can calculate the current densities,

$$\begin{aligned}\mathbf{J}_{in} &= \frac{\hbar}{2mi} (\psi_{in}^\dagger \nabla \psi_{in} - c.c.) = \frac{\hbar\mathbf{k}}{m} \\ \mathbf{J}_s &= \frac{\hbar}{2mi} (\psi_s^\dagger \partial_r \psi_s - c.c.) \hat{\mathbf{e}}_r = \frac{\hbar\mathbf{k}'}{m} \frac{1}{r^2} |f_k(\Omega)|^2 + \mathcal{O}(r^{-3}).\end{aligned}\quad (12.122)$$

The number  $dI(\Omega)$  of particles scattered per second into the solid angle  $d\Omega$  is simply  $dI(\Omega) = |\mathbf{J}_s| r^2 d\Omega$ . With this we can calculate the *differential effective cross section* defined by the ratio between  $dI(\Omega)$  and the number  $|\mathbf{J}_{in}|$  of incident particles per second,

$$\boxed{\frac{d\sigma}{d\Omega} \equiv \frac{dI(\Omega)}{|\mathbf{J}_{in}|d\Omega} = |f_k(\Omega)|^2}. \quad (12.123)$$

Finally we define the *total effective cross section*,

$$\sigma = \int d\Omega |f_k(\Omega)|^2. \quad (12.124)$$

## 12.2.2 Wave packets

We now let a *wave packet* defined at a time  $t = t_0$ ,

$$\psi(\mathbf{r}, t_0) = \int \frac{d^3k}{(2\pi)^3} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (12.125)$$

impinge on a scattering potential. The amplitude  $a_{\mathbf{k}}$  be concentrated around  $\mathbf{k}_0$ , such that the wave packet approaches the scatterer with the velocity  $\mathbf{v}_0 = \hbar\mathbf{k}_0/m$ . The time evolution of the wavefunction  $\psi(\mathbf{r}, t)$  determines the signal measured by a detector at a later time  $t = t_0$ . Our task is to determine  $\psi(\mathbf{r}, t > t_0)$ . The scattered states  $\psi_{\mathbf{k}}$  solving the Schrödinger equation (12.113) are complete in the space of the extended wavefunctions, and we can write the temporal evolution as,

$$\psi(\mathbf{r}, t) = \int \frac{d^3k}{(2\pi)^3} A_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}) e^{-iE_{\mathbf{k}}(t-t_0)/\hbar}. \quad (12.126)$$

At time  $t_0$  the results (12.125) and (12.126) must match. To verify this, we write (12.125) replacing the plane wave  $e^{i\mathbf{k}\cdot\mathbf{r}}$  using the Lippmann-Schwinger equation (12.118) with Green's function (12.117), and then we compare the coefficients,

$$\psi(\mathbf{r}, t_0) = \int \frac{d^3k}{(2\pi)^3} a_{\mathbf{k}} \left[ \psi_{\mathbf{k}}(\mathbf{r}) + \frac{m}{2\pi\hbar^2} \int d^3r' \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') \psi_{\mathbf{k}}(\mathbf{r}') \right]. \quad (12.127)$$

The scattering process is illustrated in Fig. 12.15. To simplify the calculation of

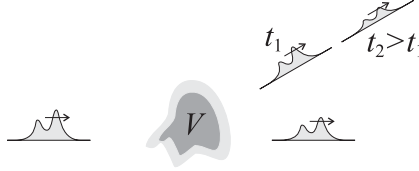


Figure 12.15: Scattering of wave packet at a potential.

the second term in this equation, we assume that  $\psi_{\mathbf{k}}$  is smooth, that is, there are no resonances, such that we can approximate,  $\psi_{\mathbf{k}} \simeq \psi_{\mathbf{k}_0}$ . With  $k \simeq \mathbf{k} \cdot \hat{\mathbf{e}}_{\mathbf{k}_0}$  we obtain,

$$\begin{aligned} \int \frac{d^3k}{(2\pi)^3} a_{\mathbf{k}} e^{ik|\mathbf{r}-\mathbf{r}'|} \psi_{\mathbf{k}}(\mathbf{r}') &= \int \frac{d^3k}{(2\pi)^3} a_{\mathbf{k}} e^{i\mathbf{k} \cdot (\hat{\mathbf{e}}_{\mathbf{k}_0} |\mathbf{r}-\mathbf{r}'|)} \psi_{\mathbf{k}_0}(\mathbf{r}') \\ &\stackrel{(12.125)}{=} \psi(\hat{\mathbf{e}}_{\mathbf{k}_0} |\mathbf{r}-\mathbf{r}'|, t_0) \psi_{\mathbf{k}_0}(\mathbf{r}'). \end{aligned} \quad (12.128)$$

Here,  $\psi(\hat{\mathbf{e}}_{\mathbf{k}_0} |\mathbf{r}-\mathbf{r}'|, t_0)$  is the incident wave package evaluated to the right, where by definition it is  $\simeq 0$ . The expression (12.127) therefore has the form,

$$\psi(\mathbf{r}, t_0) = \int \frac{d^3k}{(2\pi)^3} a_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}), \quad (12.129)$$

and a comparison of the coefficients with (12.126) gives,  $A_{\mathbf{k}} = a_{\mathbf{k}}$ . Finally, we evaluate  $\psi(\mathbf{r}, t)$  at the time of detection  $t > t_0$  to understand, that the above stationary analysis is actually physically correct. According to (12.126) we have,

$$\begin{aligned} \psi(\mathbf{r}, t) &= \int \frac{d^3k}{(2\pi)^3} A_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}) e^{-iE_{\mathbf{k}}(t-t_0)/\hbar} \\ &\stackrel{(12.120)(12.125)}{\simeq} \psi_0(\mathbf{r}, t) + \int \frac{d^3k}{(2\pi)^3} a_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{r} f_{\mathbf{k}}(\Omega) e^{-iE_{\mathbf{k}}(t-t_0)/\hbar}. \end{aligned} \quad (12.130)$$

Hence,  $\psi_0(\mathbf{r}, t)$  describes the evolution of the wave packet without scatterer,

$$\psi_0(\mathbf{r}, t) = \underbrace{\int \frac{d^3k}{(2\pi)^3} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} e^{-iE_{\mathbf{k}}(t-t_0)/\hbar}}_{\psi(\mathbf{r}, t_0)}. \quad (12.131)$$

If  $f_{\mathbf{k}}$  it's smooth around  $\mathbf{k} = \mathbf{k}_0$ , which allows us to place this amplitude ( $f_{\mathbf{k}} \simeq f_{\mathbf{k}_0}$ ) in front of the integral, and with  $k \simeq \mathbf{k} \cdot \hat{\mathbf{k}}_0$  we obtain,

$$\psi(\mathbf{r}, t) \stackrel{t \text{ large}}{\simeq} \underbrace{\psi_0(\mathbf{r}, t)}_{\text{packet not scattered}} + \underbrace{\frac{f_{\mathbf{k}_0}(\Omega)}{r} \psi_0(\hat{\mathbf{k}}_0 r, t)}_{\text{packet scattered}}. \quad (12.132)$$

The scattering process is illustrated in Fig. 12.15: According to the last equation the scattering process involves the superposition of the non-scattered packet and a packet scattered in the direction  $\Omega$ . The latter involves the amplitude  $\Psi_0(\hat{k}_0 r, t)$  of a packet propagating in forward direction, which only needs to be evaluated at the right time and distance. This packet will then be multiplied with the amplitude describing the angular dependency  $f_{k_0}$ ; the angle, therefore, only appears through this amplitude and not in the wavefunction  $\psi_0$ . In two situations the above analysis can not be applied :

- when  $V$  is long-ranged, f.ex.,  $V = 1/r$ ,
- when the incident energy  $E_k$  is resonant.

### 12.2.3 Born approximation

The Lippmann-Schwinger equation suggests the following perturbative iteration called *Born series* [77],

$$\begin{aligned}\psi(\mathbf{r}) &= \psi_i(\mathbf{r}) + (G \star \frac{2m}{\hbar^2} V \psi)(\mathbf{r}) \\ &= \psi_i(\mathbf{r}) + \frac{2m}{\hbar^2} (G \star V \psi_i)(\mathbf{r}) + (\frac{2m}{\hbar^2})^2 [G \star V (G \star V \psi_i)](\mathbf{r}) \\ &= \psi_i(\mathbf{r}) + \frac{2m}{\hbar^2} \int_V G(\mathbf{r} - \mathbf{r}') V(\mathbf{r}') \psi_i(\mathbf{r}') d^3 \mathbf{r}' \\ &\quad + (\frac{2m}{\hbar^2})^2 \int_V G(\mathbf{r} - \mathbf{r}') V(\mathbf{r}') G(\mathbf{r} - \mathbf{r}'') V(\mathbf{r}'') \psi_i(\mathbf{r}'') d^3 \mathbf{r}' d^3 \mathbf{r}'' .\end{aligned}\tag{12.133}$$

In the so-called *Born approximation* we consider only the first perturbation order, and inserting a plane wave,  $\psi_i(\mathbf{r}) = e^{ikz}/(2\pi)^{3/2}$ , we obtain,

$$\psi(\mathbf{r}) = \frac{e^{ikz}}{(2\pi)^{3/2}} - \frac{m}{(2\pi)^{3/2} 2\pi \hbar^2} \int_V \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') e^{ikz'} d^3 \mathbf{r}' .\tag{12.134}$$

The asymptotic behavior  $r \gg r'$ , it follows with (12.119) using  $z' = \mathbf{r}' \cdot \hat{\mathbf{e}}_z$  and defining  $\mathbf{k}_s = k\hat{\mathbf{e}}_r$  e  $\mathbf{k}_i = k\hat{\mathbf{e}}_z$ ,

$$\begin{aligned}\psi(\mathbf{r}) &\simeq \frac{e^{ikz}}{(2\pi)^{3/2}} - \frac{m}{(2\pi)^{3/2} 2\pi \hbar^2} \int_V \frac{e^{ik(r-\mathbf{r}\cdot\mathbf{r}'/r)}}{r} V(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'} d^3 \mathbf{r}' \\ &= \frac{e^{ikz}}{(2\pi)^{3/2}} + \frac{m}{(2\pi)^{3/2} 2\pi \hbar^2} \frac{e^{ikr}}{r} \int_V V(\mathbf{r}') e^{i(\mathbf{k}_i - \mathbf{k}_s)\cdot\mathbf{r}'} d^3 \mathbf{r}' \\ &\equiv \frac{1}{(2\pi)^{3/2}} \left( e^{ikz} + \frac{e^{ikr}}{r} f(k_i, k_s) \right) ,\end{aligned}\tag{12.135}$$

with

$$f(k_i, k_s) \equiv \frac{m}{2\pi \hbar^2} \int_V V(\mathbf{r}') e^{i(\mathbf{k}_i - \mathbf{k}_s)\cdot\mathbf{r}'} d^3 \mathbf{r}' = -\frac{m}{2\pi \hbar^2} \langle k_s | \tilde{V} | k_i \rangle .$$

### 12.2.4 Spherical potentials

For spherically symmetric scattering potentials,  $V(\mathbf{r}) = V(r)$ , the Hamiltonian  $\hat{H} = p^2/2m + V(r)$  commutes with the rotation operators  $U_{\vec{\omega}} = e^{-i\vec{\omega}\cdot\mathbf{L}/\hbar}$  around any axis  $\hat{\mathbf{e}}_{\vec{\omega}}$ . Therefore, we can separate the angular problem and decompose the scattering problem following the irreducible representations of the rotation group. This *partial wave* decomposition can be written,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\ell=0}^{\infty} (2\ell + 1) i^{\ell} P_{\ell}(\cos\theta) R_{\ell}(r) , \quad (12.136)$$

where the factor  $(2\ell + 1)i^{\ell}$  is a convention facilitating the calculation later on. By inserting this separation ansatz for the radial and angular variables into the stationary Schrödinger equation (12.113), we obtain the radial Schrödinger equation,

$$\left[ \frac{\partial^2}{\partial r^2} - \frac{\ell(\ell + 1)}{r^2} + k^2 \right] r R_{\ell}(r) = \frac{2m}{\hbar^2} V(r) r R_{\ell}(r) , \quad (12.137)$$

where  $\psi_{\mathbf{k}}$  must satisfy the boundary conditions (12.114). Fortunately, we can also expand the incident wave by partial waves <sup>7</sup>,

$$e^{ikz} = e^{ir \cos\theta} = \sum_{\ell=0}^{\infty} (2\ell + 1) i^{\ell} j_{\ell}(kr) P_{\ell}(\cos\theta) . \quad (12.138)$$

We now use the result (12.138) to find the boundary conditions for the radial waves  $R_{\ell}$ . In the infinity we have  $rV(r) \xrightarrow{r \rightarrow \infty} 0$ . For this reason,

$$R_{\ell}(r) \xrightarrow{r \rightarrow \infty} \alpha_{\ell} [h_{\ell}^{(2)}(kr) + s_{\ell} h_{\ell}^{(1)}(kr)] , \quad (12.139)$$

where the Hankel functions  $h_{\ell}^{(1,2)}(kr) \sim e^{\pm i(\rho - (\ell+1)\pi/2)}$  describe, respectively, incident ( $h_{\ell}^{(2)}$ ) and outgoing ( $h_{\ell}^{(1)}$ ) spherical waves.

To determine the coefficients  $\alpha_{\ell}$  and  $s_{\ell}$  we note first that, without potential,  $V(r) = 0$ , the solution of the radial equation (12.137) is known,

$$R_{\ell}(r) = j_{\ell}(kr) = \frac{1}{2} [h_{\ell}^{(2)}(kr) + h_{\ell}^{(1)}(kr)] , \quad (12.140)$$

such that  $\alpha_{\ell} = \frac{1}{2}$  and  $s_{\ell} = 1$ . For  $V(r) \neq 0$  the incident wave  $h_{\ell}^{(2)}$  is the same, but not the incident  $h_{\ell}^{(1)}$ , which results in  $s_{\ell} \neq 1$ . However, particle number conservation requires that the number of particles entering the potential is equal to the number of particles coming out. That is, the total radial flow must be,

$$0 = j_r^{\ell}(r) = \frac{\hbar}{2im} [R_{\ell}^* \partial_r R_{\ell} - R_{\ell} \partial_r R_{\ell}^*] = \frac{\hbar}{4mkr^2} [|s_{\ell}|^2 - 1] , \quad (12.141)$$

<sup>7</sup>For the more general case of arbitrary vectors  $\mathbf{k} \in \mathbf{r}$ , we use the addition theorem for  $Y_{\ell m}$  and express  $P_{\ell}(\cos\theta)$  by spherical functions,

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^{\ell} j_{\ell}(kr) Y_{\ell m}^*(\Omega_{\mathbf{k}}) Y_{\ell m}(\Omega_{\mathbf{r}}) .$$

approximating  $2R_\ell \simeq \frac{e^{-i(kr+w_\ell)}}{kr} + s_\ell \frac{e^{i(kr+w_\ell)}}{kr}$ . Hence,  $|s_\ell| = 1$ , that is,

$$s_\ell = e^{2i\delta_\ell(k)}, \quad (12.142)$$

where  $\delta_\ell(k)$  is the *scattering phase*. The scattering phase determines the solution of the scattering problem, because it fixes the scattering amplitude: Evaluating the solution (12.136) in the asymptotic limit by the formula (12.138),

$$\begin{aligned} \psi_{\mathbf{k}}(\mathbf{r}) &\sim \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell P_\ell(\cos\theta) [h_\ell^{(2)}(kr) + e^{2i\delta_\ell} h_\ell^{(1)}(kr)] \\ &= e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell P_\ell(\cos\theta) [e^{2i\delta_\ell} - 1] h_\ell^{(1)}(kr) = e^{i\mathbf{k}\cdot\mathbf{r}} + f_k(\theta) \frac{e^{ikr}}{r}, \end{aligned} \quad (12.143)$$

we obtain the scattering amplitude in the form <sup>8</sup>

$$f_k(\theta) = \frac{1}{k} \sum_{\ell} (2\ell+1) P_\ell(\cos\theta) e^{i\delta_\ell} \sin\delta_\ell. \quad (12.144)$$

We call

$$\frac{e^{2i\delta_\ell} - 1}{2ik} = \frac{e^{i\delta_\ell} \sin\delta_\ell}{k} \equiv f_\ell \quad (12.145)$$

the *amplitude of the partial wave* [714, 100].

### 12.2.5 Scattering phase and length

In summary, we can, within the Born approximation, express the collisional state of any type of particles by isotropic potentials,

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f_k(\Omega). \quad (12.146)$$

The scattering cross section can be written,

$$\begin{aligned} \sigma &= \int d\Omega |f_{\mathbf{k}}(\Omega)|^2 = \frac{1}{k^2} \int d\Omega \left| \sum_{\ell} (2\ell+1) P_\ell(\cos\theta) \sin\delta_\ell \right|^2 \\ &= \frac{4\pi}{k^2} \sum_{\ell} (2\ell+1) \sin^2\delta_\ell = 4\pi \sum_{\ell} (2\ell+1) |f_\ell|^2. \end{aligned} \quad (12.147)$$

The quantity

$$\sigma_\ell = \frac{4\pi}{k^2} (2\ell+1) \sin^2\delta_\ell = \frac{4\pi}{k^2} (2\ell+1) |f_\ell|^2 \quad (12.148)$$

is called *effective partial cross section*. Obviously,  $\sigma_\ell \leq \frac{4\pi}{k^2} (2\ell+1)$  holds. The phase shift  $e^{2i\delta_\ell}$  has a simple physical interpretation: We consider the function,

$$\begin{aligned} e^{i\delta_\ell} j_\ell(kr + \delta_\ell) &= \frac{e^{i\delta_\ell}}{2} [h_\ell^{(2)}(kr + \delta_\ell) + h_\ell^{(1)}(kr + \delta_\ell)] \\ &\sim \frac{e^{i\delta_\ell}}{2} \left[ \frac{(-i)^\ell e^{i(kr+\delta_\ell)}}{kr + \delta_\ell} + \frac{(+i)^\ell e^{-i(kr+\delta_\ell)}}{kr + \delta_\ell} \right] \xrightarrow{kr \gg \delta_\ell} \frac{1}{2} [h_\ell^{(2)} + e^{2i\delta_\ell} h_\ell^{(1)}] \sim R_\ell. \end{aligned} \quad (12.149)$$

<sup>8</sup>Com  $h_\ell^{(1)} \sim (-i)^{\ell+1} \frac{e^{ikr}}{kr}$ .



Now comparing the case  $V = 0$  giving  $R_\ell(r) = j_\ell(kr)$  with the case  $V \neq 0$  giving  $R_\ell(r) \sim e^{i\delta_\ell} j_\ell(kr + \delta_\ell)$ , we notice that a positive displacement,  $\delta_\ell > 0$ , pulls the wavefunction into the potential, while a negative displacement,  $\delta_\ell < 0$ , pushes the wavefunction out, as illustrated in Fig. 12.16.

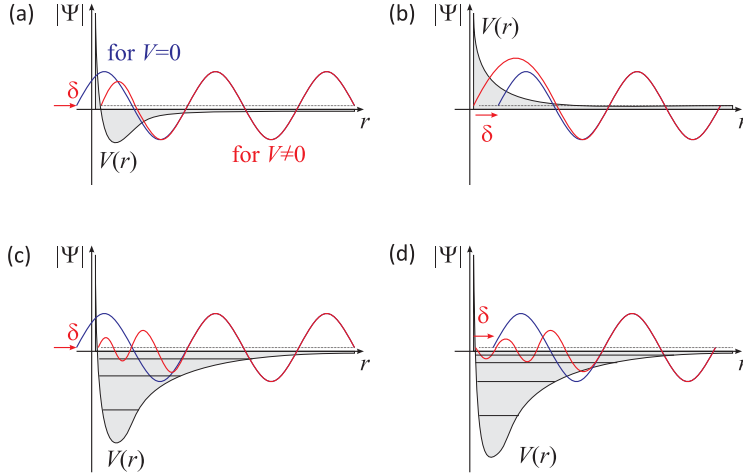


Figure 12.16: Phase shift  $\delta_\ell(k)$  of the scattered wavefunction. (a) An attractive potential increases the kinetic energy and the wavefunction oscillates faster, which causes a positive phase shift and a negative scattering length. (b) A repulsive potential slows down the wavefunction oscillation and produces a positive scattering length. (c,d) In an attractive potential deep enough to support vibrational states, the wavefunction performs several oscillations. The sign of the scattering length then depends on the distance of the last bound state to the continuum.

## 12.2.6 Optical theorem

Consider the amplitude for forward scattering  $f(0)$  by writing its imaginary part as,

$$\text{Im } f(0) = \frac{1}{k} \sum_k (2\ell + 1) P_\ell(\cos \theta) \sin^2 \delta_\ell \Big|_{\theta=0} = \frac{1}{k} \sum_k (2\ell + 1) \sin^2 \delta_\ell \equiv \frac{k}{4\pi} \sigma. \quad (12.150)$$

With this we obtain the *optical theorem*,

$$\boxed{\sigma = \frac{4\pi}{k} \text{Im } f(0)}. \quad (12.151)$$

The deeper meaning of the optical theorem is the conservation of particle number: The flux of scattered particles,  $(\hbar k/m)\sigma = I_{sct}$ , must be extracted from the incident flux  $I_0$  by scattering, and therefore, is missing in the forward direction. It is the interference of the scattered wave with the incident wave, which diminishes the non-scattered wave and therefore creates a shadow of the scatterer in the forward direction. The particles missing in the shadow of the scatterer are precisely those that have been scattered. This is the message of the optical theorem, which is always valid in the absence of possible (inelastic) processes leading to trapping or a transformation of the particles.

Table 12.1: List of scattering length for various alkaline species.

Element	$a_s^{mixed}$ [ $a_B$ ]	$a_s^{triplet}$ [ $a_B$ ]	$a_p^{triplet}$ [ $a_B$ ]	$B_{FB,s-wave}$ [ G ]	$B_{FB,p-wave}$ [ G ]
$^1\text{H}$		1.23			
$^2\text{H}$		-6.8			
$^6\text{Li}$			-35		160, 186, 215
$^7\text{Li}$	10	-27.3			
$^{23}\text{Na}$	52	85			
$^{39}\text{K}$	118	81.1			
$^{40}\text{K}$	158	1.7	-100	200	200
$^{41}\text{K}$	225	286			
$^{85}\text{Rb}$	-450	-363		156	
$^{87}\text{Rb}$	105	109.3		685.43, 911.74, 1007.34	
$^{133}\text{Cs}$	-240	-350			
$^{135}\text{Cs}$	163	138			

### 12.2.6.1 Born approximation for the scattering phase

The scattering problem can be considered as solved when we know the scattering amplitude  $f_k(\theta)$ , since this quantity gives us the flux measured by the detector. Now,  $f_k(\theta)$  is known, when we know the scattering phases  $\delta_{\ell,k}$ . These are, in general, determined by integrating the radial equation (12.137). Here, we expect that only angular momenta  $\ell < kR_0$  ( $R_0$  is the range of potential) produce significant phase shifts. Particles with larger angular momenta have collision parameters  $b \sim \ell/k$  out of the potential reach. We notice that partial  $s$ -waves are always scattered, whereas partial  $p$ -waves (or higher) are only weakly scattered when the energy is weak,  $E < \hbar^2/2mR_0^2$ . In these cases an approximate calculation of  $\delta_\ell$  is sufficient: We insert (12.136) and  $e^{ikz} = \sum_\ell \frac{1}{2} \sqrt{4\pi(2\ell+1)} \int_{-1}^1 dz P_\ell(z) e^{ikz}$  into (12.121) and integration over  $\Omega'$  yields,

$$\begin{aligned}
 f_k(\theta) &= \frac{2m}{4\pi\hbar^2} \int_V e^{-i\mathbf{k}' \cdot \mathbf{r}'} V(\mathbf{r}') \psi(\mathbf{r}') d^3\mathbf{r}' \\
 &= -\frac{2m}{\hbar^2} \sum_{\ell=0}^{\infty} (2\ell+1) P_\ell(\cos\theta) \int_0^{\infty} dr r^2 V(r) j_\ell(kr) R_\ell(r) .
 \end{aligned}
 \tag{12.152}$$

Comparing this formula with (12.144) we find,

$$e^{i\delta_\ell} \sin \delta_\ell = -\frac{2mk}{\hbar^2} \int_0^{\infty} dr r^2 V(r) j_\ell(kr) R_\ell(r) \stackrel{R_\ell \simeq j_\ell}{\simeq} -\frac{2mk}{\hbar^2} \int_0^{\infty} dr r^2 V(r) j_\ell^2(kr) .
 \tag{12.153}$$

The result (12.153) is the Born approximation for the scattering phase  $\delta_\ell(k)$ . Note that  $R_\ell \simeq j_\ell$  is not a good approximation, in ranges where  $V$  is large and  $R_\ell$  strongly suppressed (f.ex., inside hard cores). For  $\ell$  large we have  $j_\ell \sim r^\ell$ , and  $\delta_\ell$  is small for a limited potential  $V(r)$ .

### 12.2.6.2 Analyticity of $s_\ell(E)$

We consider a short-range potential that disappears at  $r > R_0$ . The radial solution out of the reach of the potential will then be given by,

$$R_\ell(r) = \frac{1}{2}[h_\ell^{(2)}(kr) + s_\ell h_\ell^{(1)}(kr)] , \quad (12.154)$$

while for  $r < R_0$  the solution  $R_\ell$  must be found by integrating the radial equation (12.137). The scattering phase  $s_\ell$  must be chosen in a way that  $R_\ell$  and  $\partial_r R_\ell$  be continuous at  $R_0$ . The normalization factor vanishes in the logarithmic derivative, such that,

$$\gamma_\ell \equiv \partial_r \ln R_\ell|_{R_0^-} = \frac{1}{R_\ell} \frac{\partial R_\ell}{\partial r} \Big|_{R_0^-} = \frac{\partial_r h_\ell^{(2)} + s_\ell \partial_r h_\ell^{(1)}}{h_\ell^{(2)} + s_\ell h_\ell^{(1)}} \Big|_{R_0^+} . \quad (12.155)$$

Now <sup>9</sup>

$$s_\ell - 1 = \frac{2(\partial_r - \gamma_\ell)j_\ell}{(\gamma_\ell - \partial_r)h_\ell^{(1)}} \Big|_{R_0} \quad (12.156)$$

or with  $s_\ell - 1 = \frac{2i}{\cot \delta_\ell - i}$  expressing  $\delta_\ell$  by  $\gamma_\ell$ ,

$$\cot \delta_\ell = \frac{(\partial_r - \gamma_\ell)n_\ell}{(\partial_r - \gamma_\ell)j_\ell} \Big|_{R_0} . \quad (12.157)$$

The partial effective cross section is,

$$\sigma_\ell = \frac{4\pi}{k^2} (2\ell + 1) \sin^2 \delta_\ell = \frac{4\pi}{k^2} \frac{2\ell + 1}{1 + \cot^2 \delta_\ell} . \quad (12.158)$$

Analyzing the expressions for  $s_\ell(\cot \delta_\ell)$  and  $\sigma_\ell(\cot \delta_\ell)$  we find that

- for  $\cos \delta_\ell = i$  the scattering phase  $s_\ell$  has a pole and  $\sigma_\ell \rightarrow \infty$ ;
- for  $\cos \delta_\ell = 0$  the scattering phase is  $s_\ell - 1$  and  $\sigma_\ell = 4\pi(2\ell + 1)/k^2$  is maximal.

The poles of  $s_\ell$  are just the bound states: A bound state asymptotically satisfies  $R_\ell(r) \sim h_\ell^{(1)}(i\kappa r) \propto e^{-\kappa r}$  with the binding energy  $E_B = -\hbar^2 \kappa^2 / 2m$ . The condition of continuity is given by,

$$\gamma_\ell = \frac{\partial_r h_\ell^{(1)}}{h_\ell^{(1)}} \Big|_{R_0} , \quad (12.159)$$

and the insertion into the general continuity condition (12.157) gives,

$$\cot \delta_\ell = \frac{h_\ell^{(1)} \partial_r n_\ell - n_\ell \partial_r h_\ell^{(1)}}{h_\ell^{(1)} \partial_r j_\ell - j_\ell \partial_r h_\ell^{(1)}} = i . \quad (12.160)$$

---

<sup>9</sup>We have for the spherical Hankel functions:  $h_\ell^{(1,2)}(x) = j_\ell(x) \pm iy_\ell(x)$ .

In the same way the zero crossings of  $\cot \delta_\ell$  correspond precisely to the scattering resonances. To see this, we expand around a resonance,

$$\cot \delta_\ell(E) \simeq \cot \delta_\ell(E_r) - \frac{1}{\sin^2 \delta_\ell} \left. \frac{d\delta_\ell}{dE} \right|_{E_r} (E - E_r) = - \left. \frac{d\delta_\ell}{dE} \right|_{E_r} (E - E_r) \equiv - \frac{2}{\Gamma_r} (E - E_r), \quad (12.161)$$

defining the width  $\Gamma_r = \frac{2}{\partial_E \delta_\ell} \Big|_{E_r}$  of the resonance peak in the effective section  $\sigma_\ell$  in the form,

$$\sigma_\ell = \frac{4\pi}{k^2} (2\ell + 1) \frac{(\Gamma_r/2)^2}{(E - E_r)^2 + (\Gamma_r/2)^2}. \quad (12.162)$$

See Fig. 12.17,

$$s_\ell - 1 = \frac{-i\Gamma_r}{E - (E_r - i\gamma_r/2)}. \quad (12.163)$$

The scattering phase  $\delta_\ell$  increases by  $\pi$ . The value  $\delta_\ell(E = 0)$  gives the number of bound states,  $\delta_\ell(0) = n_{\text{ligado}}^\ell \pi$ .

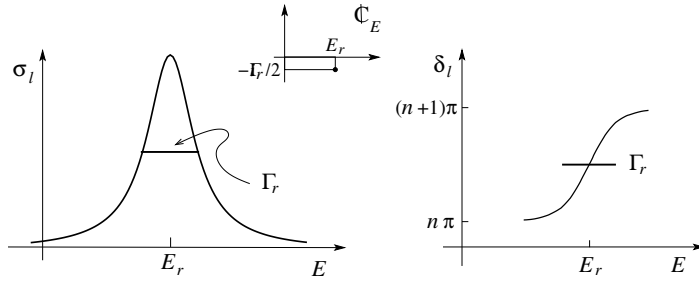


Figure 12.17: Peak of the resonance of width  $\Gamma_r$ : (Left) effective cross section  $\sigma_\ell(E)$ , (right) scattering phase  $\delta_\ell(E)$ , and (center) scheme of the position of the pole in the complex energy plane  $E$ .

## 12.2.7 Exercises

### 12.2.7.1 Ex: Green's method

Show that, knowing the solution of (12.116), that is, knowing the Green function, we can write the solution of the scattering problem (12.115) as,

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{2m}{\hbar^2} \int d^3\mathbf{r}' G(\mathbf{r} - \mathbf{r}', k) V(\mathbf{r}') \psi_{\mathbf{k}}(\mathbf{r}).$$

### 12.2.7.2 Ex: Green's function

Calculate the Green function of the equation (12.116).

### 12.2.7.3 Ex: Rutherford scattering

Consider the scattering of a particle of charge  $Q$  by a static charge distribution  $\rho(\mathbf{r}) = \rho_0 e^{-\alpha r}$  totaling the charge  $Q'$ . Derive from (12.136) the formula (1.10) describing the Rutherford scattering.

### 12.2.7.4 Ex: Scattering length for hard-core potentials

Calculate the scattering length for a spherical box barrier and a spherical box potential as a function of potential depth (see also Excs. 4.1.5.4 and 4.1.5.5 and [707]).

## 12.3 Cold atomic collisions

Modern techniques developed in the area of atomic optics allow to cool atomic gases to temperatures well below 1  $\mu\text{K}$ . We use the expansions  $j_\ell \sim x^\ell / (2\ell + 1)!!$  and  $n_\ell \sim (2\ell - 1)!! / x^{\ell+1}$  in the equation (12.157), and obtain for  $kR_0 \ll 1$ ,

$$\cos \delta_\ell \simeq \frac{2\ell + 1)!!(2\ell - 1)!!}{(kR_0)^{2\ell+1}} \frac{\ell + 1 + R_0\alpha_\ell(E)}{\ell - R_0\alpha_\ell(E)}. \quad (12.164)$$

A coarse approximation leads to

$$\cos \delta_\ell = \frac{\cos \delta_\ell}{\sin \delta_\ell} \stackrel{\delta_\ell \ll 1}{\simeq} \frac{1}{\sin \delta_\ell} \simeq \frac{1}{(R_0 k)^{2\ell+1}}, \quad (12.165)$$

that is,

$$\sin \delta_\ell \simeq (R_0 k)^{2\ell+1}. \quad (12.166)$$

In other words, the scattering phases decrease rapidly, in the regime of cold collisions, with increasing  $\ell$ , and  $\ell = 0$  type collisions dominate,

$$k \cot \delta_0 \stackrel{\alpha_\ell(E) \simeq \alpha_\ell(0)}{\simeq} \frac{1 + R_0\alpha_0(0)}{R_0^2\alpha_\ell(E)}. \quad (12.167)$$

The  $s$ -wave *scattering length* defined by,

$$a_s \equiv \frac{R_0^2\alpha_\ell(E)}{1 + R_0\alpha_0(0)} = \frac{\sin \delta_0}{k} \quad (12.168)$$

then it is the only relevant parameter of the collision. For  $R_0\alpha_0 \gg 1$  we find  $a \simeq R_0$ . For example, for a hard sphere we have  $R_\ell(R_0) = 0$ ,  $\alpha_\ell = \infty$ ,  $a = R_0 > 0$  and  $\cot \delta_0 = -1/kR_0$ . For small  $kR_0$  we obtain  $\delta_0 \simeq -kR_0 < 0$ , which corresponds to a negative phase shift for the repulsive potential, as expected. The effective cross section is,

$$\sigma_0 = \frac{4\pi}{k^2} \frac{1}{1 + \cot^2 \delta_0} \simeq \frac{4\pi}{k^2 + 1/a_s^2}. \quad (12.169)$$

In comparison to the effective cross section for higher angular momenta,  $\sigma_\ell \propto \frac{\sin^2 \delta_\ell}{k^2}$  behaves like,

$$\sigma_\ell \propto R_0^2 (R_0 k)^{4\ell} \rightarrow 0. \quad (12.170)$$

In contrast, we find that the scattering at low energies has an  $s$ -wave character,  $\sigma$  being dominated by  $\sigma_0$ ,

$$\sigma(E = 0) = 4\pi a_s^2. \quad (12.171)$$

For a hard sphere ( $a = R_0$ ) we find an effective cross section *four times larger* than classically expected ( $\sigma_{cl} = \pi R_0^2$ ).

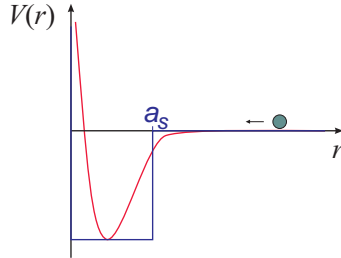


Figure 12.18: The cold collision can be described by a hard core potential.

In summary, for kinetic energies below the centrifugal barrier, only  $s$ -wave collisions are significant. The higher-order partial waves are *frozen* behind the centrifugal barrier. That is, the energy of cold collisions is not enough to excite a rotational motion, not even the one with the lowest rotational energy allowed by quantum mechanics. Such a collision is called *cold collision* or *s-wave collision*.

The relative wavefunction tends asymptotically to  $\psi(R) \xrightarrow{R \rightarrow \infty} k_{dB}^{-1} \sin[k_{dB}(R - a)] \xrightarrow{T \rightarrow 0} R - a$ . This means that for temperatures so low that the length of the Broglie wave of the relative motion is much longer than the potential range  $k_{dB}^{-1} \gg R_{turning}$ , the scattering becomes independent of temperature, and the scattering length  $a$  becomes well defined<sup>10</sup>

Generally, a repulsive interaction potential corresponds to a positive scattering length and an attractive potential to a negative one. However, if the attractive potential supports bound states, the value of the scattering length depends on the energy of the last bound state with respect to the dissociation threshold [707, 708].

### 12.3.1 Collision cross section, unitarity regime

Note that the scattering length  $a$  may have a value quite different from  $r_e$ , especially in the presence of a Feshbach resonance. The meaning of *universality*,  $|a| \gg r_e$ , is that short-range properties play no role in the dynamics.

At low temperatures,  $kr_e \rightarrow 0$ , we have the equation (12.169). In contrast, in the *unitarity limit*,  $k \rightarrow \infty$ , but  $r_e \rightarrow 0$ , we have,

$$\sigma = \frac{8\pi}{k^2}, \quad (12.172)$$

and the cross section becomes independent of atomic particularities. What the equation (12.169) says is, that the maximum attainable cross-section is limited to the

<sup>10</sup>At temperatures at which the trajectory of atoms is described by de Broglie waves the only difference between an atom before and after an elastic collision is the phase shift  $\delta_0$  of this wave.

smallest of the values  $8\pi a$  and  $8\pi/k$ . Even though  $a(B)$  can be increased to divergent values near a Feshbach resonance, for finite collision energies it will never exceed an effective value  $a_{eff} = 1/\sqrt{a^2 + 1/k^2}$ . For a thermal gas,  $k = \hbar^{-1}\sqrt{2\pi m k_B T}$ , while for a pure condensate  $k = 2\pi/L$ , where  $L$  is the size of the condensate. Therefore, the effective scattering length can not exceed the size of the condensate. Unitarity also means that the kinetic energy exceeds the binding energy,  $k_B T \equiv \frac{\hbar^2 k^2}{2m} \leq \frac{\hbar^2}{2ma^2}$ .

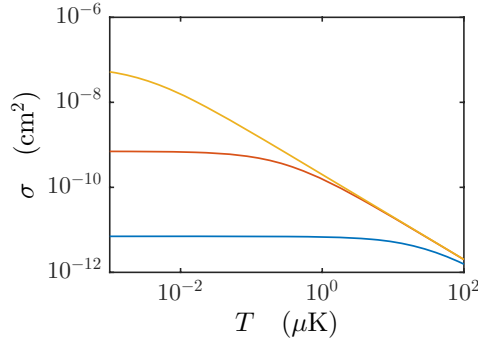


Figure 12.19: (code) Temperature dependence of the collision cross section for various scattering lengths. For higher scattering lengths, the unitarity limit is reached at lower temperatures.

The collision rate depends on the density, temperature and collisional cross section [389],

$$\gamma_{coll.peak} = \sqrt{2}\sigma_{elast}\bar{v}n_0, \quad (12.173)$$

$$\gamma_{coll.aver} = \gamma_{coll.peak}/2\sqrt{2}.$$

Note that at the unitary limit, as  $\bar{v} \propto \sqrt{T}$ , we have that  $\sigma_{elas} \propto T$  and  $n_0 \propto \bar{r}^{-3} \propto T^{-3/2}$ , such that the collision rate is independent of temperature.

At low temperatures,  $k \rightarrow 0$ , the delocalization of the colliding particles is greater than its short-range structure. This is the *Wigner threshold law* [721, 714]. For elastic collisions of neutral ground state atoms, the cross section (12.169) becomes temperature-independent. Thus, the rate coefficient decreases as  $\langle\sigma\bar{v}\rangle \propto \sqrt{T}$ , while the collision rate increases as  $\langle\sigma\bar{v}n_0\rangle \propto T^{-1}$ .

For inelastic collisions,  $\sigma \propto T^{-1}$ . For three-body collisions see [230].

### 12.3.2 Collisions between identical particles

We consider collisions of two identical particles. Separating the center-of-mass coordinates,  $\mathbf{R} = \mathbf{r}_1 + \mathbf{r}_2$ , from the relative ones,  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ , we see that  $\mathbf{R}$  is symmetric and  $\mathbf{r}$  antisymmetric in  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . We separate the wavefunction into orbital and spin parts,

$$\Psi(x_1, x_2) = e^{i\mathbf{P}\cdot\mathbf{R}}\psi(\mathbf{r})\chi(s_1, s_2). \quad (12.174)$$

For indistinguishable particles the result of the scattering has the asymptotic form,

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\frac{e^{ikr}}{r}. \quad (12.175)$$

12.3.2.1 Spin 0 bosons

For bosons with spin 0 we have  $\chi = 1$  and, because of the symmetry of  $\Psi$ , holds  $\psi(\mathbf{r}) = \psi(-\mathbf{r})$ . Consequently, we must symmetrize the result of the scattering. We make use of the fact that the exchange of particles via  $\mathbf{r} \rightarrow -\mathbf{r}$  in polar coordinates corresponds to the transformation  $\theta \rightarrow \pi - \theta$ ,  $r \rightarrow r$ ,

$$\psi \sim (e^{i\mathbf{k}\cdot\mathbf{r}} + e^{-i\mathbf{k}\cdot\mathbf{r}}) + [f(\theta) + f(\pi - \theta)] \frac{e^{ikr}}{r} . \quad (12.176)$$

For the effective differential cross section we obtain,

$$\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2 = |f(\theta)|^2 + |f(\pi - \theta)|^2 + 2\Re[f^*(\theta)f(\pi - \theta)] . \quad (12.177)$$

The first two terms are classical. The third (interference) term appears because of quantum statistics. The angles showing up in (12.177) are illustrated in Fig. 12.20. For bosons, the interference terms double the cross section as compared to the classical case, when  $\theta = \pi/2$ ,

$$\boxed{\frac{d\sigma}{d\Omega} = 4|f(\frac{\pi}{2})|^2} . \quad (12.178)$$

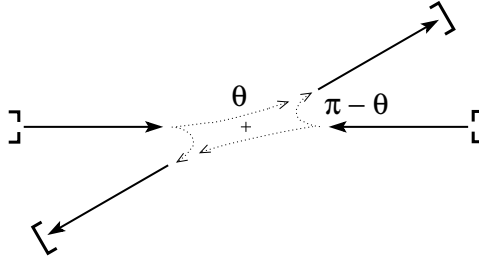


Figure 12.20: The symmetrization of the collision wavefunction produces two paths with angles  $\theta$  and  $\pi - \theta$ , which must be added coherently.

For the isotropic potential  $V(r)$  we use the partial wave representation,

$$f(\theta) = \sum_{\ell} i^{\ell} f_{\ell} P_{\ell}(\cos \theta) . \quad (12.179)$$

With  $P_{\ell}(\cos \theta) = (-1)^{\ell} P_{\ell}(\pi - \cos \theta)$  we get,

$$f(\theta) - f(\pi - \cos \theta) = 2 \sum_{\ell_{\text{par}}} i^{\ell} f_{\ell} P_{\ell}(\cos \theta) , \quad (12.180)$$

and we find that only *even angular momenta* appear <sup>11</sup>

<sup>11</sup>For  $\ell$  odd the Legendre polynomial changes sign, and the contributions vanish.



### 12.3.2.2 Spin 1/2 fermions

In the case of fermions with spin  $\frac{1}{2}$  two situations are possible <sup>12</sup>:

1. The singlet spin state  $\chi_s = \frac{1}{\sqrt{2}}[(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)]$  is antisymmetric and, consequently, the orbital part,

$$\psi(\mathbf{r}) = \psi(-\mathbf{r}) \quad (12.181)$$

must be symmetric. The cross section is the same as for spin 0 bosons,

$$\left. \frac{d\sigma}{d\Omega} \right|_s = |f(\theta) + f(\pi - \theta)|^2 . \quad (12.182)$$

2. The triplet spin states,

$$\chi_s = \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\downarrow\downarrow\rangle \end{cases} \quad (12.183)$$

require an antisymmetric orbital wavefunction,  $\psi(\mathbf{r}) = -\psi(-\mathbf{r})$ , and we obtain a scattering amplitude,  $f(\theta) \rightarrow f(\theta) - f(\pi - \theta)$ , which only contains *odd angular momenta*  $\ell$ . With this, the cross section becomes,

$$\left. \frac{d\sigma}{d\Omega} \right|_t = |f(\theta) - f(\pi - \theta)|^2 \stackrel{\theta=\pi/2}{=} 0 , \quad (12.184)$$

Note that polarized fermions only scatter in channels of odd angular momenta: cold bosonic atoms show a *contact potential* due to *s*-wave collisions (12.180), polarized fermionic atoms only interact weakly in the *p*-channel. In the case of a statistically mixed ensemble of non-polarized fermions we have a the weighted average,

$$\frac{d\sigma}{d\Omega} = \frac{3}{4} \left. \frac{d\sigma}{d\Omega} \right|_t + \frac{1}{4} \left. \frac{d\sigma}{d\Omega} \right|_s = |f(\theta)|^2 + |f(\pi - \theta)|^2 - \Re[f^*(\theta)f(\pi - \theta)] . \quad (12.185)$$

### 12.3.2.3 Molecular spectra

Here we consider rotational spectra of low energies  $E_{rot} = \hbar^2 \ell(\ell+1)/2\Theta \ll E_{electronico} \sim eV$ . In slow time scales we can consider the electronic shell to be rigid. We look at two examples of molecules with bosonic and fermionic nuclei:

- Molecules  $(C^{12})_2$ : the nuclei are 0-spin bosons, so only collisions with even  $\ell$  are allowed.
- Molecules  $H_2$ : the nuclei are spin- $\frac{1}{2}$  fermions, so we have for a spin wavefunction,

$$\chi = \chi_s : \ell = \text{even, para-hydrogen, } \chi = \chi_t : \ell = \text{odd, ortho-hydrogen.} \quad (12.186)$$

The transformation of ortho-hydrogen into para-hydrogen is difficult (the nuclei being well shielded), such that we observe two types of gases with,

$$E_{rot,para} = 0, \frac{3}{\Theta}, \frac{10}{\Theta}, \frac{21}{\Theta}, \dots E_{rot,orto} = \frac{1}{\Theta}, \frac{6}{\Theta}, \frac{15}{\Theta}, \dots \quad (12.187)$$

<sup>12</sup>This is analogous to the case of helium, where the spatial function of the state  $2s^2 \uparrow\uparrow$  is always antisymmetric, but for the  $2s \uparrow 2p \uparrow$  exist symmetric spatial orbitals.

### 12.3.3 Collisions between hot atoms

Angular moments with  $\ell \leq kR_0$  should contribute a lot to  $\sigma$ , since the collision parameter is inside  $R_0$ . For a hard sphere we have  $\alpha_\ell = \infty$  and  $\cot \delta_\ell = n_\ell(kR_0)/j_\ell(kR_0)$ . With the asymptotic expressions of  $j_\ell$  and  $n_\ell$  we obtain  $\cot \delta_\ell \sim -\cot(kR_0 - \ell\pi/2)$ , that is,  $\delta_\ell \sim kR_0 - \ell\pi/2 (+\pi)$ . With these scattering phases we can calculate the scattering cross section,

$$\sigma \simeq \frac{4\pi}{k^2} \sum_{\ell=0}^{kR_0} (2\ell + 1) \sin^2 \delta_\ell \quad (12.188)$$

$$\begin{aligned} &\simeq \frac{4\pi}{k^2} \sum_{\ell=0}^{kR_0} (\ell + 1) \cos^2[kR_0 - (\ell + 1)\pi/2] + \ell \sin^2(kR_0 - \ell\pi/2) \\ &= \frac{4\pi}{k^2} \sum_{\ell=0}^{kR_0} \ell(\cos^2 + \sin^2) = \frac{4\pi}{k^2} \frac{kR_0(kR_0 + 1)}{2} = 2\pi R_0^2, \end{aligned} \quad (12.189)$$

which is the double of the classical value.

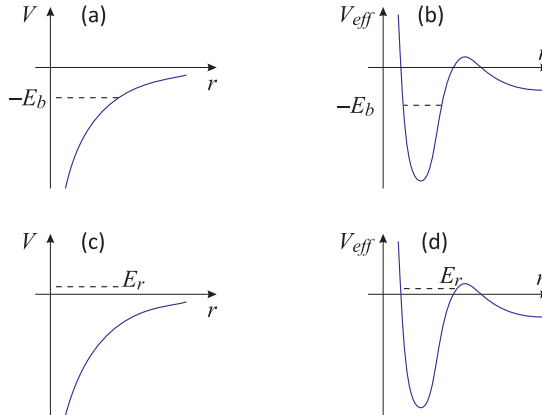


Figure 12.21: (a) Bound state for  $\ell = 0$ . (b) Bound state for  $\ell > 0$  in a potential including the centrifugal barrier  $\hbar^2 \ell(\ell + 1)/2mr^2$ . (c) Resonances for  $\ell = 0$  are broad and possibly not defined with  $\Gamma_r > E_r$ . A defined resonance with  $\Gamma_r < E_r$  requires that  $|\partial_E \alpha_0|$  be large. (d) For  $\ell > 0$  we obtain narrow resonances called *shape resonances*, because the decay of the state is suppressed by the centrifugal barrier.

### 12.3.4 Photoassociation during ultracold collisions

Ultra-cold collisions are an interesting example of how light can control the result of inelastic or reactive collisions. Here we discuss as a specific example the *photoassociation*, which illustrates the utility of the dressed states pictures. The upper panel of Fig. 12.22 shows schematic curves of (bare) potentials relevant to our discussion. Two atoms in the ground state form a relatively shallow molecular ground state char-

acterized by electrostatic dispersion

$$V_1(r) = -\frac{C_6}{R^6} . \quad (12.190)$$

or long-range *van der Waals potential*. Two other molecular states arise from the interaction of an excited atom with the ground state atom. The predominant term of the interaction is the potential of resonant dipole-dipole interactions,

$$V_{2,3}(r) = -\mp \frac{C_3}{R^3} . \quad (12.191)$$

which gives rise to an attractive and a repulsive potential. The  $R^{-3}$  dependence of the resonant dipole interaction means that the associated potentials greatly modify the asymptotic level even at internuclear distances where the ground state van der Waals potential is still relatively shallow. The photoassociation process involves a slow approach of two identical ground state atoms. A mono-modal optical field, tuned to the red of the atomic resonance, is applied. When the two atoms reach an internuclear distance  $R_C$  such that the energy of the applied field  $\hbar\omega_C$  exactly coincides with the potential difference  $V_2(R_C) - V_1(R_C)$ , the probability of transferring population from the fundamental molecular state to the excited molecular state is maximal. This molecular resonance is sometimes called *Condon point*. The conventional way of calculating this probability follows the procedure elaborated in Sec. 13.1 for a two-level atom. First, we would solve the time-independent molecular Schrödinger equation to obtain the molecular wavefunctions. Then, write down the coupled differential equations by describing the time dependence of the expansion coefficients of the relevant molecular wavefunctions, solve for the coefficients and calculate the square of their absolute values. Finally, we would need to integrate the transition probability inside a region  $\Delta R$  around the Condon point, where the transition probability is not be negligible. The dressed states picture allows to reduce this rather laborious program, essentially, to a problem of a curve crossing of two levels. The bottom panel of Fig. 12.22 illustrates the photoassociation in the dressed states picture. The basis states are now product states made up of the field and the molecular levels. Furthermore, we approximate the molecular states themselves as products of atomic states. This approximation is justified by the long range, weakly perturbative influence of the van der Waals and resonant dipoles interactions. Calling the ground and excited states  $|1\rangle$  and  $|2\rangle$ , respectively, we have

$$|1, n\rangle = |1||1\rangle|n\rangle , \quad (12.192)$$

and for the field-molecule excited state

$$|2, n-1\rangle = |2||1\rangle|n-1\rangle . \quad (12.193)$$

The two molecular curves intersect at the Condon point and optically couple to the applied field. This optical coupling produces an *avoided crossing* near  $R_C$  and mixes the states of the molecule-field basis. The well-known *Landau-Zener* formula (LZ) expresses the probability of traversing from one adiabatic molecular state to another as a function of the interaction strength, the relative velocity of the collision partners,

and the relative slopes of the two curves. The probability of LZ is given by,

$$\exp \frac{2\pi \langle 1, n | \frac{\Omega}{2} | 2, n-1 \rangle}{v \left| \frac{d}{dR} \Delta V_{12}(R_C) \right|}, \quad (12.194)$$

where  $v$  is the relative radial velocity of the approaching particles and  $\frac{d}{dR} \Delta V_{12}(R_C)$  is the difference of slopes of the two non-interacting potentials at the Condon point. The dipole-field interaction operator  $\Omega$  must be taken with the dipole of the molecular transition. A reasonable approximation is to take the moment of molecular transition as twice the atomic moment and average over the whole space. The result is,

$$\exp \frac{\frac{2\pi}{\sqrt{3}} \langle 1, n | \Omega_{at} | 2, n-1 \rangle}{v \left| \frac{d}{dR} \Delta V_{12}(R_C) \right|}, \quad (12.195)$$

where  $\Omega_{at}$  denotes the atomic operator of the dipole-field interaction. In the case of a crossing of an essentially flat potential  $V_1$  and  $V_2(R) = -\frac{C_3}{R^3}$ , the absolute value of the derivative of the slope difference is,

$$\left| \frac{d}{dR} \Delta V_{12}(R_C) \right| = \frac{3C_3}{R_C^3}. \quad (12.196)$$

Resolve Exc. [12.3.13.1](#).

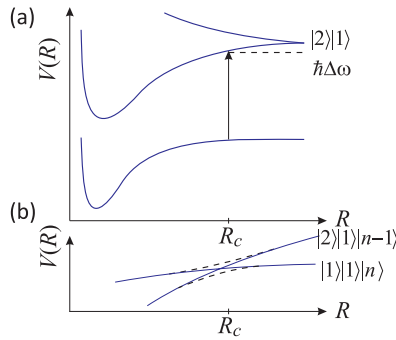


Figure 12.22: (Above) Molecular states resonantly coupled by a light field at the Condon point. (Below) Same coupling of the molecular states represented by an avoided intersection in the dressed states basis.

### 12.3.5 Ground state collisions

### 12.3.6 Hyperfine structure

We consider the scheme (11.90), we set  $\mathbf{l}_j = 0$ , and concentrate on  $s$ -waves,  $\ell = 0$ ,

$$\begin{aligned} \mathbf{s}_1 + \mathbf{s}_2 &= \mathbf{S} \xrightarrow{\hat{z}} \mathbf{\Omega} \\ + &+ + \\ \mathbf{i}_1 + \mathbf{i}_2 &= \mathbf{I} \\ = &= = \\ \mathbf{f}_1 + \mathbf{f}_2 &= \mathbf{f} \end{aligned} \quad (12.197)$$

At short distances the coupling  $((S, I)f_1, f_2)f$  breaks up and a  $((s_1, s_2)S, I)f$  coupling emerges. This does not hold for fully stretched spin states  $f_1 + f_2 = f$ , because  $f$  is a good quantum number at all distances (and small enough magnetic fields). In contrast  $m_f$  is a good quantum number at all distances and at all fields.

In order to obtain the potentials coupled by hyperfine interaction, we first calculate for a *single vibrational level* the relative wavefunctions  $|\psi_{(f_1, f_2)f}(R)\rangle$  from the known perturbed but uncoupled potentials  $V(R) + V_{hf}$ , where,

$$V_{hf} = ha_{hf,1}\mathbf{s}_1 \cdot \mathbf{i}_1 + ha_{hf,2}\mathbf{s}_2 \cdot \mathbf{i}_2 . \quad (12.198)$$

The antisymmetric part is negligible [698], so that  $V_{hf} \simeq \frac{1}{2}ha_{hf,1}\mathbf{S} \cdot \mathbf{i}_1 + \frac{1}{2}ha_{hf,2}\mathbf{S} \cdot \mathbf{i}_2$ . Then couple the channels via,

$$|\psi_{(S,I)f}(R)\rangle = A \sum_{f_1, f_2} \sqrt{\hat{S}\hat{I}\hat{f}_1\hat{f}_2} \begin{Bmatrix} s_1 & s_2 & S \\ i_1 & i_2 & I \\ f_1 & f_2 & f \end{Bmatrix} |\psi_{(f_1, f_2)f}(R)\rangle \quad (12.199)$$

$$|\psi_{(f_1, f_2)f}(R)\rangle = A^{-1} \sum_{S, I} \sqrt{\hat{S}\hat{I}\hat{f}_1\hat{f}_2} \begin{Bmatrix} s_1 & s_2 & S \\ i_1 & i_2 & I \\ f_1 & f_2 & f \end{Bmatrix} |\psi_{(S, I)f}(R)\rangle .$$

which satisfies the orthogonality relation (see Tables in 7.2).

### 12.3.7 Scattering length in specific channels

The scattering length in specific channels can be expressed via singlet and triplet scattering length,

$$a_{|f_1, m_{f_1}\rangle + |f_2, m_{f_2}\rangle} = P_{S=0}a_s + P_{S=1}a_t . \quad (12.200)$$

The projectors are  $P_S = |\langle S|(f_1 f_2)f\rangle|$ . According to [111] or [481] the recoupling from the uncoupled hyperfine representation into the short range representation is given by,

$$\langle Sm_S Im_I \ell' m_{\ell'} | f_1 m_{f_1} f_2 m_{f_2} \ell m_{\ell} \rangle = \delta_{\ell \ell'} \delta_{m_{\ell} m_{\ell}'} \sum_{f, m_f} \langle Sm_S Im_I | f m_f \rangle \langle f_1 m_{f_1} f_2 m_{f_2} | f m_f \rangle \times \quad (12.201)$$

$$\times \begin{Bmatrix} s_1 & s_2 & S \\ i_1 & i_2 & I \\ f_1 & f_2 & f \end{Bmatrix} \sqrt{\hat{S}\hat{I}\hat{f}_1\hat{f}_2} \left( \frac{1 - (1 - \delta_{f_1 f_2})(-1)^{S+I+\ell}}{\sqrt{2 - \delta_{f_1 f_2}}} \right) .$$

The last bracket is dropped for unsymmetrized recoupling. Calculations have been done for  $^{87}\text{Rb}$  collisions and for  $^6\text{Li}^{87}\text{Rb}$  collisions. It turns out that the fully stretched states have pure triplet character.

Note that in strong magnetic fields the coupling  $(i_1, i_2)I$  easily breaks up, and the recoupling to be considered is rather  $\langle Sm_S m_{i_1} m_{i_2} \ell' m_{\ell'} | f_1 m_{f_1} f_2 m_{f_2} \ell m_{\ell} \rangle$ .

### 12.3.8 Hyperfine coupling in magnetic fields

### 12.3.8.1 Zeeman splitting of bound states

The splitting of the bound state is described by [698],

$$\begin{aligned} H_{int}^+ &= V_{hf}^+ + V_{Zeeman} \\ &= E_B + \frac{1}{2}ha_{hf,1}\mathbf{S} \cdot \mathbf{i}_1 + \frac{1}{2}ha_{hf,2}\mathbf{S} \cdot \mathbf{i}_2 + \mu_B\mathbf{B}(g_S\mathbf{S} + g_1\mathbf{i}_1 + g_2\mathbf{i}_2) , \end{aligned} \quad (12.202)$$

such that,

$$\begin{aligned} &\langle m'_{i1}m'_{i2}m'_S | H_{hfs} + H_B | m_S m_{i2} m_{i1} \rangle \\ &= E_B + (g_S m_S + g_{i1} m_{i1} + g_{i2} m_{i2}) \mu_B B \delta_{m'_{i1} m_{i1}} \delta_{m'_{i2} m_{i2}} \delta_{m'_S m_S} \\ &+ \frac{1}{2}h(a_{hf,1} m_{i1} m_S + a_{hf,2} m_{i2} m_S) \delta_{m'_{i1} m_{i1}} \delta_{m'_{i2} m_{i2}} \delta_{m'_S m_S} \\ &+ \frac{1}{4}ha_{hf,1}(i_{1,+} S_- \delta_{m'_S m_S+1} \delta_{m'_{i1} m_{i1}-1} + i_{1,-} S_+ \delta_{m'_{i1} m_{i1}-1} \delta_{m'_S m_S+1}) \delta_{m'_{i2} m_{i2}} \\ &+ \frac{1}{4}ha_{hf,2}(i_{2,+} S_- \delta_{m'_S m_S+1} \delta_{m_{i2}-1} + i_{2,-} S_+ \delta_{m'_{i2} m_{i2}-1} \delta_{m'_S m_S+1}) \delta_{m'_{i1} m_{i1}} . \end{aligned} \quad (12.203)$$

For an example on how to evaluate the matrix at various magnetic fields and obtain the hyperfine structure of a bound state in the Zeeman and the Paschen-Back regime, we propose the systems  ${}^6\text{Li}^{23}\text{Na}$  and  ${}^6\text{Li}^{87}\text{Rb}$ .

### 12.3.8.2 Magnetic dipole interaction

Reads,

$$V_{dd} = \frac{\mu_0}{4\pi R^3} [\mu_1 \cdot \mu_1 - 3(\mu_2 \cdot \mathbf{R})(\mu_2 \cdot \mathbf{R})] \quad (12.204)$$

neglecting nuclear spin.

### 12.3.8.3 Second-order spin-orbit interaction

First-order spin-orbit interaction disappears for ground state collisions. But second-order spin-orbit interaction may occur. These lead to inelastic losses (see next section).

### 12.3.8.4 Selection rules

The selection rules for bosonic homonuclear collisions are,

$$\begin{aligned} S &= 0, \dots, s_1 + s_2 \\ I &= 0, \dots, i_1 + i_2 \\ f_j &= |i_j - s_j|, \dots, i_j + s_j \\ |I - S| &\leq F \leq I + S \\ |f_1 - f_2| &\leq F \leq f_1 + f_2 \\ (-1)^I &= (-1)^S \quad \text{for all } F \\ (-1)^{f_1} &= -(-1)^{f_2} \quad \text{for all odd } F . \end{aligned} \quad (12.205)$$

What does they look like for fermions? What does they look like for heteronuclear collisions?

### 12.3.9 Inelastic collisions

#### 12.3.9.1 Spin changing collisions

These have their origin in *spin exchange* and spin dipole-dipole processes. Spin exchange occurs when the colliding electronic clouds overlap. At short distances the  $((S, I)f_1, f_2)f$  breaks up and a  $((s_1, s_2)S, I)f$  coupling remixes, as shown in Exc. 11.3.5.1. Hence, collisions between atoms  $|f_1, m_{f1}\rangle|f_2, m_{f2}\rangle$  are subject to spin exchange induced by coupling of the spin states via the exchange interaction, e.g.  $|2, 1\rangle|2, 1\rangle \rightarrow |2, 2\rangle|2, 0\rangle$ . Typical exchange rates are on the order of  $10^{-10} \text{ cm}^3/\text{s}$ .

Since  $f$  is a good quantum number at all distances (for  $B = 0$ ), spin exchange processes conserve  $\ell$  and  $f$ . Hence, the fully stretched spin states  $f_1 + f_2 = f$  cannot decay into other states, except by higher-order processes, such as dipolar relaxation. Consequently, the relaxation rates for  $|2, 2\rangle + |2, 2\rangle$  or  $|1, -1\rangle + |1, -1\rangle$  states are only on the order of  $10^{-15} \text{ cm}^3/\text{s}$ .

The cross section for inelastic spin exchange collisions is [717, 151],

$$\sigma = M_{if}\pi(a_t - a_s)^2, \quad (12.206)$$

where,

$$M_{if} = \left[ \sum_{m_S, I, m_I} (C_{S=0}C'_{S=0} - C_{S=1}C'_{S=1}) \right]^2 \quad (12.207)$$

$$C = \langle S, m_S; I, m_I | F_1 m_1; F_2 m_2 \rangle .$$

See also [635]. The reason for the above dependence can be understood as follows.  $a_s$  and  $a_t$  determine the energy of the last bound states of the singlet and triplet potentials. The more those energies are different, the stronger the coupling  $\propto |E_t - E_s|^{-1}$ . An alternative, physical picture is given in [112].

#### 12.3.9.2 Dipolar relaxation

The fully stretched spin states, such as  $^{87}\text{Rb } |f = 2, m_f = 2\rangle$  are expected to be quite stable. However, relativistic effects (retardation?) (and  $2^{nd}$  order spin-orbit coupling) break the degeneracy of the molecule-fixed projection  $|\Omega| = 0, 1$  of the  $^3\Sigma$  potential [481]. When the atoms approach their spins recouple, i.e. from  $[(s_1, i_1)f_1, (s_2, i_2)f_2]f$  towards  $[(s_1, s_2)s, (i_1, i_2)i]f$  as described by the 9j coefficients Eq. (12.197). Due to the symmetry of the problem,  $f$  and its projection  $m_f$  are good quantum numbers at all distances. However, if there is a higher-order admixture of the orbit  $l_j$ , the symmetry is broken, and the quantum number depends on the coupling schemes. Consequently, transitions between different  $m_f$  become possible, i.e. dipolar relaxation may change  $f$ ,  $m_f$  or  $\ell = 0$ , e.g. a collision can be  $s$ -wave in the entrance and  $d$ -wave in the exit channel.

#### 12.3.9.3 Three-body collisions

The trapped low-field seeking alkali gases are metastable versus 3-body recombination. 3-body recombination is the combination of two colliding atoms to a dimer in presence

of a third atom receiving the excess energy as kinetic energy and results in trap loss of the molecule and of the atom. They are suppressed as the gas gets more and more dilute since the rate goes like  $n^3$ . There might be interesting 3-body resonance phenomena like the *Efimov state* predicted for Helium droplets [220], [434] and recently seen in experiment [413, 666, 100, 445].

3-body recombination is in contrast to the more controlled way of creating molecules via photoassociation or coherent free-bound coupling.

Ultracold collisions are crucial for BEC. They provide the thermalizing elastic collisions necessary for evaporative cooling, they are the cause for the condensate self-energy and give rise to nonlinearities in the condensate dynamics. But they are also interesting by themselves. The spectrum of two-body collisions exhibits interesting features like shape- and Feshbach resonances [155, 351]. Their analysis facilitates detailed conclusions on the nature of the interaction potentials. Three body collisions are important to investigate, because they constitute a decay mechanism of the intrinsically metastable system that represents a trapped Bose-gas.

Three body collisions are not a quantum statistical effect and don't require the presence of a BEC, but they occur only at very high densities comparable to those necessary for BEC. It should be possible to detect them in *photoassociation* (PA) spectra. Photoassociation provides a tool to explore the level structure of excited states by shining in a laser with frequency  $\nu$  tuned between the colliding channel and a vibrational bound level of the excited state potential. Since the excited state preferentially decays into the continuum, where the atoms have high kinetic energy, the transition rate may be monitored via trap losses. Or we can shine in an additional laser that further excites the excited atoms into the ionized continuum where they can be registered by an ion detector.

Three-body photoassociation processes should reveal themselves by additional lines in the two-body photoassociation spectra. Those lines should only appear at very high densities and their strength should scale as the density cubed,



#### 12.3.9.4 Other processes

Majorana spin flips and collisions involving higher partial waves  $\ell$  can eventually lead to spin relaxation. In Eq. (11.90) we see that  $f$  is not necessarily a good quantum number in contrast to  $F$ ,  $|2, 2\rangle|2, 2\rangle \rightarrow |2, 1\rangle|2, 0\rangle + E_{rot}$ . However, the particles must tunnel across the centrifugal barrier, which sets temperature constraints.

#### 12.3.9.5 Collisions between fermions

Very cold three-body collisions are suppressed for fermions, because two of them necessarily must have the same quantum state, which violates the Pauli exclusion principle. This is useful for employing Feshbach resonances to form molecular BECs made of fermions.

#### 12.3.10 Excited states collisions



### 12.3.10.1 Adiabatic potentials

We consider the scheme (11.90), we set  $\mathbf{I} = 0$ , and we concentrate on  $s$ -waves,  $\ell = 0$ ,

$$\begin{array}{ccccccc}
 \mathbf{l}_1 & + & \mathbf{l}_2 & = & \mathbf{L} & \xrightarrow{\hat{z}} & \mathbf{\Lambda} \\
 + & & + & & + & & + \\
 \mathbf{s}_1 & + & \mathbf{s}_2 & = & \mathbf{S} & \xrightarrow{\hat{z}} & \mathbf{\Sigma} \\
 = & & = & & = & & = \\
 \mathbf{j}_1 & + & \mathbf{j}_2 & = & \mathbf{j} & \xrightarrow{\hat{z}} & \mathbf{\Omega}
 \end{array} \tag{12.209}$$

The *spin-orbit interaction* splits the potential curves. The recoupling is described by,

$$|\psi_{(L,S)j}(R)\rangle \sim \sum_{j_1, j_2} \sqrt{\hat{L}\hat{S}j_1 j_2} \begin{Bmatrix} l_1 & l_2 & L \\ s_1 & s_2 & S \\ j_1 & j_2 & j \end{Bmatrix} |\psi_{(j_1, j_2)j}(R)\rangle . \tag{12.210}$$

### 12.3.10.2 Homonuclear collisions

Let us consider the example of the fine structure in homonuclear  $^{87}\text{Rb}$  collisions. Without hyperfine, rotational and Zeeman splitting the recoupling goes like illustrated in Fig. 12.23.

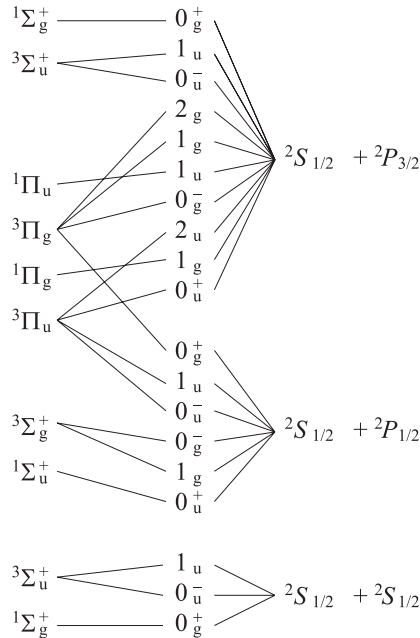


Figure 12.23: Movre coupling scheme.

From Fig. 12.23 we see that the molecular states are remixed at long range: Every state  $0_g^-, 0_u^-, 0_g^+, 0_u^+, 1_g, 1_u, 2_g, 2_u$  has several molecular states to which it connects, e.g.  $0_g^-$  connects within the fine structure to  $(2)^3\Sigma_g^+$  and  $(2)^3\Pi_g$ . Those multiplets

form a closed interacting subspace. According to Movre and Pichler [507, 685] we get with  $\Delta = E(^2P_{3/2}) - E(^2P_{1/2}) = \frac{3}{2}A_{so}$ ,

$$0_{\sigma}^{-} = \begin{pmatrix} E(^3\Pi_{\sigma}) - \frac{1}{3}\Delta & \frac{\sqrt{2}}{3}\Delta \\ -\frac{\sqrt{2}}{3}\Delta & E(^3\Sigma_{\sigma}^{+}) \end{pmatrix}, \quad 0_{\sigma}^{+} = \begin{pmatrix} E(^3\Pi_{\sigma}) - \frac{1}{3}\Delta & -\frac{\sqrt{2}}{3}\Delta \\ -\frac{\sqrt{2}}{3}\Delta & E(^1\Sigma_{\sigma}^{+}) \end{pmatrix} \quad (12.211)$$

$$1_{\sigma} = \begin{pmatrix} E(^3\Pi_{\sigma}) & \frac{1}{3}\Delta & -\frac{1}{3}\Delta \\ \frac{1}{3}\Delta & E(^1\Pi_{\sigma}) & -\frac{1}{3}\Delta \\ -\frac{1}{3}\Delta & -\frac{1}{3}\Delta & E(^3\Sigma_{\sigma}^{+}) \end{pmatrix}, \quad 2_{\sigma} = (^3\Pi_{\sigma}).$$

At short range the potentials approximately go like,

$$\begin{aligned} E(^1\Sigma_g^{+}), E(^3\Sigma_u^{+}) &\propto 2C_3/R^3 \\ E(^1\Pi_u), E(^3\Pi_g) &\propto C_3/R^3 \\ E(^1\Pi_g), E(^3\Pi_u) &\propto -C_3/R^3 \\ E(^1\Sigma_u^{+}), E(^3\Sigma_g^{+}) &\propto -2C_3/R^3. \end{aligned} \quad (12.212)$$

Inserting the short range potentials and defining  $X = \sigma C_3/3\Delta R^3$ ,  $Y = E/\Delta$  and  $\sigma = +$  for  $g$  and  $-$  for  $u$ ,

$$\begin{aligned} 0_{\sigma}^{-} &= \begin{pmatrix} 3X + \frac{1}{3} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{2}}{3} & -6X + \frac{2}{3} \end{pmatrix}, \quad 0_{\sigma}^{+} = \begin{pmatrix} 3X + \frac{1}{3} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{2}}{3} & 6X + \frac{2}{3} \end{pmatrix} \\ 1_{\sigma} &= \begin{pmatrix} 3X + \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & -3X + \frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & -6X + \frac{2}{3} \end{pmatrix}, \quad 2_{\sigma} = (3X + 1). \end{aligned} \quad (12.213)$$

Note that the structure looks very much like the transition from the Zeeman to the Paschen-Back regime, where  $X$  plays the role of the magnetic field and  $Y$  the level shift. The characteristic equations are,

$$\begin{aligned} Y^2 - (1 - 3X)Y - 18X^2 &= 0 && \text{for } 0_{\sigma}^{-} \\ Y^2 - (1 + 9X)Y + (4X + 18X^2) &= 0 && \text{for } 0_{\sigma}^{+} \\ Y^3 + (-2 + 6X)Y^2 + (1 - 8X - 9X^2)Y + (2X + 6X^2 - 54X^3) &= 0 && \text{for } 1_{\sigma} \\ Y - (1 + 3X) &= 0 && \text{for } 2_{\sigma} \end{aligned} \quad (12.214)$$

### 12.3.11 Heteronuclear collisions

For a collision in the channel  ${}^6\text{Li } P \text{ } {}^{87}\text{Rb } S$  we get the  $\{9j\}$ -symbol,

$$\left\{ \begin{matrix} l_6 & l_{87} & L \\ s_6 & s_{87} & S \\ j_6 & j_{87} & j \end{matrix} \right\} = \left\{ \begin{matrix} 0 & 1 & 1 \\ \frac{1}{2} & \frac{1}{2} & S \\ \frac{1}{2} & j_{87} & j \rightarrow \Omega \end{matrix} \right\}. \quad (12.215)$$

We thus expect a fine structure  $j_{87} = \frac{1}{2}, \frac{3}{2}$  at long range and exchange interactions  $S = 0, 1$  at short range. For the projection onto the internuclear axis  $|L - S| \leq \Omega \leq L + S$ .

Let  $V_k(R)$  be the uncoupled potentials and,

$$\Delta_{kl}(R) = D_{kl} + A_{kl} \left( [1 - e^{-B_{kl}(R-R_{kl})}]^2 - 1 \right) \quad (12.216)$$

the spin-orbit functions modeled as Morse potentials, where  $D_{kl}$  is related to the fine-structure splitting,  $D_{kl} = \frac{1}{3}(E_k - E_l)$ , for diagonal and,  $D_{kl} = \frac{\sqrt{2}}{3}(E_k - E_l)$ , for off-diagonal elements. For heteronuclear molecules like  ${}^6\text{Li}{}^87\text{Rb}$  we have matrices like [65, 64],

$H$	$ {}^3\Sigma^+\rangle$	$ {}^3\Pi\rangle$	$ {}^1\Sigma^+\rangle$	$ {}^3\Pi\rangle$	$ {}^3\Sigma^+\rangle$	$ {}^1\Pi\rangle$	$ {}^3\Pi\rangle$	$ {}^3\Pi\rangle$
$\langle {}^3\Sigma^+_{\Omega=0-}  $	$V({}^3\Sigma)$	$\Delta_{cb}\sqrt{2}$						
$\langle {}^3\Pi_{\Omega=0-}  $	$\Delta_{cb}\sqrt{2}$	$V({}^3\Pi) - \Delta_{bb}$						
$\langle {}^1\Sigma^+_{\Omega=0+}  $			$V({}^1\Sigma)(-2\Delta_{bb})$	$-\Delta_{bb}$				
$\langle {}^3\Pi_{\Omega=0+}  $			$-\Delta_{bb}$	$V({}^3\Pi) (+\Delta_{bb})$				
$\langle {}^3\Sigma^+_{\Omega=1}  $					$V({}^3\Sigma)$	$\Delta_{cB}$	$\Delta_{cb}$	
$\langle {}^1\Pi_{\Omega=1}  $					$\Delta_{cB}$	$V({}^1\Pi)$	$-\Delta_{bB}$	
$\langle {}^3\Pi_{\Omega=1}  $					$\Delta_{cb}$	$-\Delta_{bB}$	$V({}^3\Pi)$	
$\langle {}^3\Pi_{\Omega=2}  $								$V({}^3\Pi) + \Delta_{bb}$

(12.217)

for every fine structure. For example, there is a matrix for the two  ${}^6\text{Li } S_{1/2}$   ${}^87\text{Rb } P_{1,3/2}$  asymptotes and another one for the  ${}^6\text{Li } P_{1/2,3/2}$   ${}^87\text{Rb } S_1$  asymptotes. Additional terms enter via rotational effects [65].

Concretely,

$$\Delta_{bb}(R \rightarrow \infty) = \frac{1}{3}(E_{3/2} - E_{1/2}) \quad (12.218)$$

$$\Delta_{cB}(R \rightarrow \infty) = \frac{1}{3}(E_{3/2} - E_{1/2})$$

$$\Delta_{bB}(R \rightarrow \infty) = \frac{1}{3}(E_{3/2} - E_{1/2})$$

$$\Delta_{cb}(R \rightarrow \infty) = \frac{1}{3}(E_{3/2} - E_{1/2}) .$$

### 12.3.11.1 Inelastic trap losses

Between ground and excited states *fine changing collisions* and *radiative escape* are possible. Between two ground states only *hyperfine changing collisions* may occur.

The nature of the collision process, whether it is a one-<sup>13</sup>, two-, or three-body collision, reveals itself via the temporal behavior of trap losses. Using the abbreviation,

$$\langle \eta \rangle \equiv \frac{1}{N} \int \eta(\mathbf{r}) n(\mathbf{r}) d^3r , \quad (12.219)$$

we can write the loss rates due to inelastic one-, two-, and three-body collisions,

$$B\langle 1 \rangle N \quad , \quad K\langle n \rangle N \quad , \quad L\langle n^2 \rangle N . \quad (12.220)$$

<sup>13</sup>By one-body collision we mean collisions with atoms of the background gas.

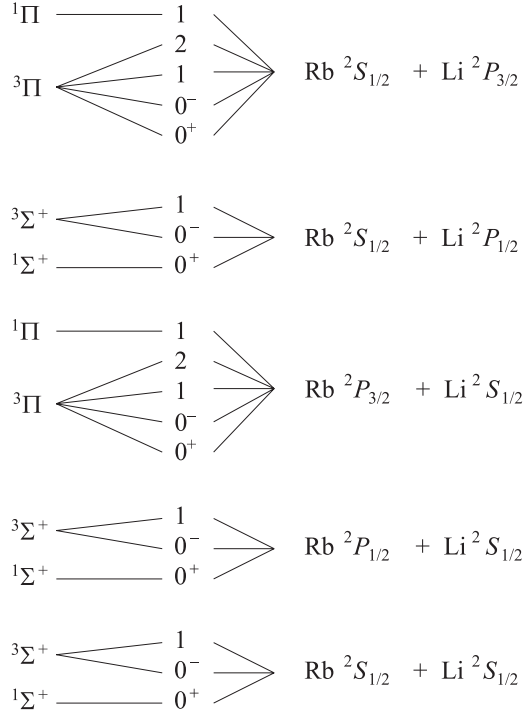


Figure 12.24: Movre type spin-orbit recoupling scheme for heteronuclear molecules.

the prefactors depend on the collision velocity (that is, the temperature of the sample) and atomic parameters (for example, the collision cross section for two-body collisions, which may itself depend on temperature). Hence, the total number of trapped atoms evolves according to,

$$\dot{N} = -B\langle 1 \rangle N - K\langle n \rangle N - L\langle n^2 \rangle N . \quad (12.221)$$

Assuming a gaussian density distribution,

$$n(\mathbf{r}) = \frac{N}{(2\pi)^{3/2}\bar{r}^3} e^{-r^2/2\bar{r}^2} , \quad (12.222)$$

we calculate,

$$\dot{N} = -BN - \frac{K}{(4\pi)^{3/2}\bar{r}^3} N^2 - \frac{L}{3^{3/2}(2\pi)^{3/2}\bar{r}^6} N^3 . \quad (12.223)$$

Fig. 12.26 shows a simulation of Eq. (12.223).

For condensates in the Thomas-Fermi limit [646] found the following differential equations for two- and three-body collisions,

$$\frac{\dot{N}}{N} = -Gc_2 N^{2/5} - \frac{1}{\tau} \quad \text{and} \quad \frac{\dot{N}}{N} = -Lc_3 N^{4/5} - \frac{1}{\tau} . \quad (12.224)$$

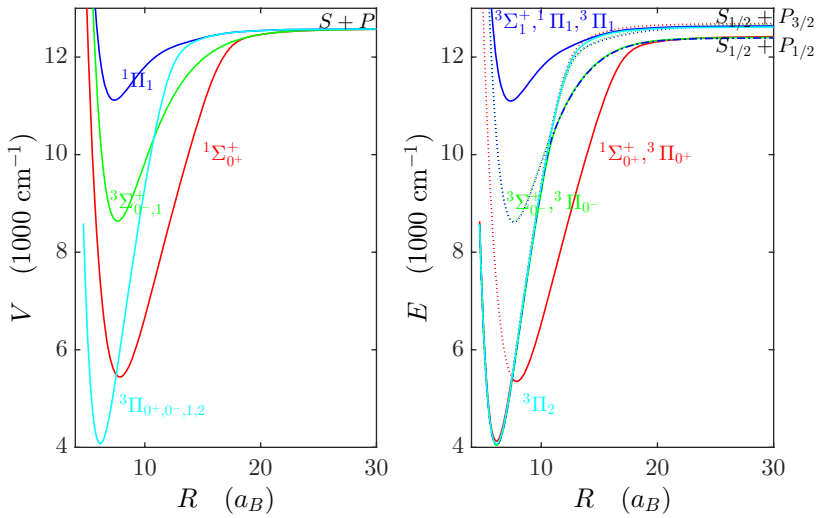


Figure 12.25: (code) Adiabatic potentials.

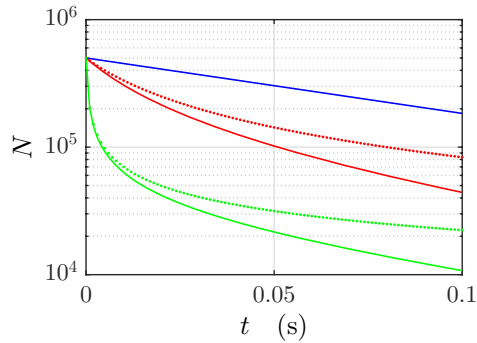


Figure 12.26: (code) One-, two-, and three-body losses.

### 12.3.12 Heteronuclear electric dipole moment

The *electric dipole moment* of a dimer is highest for big mass difference, as in the case of LiRb and for low vibrational quantum number [407, 30]. The electric dipole moment determines the rate for spontaneous and *black-body radiation*,  $\bar{n} = (e^{-\beta\hbar\omega} - 1)^{-1}$ , induced transitions between rovibrational states [408],  $\Gamma_{vlm}^{tot} = \Gamma_{vlm}^{spnt} + \Gamma_{vlm}^{bb}$ . With the transition rate between individual levels,

$$\Gamma_{vlm \rightarrow v'l'm'}^{\alpha} = \frac{8\pi}{3} \frac{\omega^3}{hc^3} |\langle |d| \rangle|^2, \quad (12.225)$$

we can estimate the rates for spontaneous emission,

$$\Gamma_{vlm}^{spnt} = \sum_{v'l'm'} \Gamma_{vlm \rightarrow v'l'm'}^{em}, \quad (12.226)$$

and for black-body radiation,

$$\Gamma_{v'lm}^{bb} = \sum_{v'l'm'} \bar{n} \Gamma_{v'lm \rightarrow v'l'm'}^{em} + \sum_{v''l''m''} \bar{n} \Gamma_{v'lm \rightarrow v''l''m''}^{abs}. \quad (12.227)$$

Note that selection rules require  $|l - l'| \leq 1$  and  $|m - m'| \leq 1$ , rotational transitions are inhibited by small  $\omega^3$ , spontaneous emission is high for intermediate levels for which on one hand  $\omega^3$  is large enough and enough final states are available.

From calculations of the  $R$ -dependence of the electric dipole moments [30] the dipole moment of a specific vibrational state is easily estimated from,

$$d = \frac{\int \psi(R) R \psi(R) dR}{\int \psi(R) \psi(R) dR}. \quad (12.228)$$

In electric fields the dipole moments will lead to Stark shifts. For  $|d| = 1$  Debye in a field of 1 V/m we expect a Stark shift of  $H_{Stark} \approx 500$  kHz. It may be possible to measure this by photoassociation spectroscopy. Note also that since homonuclear dimers do not have a permanent electric dipole moment, transitions between vibrational ground states are forbidden.

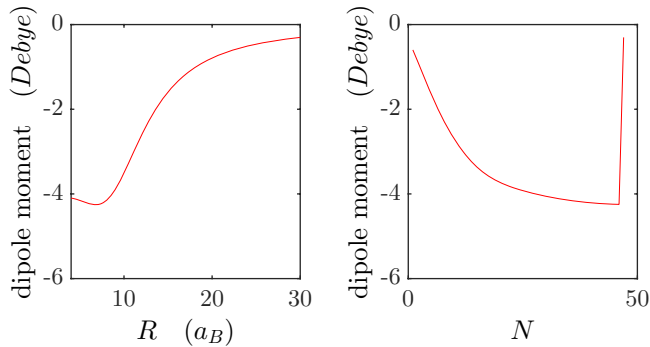


Figure 12.27: (code) (a) Dipole moment at the example of LiRb as a function of interatomic distance. (b) Dipole moment at the example of LiRb as a function of vibrational quantum number.

## 12.3.13 Exercises

### 12.3.13.1 Ex: Photoassociation

Consider a laser focused into a cold, confined cloud of Na atoms at a temperature of  $450 \mu\text{K}$ . For a detuning of 600 MHz, calculate the laser intensity (in  $\text{W}/\text{cm}^2$ ) required to produce a 25% probability of photoassociation. The transition moment (a.u.) of Na is 2.55.

### 12.3.13.2 Ex: Vibrational structure of LiRb

Calculations of the vibrational structures of several ground states of the heteronuclear molecule LiRb.

## 12.4 Resonances in cold collisions

### 12.4.1 Shape resonances

The 'centrifugal' term can give rise to repulsive walls for attractive potentials. Behind these walls, quasi-bound states can develop and give rise to collision resonances. That is, resonances emerge in the collision cross section as a function of the collision temperature called *shape resonances*.

### 12.4.2 Feshbach resonances

The so-called *Feshbach resonance* is due to an energetic match between a collision channel and a bound molecular state [235, 681, 682, 492, 233, 493, 699]. They allow to vary the scattering length  $a_s$  almost arbitrarily from zero, where the atomic cloud turns into an ideal gas, up to values exceeding the total size of the cloud.

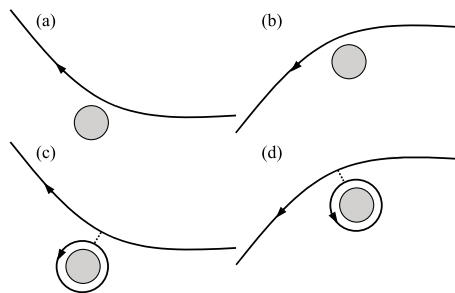


Figure 12.28: Classical illustration of a scattering resonance.

The impact of a Feshbach resonance can be understood as a perturbation of the collisional channel leading to a modification of the depth of the scattering potential. When this leads to the promotion of one more vibrational state into (or from) the continuum, this obviously leads to a dramatic modification of the scattering length  $a_s$ .<sup>14</sup>

Let us consider two very cold atoms colliding on an attractive interatomic potential  $V(R)$  (see Fig. 12.29, right). At long distances the relative wavefunction is a sine characterized by the Broglie wave vector  $k_{dB}$ . As the atoms approach each other, they mutually accelerate, and the Broglie wave performs some small and rapid oscillations within the potential. The number of nodes of the wavefunction within the potential corresponds to the number of bound vibrational levels that the potential with a given depth can support. The scattering length  $a_s$  is defined as the phase slip, which the Broglie wave would acquire during the collision at the boundary  $k_{dB} \rightarrow \infty$ .

With the possibility of gradually decreasing the depth of the molecular potential, at some point the last state below the ionization threshold goes to the continuum of unbound states, the wavefunction decreases the number of nodes by one unit, while the scattering cross section crosses a singularity. In fact, the potential  $V(R)$  can

<sup>14</sup>Note that the divergence of the scattering length is an artifact of the hard core approximation, that is, the regularization of the interaction potential, since the matrix  $\mathcal{T}$  by itself does not diverge.

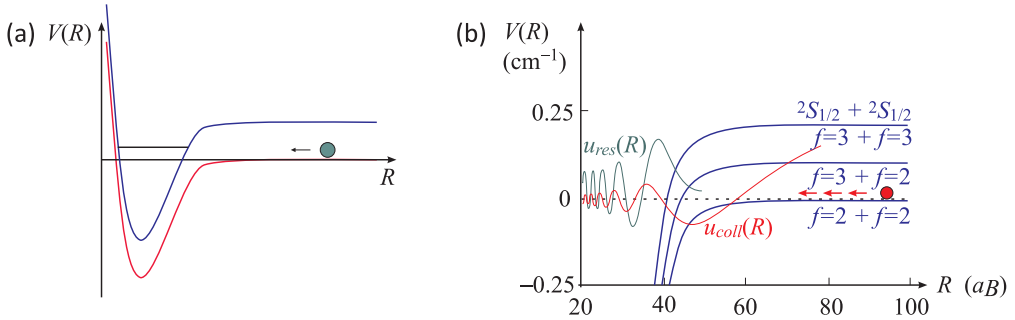


Figure 12.29: (a) The Feshbach resonance is due to a coincidence of collisional and bound channels. (b) Feshbach resonance in  $^{85}\text{Rb}$ . The atoms collide in the hyperfine state  $F = 2$ , and the resonant bound state is in the  $F = 3$  multiplet (courtesy [155]).

be manipulated with the help of radiation fields [233, 84, 493] or, near a collisional *Feshbach resonance*, by magnetic fields [682, 683]. Feshbach resonances were predicted in nuclear systems [235]. Its recent revival in the context of cold atomic collisions is due to the prospect of its use for manipulating the scattering length and thus controlling the mean-field energy of a Bose-Einstein condensate <sup>15</sup>

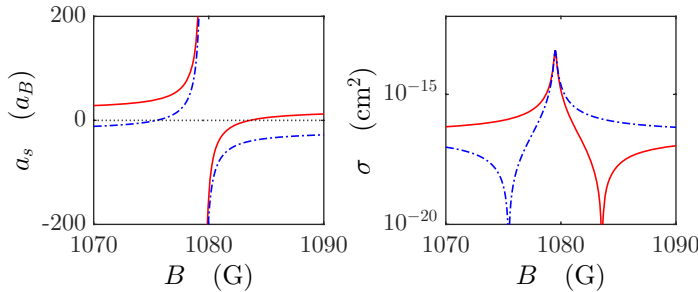


Figure 12.30: (code) (a) Scattering length and (b) collision cross section upon crossing a Feshbach resonance. The scattering length can be positive (solid red line) or negative (dashed blue line). A movie on a simulation of a Feshbach resonance can be watched here ([watch movie](#)).

The collisional *Feshbach resonance* arises when the energy of the state of two colliding atoms coincides with the energy of a vibrational molecular level belonging to a higher energy asymptote (see Fig. 12.29, right). This coincidence can strongly perturb the collisional channel, because the resonance shifts the phase of the relative de Broglie wavefunction and allows the atoms to tunnel into the molecular state for a short period of time, the duration of which is determined by the Heisenberg uncertainty relation. If the sum of the magnetic dipole moments of the atoms is

<sup>15</sup>It is even possible to invert the sign of the scattering length. This was a prerequisite for condensation of the atomic species of  $^{85}\text{Rb}$  [586]. In addition, Feshbach resonances are interesting because they can install a coherent free-bound coupling between an *open-channel* of colliding atoms and a bound molecular state of the same atoms, as shown in Fig. 12.29. This coupling can lead to the creation of molecular condensates.



different from the dipole moment of the molecule, the resonance can be tuned via external magnetic fields exploring the Zeeman effect. When a Feshbach resonance is crossed, the scattering length crosses a singularity, as shown in Fig. 12.30(left) <sup>16</sup>.

## 12.5 Further reading

### 12.5.1 on cold collisions

- J.M. Vogels et al., *Coupled Singlet-Triplet Analysis of Two-Color Cold-Atom Photoassociation Spectra* [\[DOI\]](#)
- H. Ouerdane et al., *Scattering Parameters for Cold LiRb and NaRb Collisions Derived from Variable Phase Theory* [\[DOI\]](#)
- M. Marinescu et al., *Long-Range Potentials for Two-Species Alkali-Metal Atoms* [\[DOI\]](#)
- S.B. Weiss et al., *Calculation of the Interspecies S-Wave Scattering Length in an Ultracold Na-Rb Vapor* [\[DOI\]](#)

### 12.5.2 on Feshbach resonances

- Ph.W. Courteille et al., *Observation of a Feshbach resonance in Cold Atom Scattering* [\[DOI\]](#)
- S. Inouye et al., *Observation of Feshbach resonances in a Bose-Einstein condensate* [\[DOI\]](#)
- C. Chin et al., *Feshbach Resonances in Ultracold Gases* [\[DOI\]](#)

Part III

Quantum Optics



# Chapter 13

## Interaction of light with mono-electronic atoms

In Secs. 1.2 we introduced the Einstein coefficients  $A$  and  $B$ , which we associated with Planck's spectral distribution of black-body radiation. This procedure allowed us to connect the coefficients for spontaneous and stimulated transitions, but did not provide any method to calculate them from the intrinsic properties of the atoms. The purpose of this chapter is to find expressions for the rates of absorption and emission of atomic radiation using quantum mechanics and to relate them to the Einstein coefficients. As for all rates, we will find that these rates should be expressed in terms of probabilities for absorption and emission. Several disciplines such as spectrometry, spectroscopy and astrophysics have developed their own terminologies to describe absorption and emission of light by matter. We will explain how the most frequently used parameters are interrelated by placing particular emphasis on the simplest system, which is the two-level atom with no degeneracy and no spin.

### 13.1 Semiclassical theory of the excitation of atomic transitions

In a model of an isolated atom, the atomic energy levels are eigenstates of the Hamiltonian and describe the system completely, i.e. they do not undergo any evolution. To accurately describe an atom, one has to consider its coupling to the field of the electromagnetic vacuum. The total system has different eigenstates and their projection on the unperturbed eigenstates changes over time. We will show in the following, that an excited atomic state has a constant probability, depending on the coupling to the electromagnetic field, to decay to another state. Thus, the probability of measuring a specific lifetime follows a Poisson distribution.

#### 13.1.1 Time-dependent perturbation by a plane wave

Looking at the Hamiltonian (9.11) describing the interaction of a charged particle with an electromagnetic field, we find that the term  $\mathbf{A} \cdot \nabla \propto e^{i\omega t}$  oscillates with frequency  $\omega$ , while the term  $\mathbf{A}^2 \propto e^{2i\omega t}$  oscillates with twice that frequency. We will only consider the interaction term (9.12), which is linear in  $\mathbf{A}$ , and we will treat this term as first-order perturbation by *time-dependent perturbation theory* (TPDT).

With this scope we separate the Hamiltonian in a stationary part and a time-dependent part <sup>1</sup>,

$$\hat{H}(t) = \hat{H}^{(0)} + \hat{H}_{int}(t) \quad \text{with} \quad \hat{H}_{int} = \frac{e}{m} \mathbf{A}(\mathbf{r}, t) \cdot \hat{\mathbf{p}}, \quad (13.1)$$

where  $\hat{H}^{(0)}$  contains the kinetic energy and the Colombian potential of Eq. (9.11). In Sec. 6.4.4, inserting the expansion,

$$|\psi\rangle = \sum_k a_k(t) |k\rangle e^{-iE_k t/\hbar}, \quad (13.2)$$

along with the Hamiltonian (13.1) in the Schrödinger equation, we obtained the first order perturbative approximation (6.72). Setting the initial condition to  $c_k(t \leq 0) = \delta_{ki}$  and supposing that the probability of finding the atom initially in the ground state  $|i\rangle$  for short times is 1, we got,

$$a_f^{(1)}(t) \simeq \frac{1}{i\hbar} \int_0^t \langle f | \hat{H}_{int} | i \rangle e^{i\omega_{fi}t'} dt'. \quad (13.3)$$

We now consider a perturbation by an electromagnetic plane wave within the Coulomb gauge,

$$\Phi = 0 \quad \text{and} \quad \nabla \cdot \mathbf{A} = 0. \quad (13.4)$$

The solution of the wave equation can be written,

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_0^*(\mathbf{r}) e^{i\omega t} + \mathbf{A}_0(\mathbf{r}) e^{-i\omega t}. \quad (13.5)$$

For plane waves,

$$\mathbf{A}_0(\mathbf{r}) = \mathbf{A}_0 e^{i\mathbf{k} \cdot \mathbf{r}} \quad (13.6)$$

and  $k = \omega/c$  and  $\mathbf{k} \cdot \mathbf{A}_0 = 0$ . With this, it is possible to show (see Exc. 13.1.4.1), that the energy density is,

$$u(\omega) = \frac{\epsilon_0}{2} \vec{\mathcal{E}}^2 + \frac{1}{2\mu_0} \vec{\mathcal{B}}^2 = 2\epsilon_0 \omega^2 A_0^2. \quad (13.7)$$

On the other hand, the energy density is proportional to the number of photons  $N(\omega)$  inside the volume  $V$ ,

$$u(\omega) = \frac{N(\omega) \hbar \omega}{V}. \quad (13.8)$$

The intensity corresponds to a flow of energy,

$$I(\omega) = u(\omega) c. \quad (13.9)$$

Separating the polarization  $\hat{\mathbf{e}}$  from the amplitude  $A_0$ ,

$$\mathbf{A} = \hat{\mathbf{e}} A_0 e^{i\mathbf{k} \cdot \mathbf{r}} e^{-i\omega t} + c.c., \quad (13.10)$$

---

<sup>1</sup>The energy of the light field is not considered in the Hamiltonian, because it is treated as classical, that is, its energy commutes with the other observables of the system.

and inserting the perturbation (13.1) into the approximation (13.3),

$$\begin{aligned} a_f^{(1)}(t) &= -\frac{e}{m} \int_0^t dt' \langle f | \mathbf{A} \cdot \nabla | i \rangle e^{i\omega_{fi}t'} dt' \\ &= -\frac{eA_0}{m} \langle f | e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\epsilon} \cdot \nabla | i \rangle \int_0^t dt' e^{i(\omega_{fi}-\omega)t'} dt' - \frac{eA_0}{m} \langle f | e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{\epsilon} \cdot \nabla | i \rangle \int_0^t dt' e^{i(\omega_{fi}+\omega)t'} dt' . \end{aligned} \quad (13.11)$$

Which of the two processes occurs, depends on the initial and final energies. For  $E_f = E_i + \hbar\omega$  the first term describing the process of *absorption* will dominate, for  $E_f = E_i - \hbar\omega$  the second term describing *emission* prevails.

## 13.1.2 Absorption and stimulated emission

### 13.1.2.1 Absorption

We define the *matrix element*,

$$M_{fi} \equiv \langle f | e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\epsilon} \cdot \nabla | i \rangle , \quad (13.12)$$

and concentrate on the absorption process. Defining the detuning by  $\Delta \equiv \omega - \omega_{fi}$  and evaluating the integral,

$$\left| \int_0^t e^{-i\Delta t'} dt' \right|^2 = \left| \frac{e^{-i\Delta t} - 1}{-i\Delta} \right|^2 = 4 \frac{\sin^2 \frac{\Delta t}{2}}{\Delta^2} \simeq 2\pi t \delta(\Delta) , \quad (13.13)$$

at short times <sup>2</sup>, the absorption probability becomes,

$$|a_f^{(1)}(t)|^2 = \frac{e^2}{m^2} A_0(\omega)^2 |M_{fi}|^2 \left| \int_0^t dt' e^{i(\omega_{fi}-\omega)t'} dt' \right|^2 = \frac{e^2}{m^2} A_0(\omega)^2 |M_{fi}|^2 2\pi t \delta(\Delta) . \quad (13.14)$$

The  $\delta(\Delta = 0)$  function simply represents conservation of energy. Of course this is only an approximation not taking into account the finite width of the transition line.

Expressing the field by the intensity (13.10), we obtain the transition rate for absorption,

$$\boxed{W_{fi}^{(ab)} = \frac{d}{dt} |a_f^{(1)}(t)|^2 = 2\pi \left( \frac{eA_0}{m} \right)^2 |M_{fi}|^2 \delta(\omega - \omega_{fi}) = \frac{\pi e^2}{\varepsilon_0 m^2 c} \frac{I(\omega)}{\omega^2} |M_{fi}|^2 \delta(\omega - \omega_{fi})} . \quad (13.15)$$

We note that the absorption rate is proportional to the intensity of the radiation, which characterizes a typically linear effect.

If we want to express the rate of absorption by atoms in terms of energy, we simply multiply  $W_{fi}$  by  $\hbar\omega$  and, hence, we can define the cross section for the absorption of radiative energy as,

$$\sigma_{i \rightarrow f} \equiv \frac{\text{absorption rate}}{\text{incident intensity}} = \frac{\hbar\omega W_{fi}}{I(\omega)} = \frac{\pi e^2}{\varepsilon_0 m^2 c} \frac{\hbar}{\omega} |M_{fi}(\omega_{fi})|^2 \delta(\omega - \omega_{fi}) . \quad (13.16)$$

<sup>2</sup> $\lim_{n \rightarrow \infty} \frac{n}{\pi} \frac{\sin^2 nx}{(nx)^2} = \delta(x)$ .

### 13.1.2.2 Stimulated emission

For  $E_f = E_i - \hbar\omega$  the equation describes the process of *stimulated emission*. Analogously to the calculation of the absorption, we obtain,

$$W_{if}^{(st)} = \frac{\pi e^2}{\varepsilon_0 m^2 c} \frac{I(\omega)}{\omega^2} |M_{if}^*|^2 \delta(\omega + \omega_{fi}), \quad (13.17)$$

with  $M_{fi}^* = \langle f | e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{\epsilon} \cdot \nabla | i \rangle$ . Of course,

$$W_{if}^{(st)} = W_{fi}^{(ab)}. \quad (13.18)$$

The fact that, in a coupled atom-radiation system in equilibrium, the radiation field excites the same number of transitions in absorption  $i \rightarrow f$  as in stimulated emission  $f \rightarrow i$  is called the principle of *detailed balance*.

Obviously, the situation is different, if instead of two states we have several states that can be excited by radiation or decay.

### 13.1.3 Spontaneous emission

Absorption and stimulated emission are due to the interaction of the atom with a radiation field. There is another emission process due to interaction with fluctuations of the electromagnetic vacuum called *spontaneous emission*. This interaction is understood in the framework of *quantum electrodynamics*. Here, we will adopt a heuristic treatment.

Replacing in Eq. (13.17) the intensity by the number of photons (13.8), we obtain,

$$W_{if}^{(st)} = \frac{\pi \hbar e^2 N(\omega)}{\varepsilon_0 m^2 \omega V} |M_{fi}|^2 \delta(\omega - \omega_{fi}). \quad (13.19)$$

In fact, the introduction of the concept of photons already implies the quantization of the electromagnetic field. Adding to the number of photons a photon representing the vacuum fluctuations,  $N(\omega) \rightarrow N(\omega) + 1$ , we are able to include spontaneous emission,

$$W_{if}^{(st)} + W_{if}^{(sp)} = \frac{\pi \hbar e^2 [N(\omega) + 1]}{\varepsilon_0 m^2 \omega V} |M_{fi}|^2 \delta(\omega + \omega_{fi}). \quad (13.20)$$

This means that even in the absence of a classical radiation field,  $N(\omega) = 0$ , there is an emission probability. We note that  $W_{if}^{(sp)}$  depends on the volume confining the atom, that is, the cavity, since it describes the transfer of energy to this volume. Here, it is clear that an argument is still missing, because the transfer rate must depend in some way on the number of states available to accommodate the emitted photon, that is, on the *density of states* within the cavity. The calculation of this density of states should allow us to evaluate the quantization volume  $V$ .

#### 13.1.3.1 Density of states

To estimate the number of modes, that is, of photonic states within a solid angle  $d\Omega$  of free space, we consider a cubic box of size  $L$ . The modes within this volume

are imposed by the periodic boundary conditions on the spatial part of the plane wavefunctions  $e^{-i\mathbf{k}\cdot\mathbf{r}}$ ,

$$k_{x,y,z} = \frac{2\pi}{L} n_{x,y,z} , \quad (13.21)$$

where  $(n_x, n_y, n_z)$  is a set of integers representing the various states of the photon. In the limit of large  $L$  the variation between successive  $\mathbf{k}$  is very small, such that we can treat the numbers as continuous variables. That is, the number of states with  $\mathbf{k}$  between  $(k_x, k_y, k_z)$  and  $(k_x + dk_x, k_y + dk_y, k_z + dk_z)$  is,

$$dn_x dn_y dn_z = \frac{L^3}{(2\pi)^3} dk_x dk_y dk_z = \frac{V}{(2\pi)^3} k^2 dk d\Omega = \frac{V}{(2\pi)^3} \frac{\omega^2}{c^3} d\omega d\Omega \equiv \rho_c(\omega) d\omega d\Omega , \quad (13.22)$$

where the third expression is in spherical coordinates, the fourth one uses the relation  $\omega = ck$ , and the last one defines the density of states,

$$\rho_c(\omega) = \frac{V}{(2\pi)^3} \frac{\omega^2}{c^3} . \quad (13.23)$$

Thus, the spontaneous emission rate of photons into the solid angle  $d\Omega$  is,

$$\begin{aligned} \mathcal{W}_{if}^{(sp)} d\Omega &= \left( \int_{\omega} W_{if}^{(sp)} \rho_c(\omega) d\omega \right) d\Omega = \int_{\omega} \frac{\pi \hbar e^2}{\varepsilon_0 m^2 \omega V} |M_{fi}|^2 \delta(\omega + \omega_{fi}) \frac{V}{(2\pi)^3} \frac{\omega^2}{c^3} d\omega d\Omega \\ &= \frac{\hbar e^2}{8\pi^2 \varepsilon_0 m^2 c^3} |M_{fi}|^2 \omega_{fi} d\Omega , \end{aligned} \quad (13.24)$$

This simplified treatment with only two atomic states considers light as a scalar field. In fact, light is a vector field and can have two independent orthogonal polarizations. The transition matrix may depend on polarization, such that,

$$\mathcal{W}_{if}^{(sp)} = \frac{\hbar e^2}{8\pi^2 \varepsilon_0 m^2 c^3} \int \sum_{\lambda=1,2} |M_{fi}^{\lambda}|^2 \omega_{fi} d\Omega . \quad (13.25)$$

### 13.1.4 Exercises

#### 13.1.4.1 Ex: Energy density of plane waves

Derive the result (13.7) for the temporal averages of the squares of the fields  $\overline{\vec{\mathcal{E}}(\mathbf{r}, t)^2} = \overline{[-\partial_t \mathbf{A}(\mathbf{r}, t)]^2}$  and  $\overline{\vec{\mathcal{B}}(\mathbf{r}, t)^2} = \overline{[\nabla \times \mathbf{A}(\mathbf{r}, t)]^2}$ .

## 13.2 Dipolar transitions

### 13.2.1 Dipolar approximation

So far, we have used the matrix element  $M_{fi}^{\lambda}(\omega_{fi})$  without saying how it can be calculated, nor when it is significant. In many cases of interest the calculation of this matrix element is considerably simplified by an expansion of the term  $e^{-i\mathbf{k}\cdot\mathbf{r}}$ , which



is part of the matrix element (13.12)<sup>3</sup>,

$$e^{-i\mathbf{k}\cdot\mathbf{r}} = 1 - i\mathbf{k}\cdot\mathbf{r} - \frac{1}{2!}(\mathbf{k}\cdot\mathbf{r})^2 + \dots \quad (13.26)$$

This expansion is justified by the fact that the wavelength ( $\sim 600$  nm in the visible spectrum) is much larger than the size of the scattering atom,  $ka_B \ll 1$ . The *dipolar approximation* supposes,

$$e^{-i\mathbf{k}\cdot\mathbf{r}} \simeq 1, \quad (13.27)$$

such that we can remove the spatial dependence. In this approximation there is only an interaction of the *electric field* of the radiation with the atom via an electric dipole term  $\mathbf{d}\cdot\hat{\mathcal{E}}$ . Thus,

$$M_{fi}^\lambda(\omega_{fi}) = \langle f|e^{-i\mathbf{k}\cdot\mathbf{r}}\hat{\epsilon}\cdot\nabla|i\rangle \simeq \hat{\epsilon}\frac{i}{\hbar}\langle f|\mathbf{p}|i\rangle = \hat{\epsilon}\frac{im}{\hbar}\langle f|\hat{\mathbf{r}}|i\rangle. \quad (13.28)$$

We can calculate the expectation value of the velocity of the moving charge by the Heisenberg equation using the unperturbed Hamiltonian,

$$M_{fi}^\lambda(\omega_{fi}) \simeq \hat{\epsilon}\frac{im}{\hbar}\langle f|\frac{1}{i\hbar}[\mathbf{r},\hat{H}_0|i\rangle = \hat{\epsilon}\frac{m}{\hbar^2}\langle f|\mathbf{r}\hat{H}_0 - \hat{H}_0\mathbf{r}|i\rangle = \hat{\epsilon}\frac{m}{\hbar^2}(E_i - E_f)\langle f|\mathbf{r}|i\rangle. \quad (13.29)$$

The interpretation of the last equation is, that the states  $|i\rangle$  and  $|f\rangle$  are connected through a displacement of the electronic cloud which, therefore, represents the induction of an electric dipole during the electronic transition. It is convenient to introduce the *electric dipole moment*<sup>4</sup>.

$$\mathbf{d}_{fi} \equiv -e\langle f|\mathbf{r}|i\rangle. \quad (13.30)$$

As a result, the matrix element becomes,

$$M_{fi}^\lambda(\omega_{fi}) \simeq \frac{m\omega_{fi}}{e\hbar}\hat{\epsilon}\cdot\mathbf{d}_{fi} \quad (13.31)$$

and the absorption rate (13.15) is then, in the dipolar approximation,

$$\begin{aligned} W_{fi}^{(dp)} &= \frac{\pi e^2}{\varepsilon_0 m^2 c} \frac{I(\omega_{fi})}{\omega_{fi}^2} |M_{fi}|^2 \delta(\omega - \omega_{fi}) \\ &= \frac{\pi}{\varepsilon_0 \hbar^2 c} I(\omega_{fi}) |\hat{\epsilon}\cdot\mathbf{d}_{fi}|^2 \delta(\omega - \omega_{fi}) = \frac{4\pi^2 \alpha}{\hbar} I(\omega_{fi}) |\hat{\epsilon}\cdot\mathbf{r}_{fi}|^2 \delta(\omega - \omega_{fi}). \end{aligned} \quad (13.32)$$

using the definition of the fine structure constant  $\alpha = e^2/4\pi\varepsilon_0\hbar c$ .

**Example 56 (Alternative derivation of the dipolar approximation):** In the presence of the external field the momentum part of the unperturbed Hamiltonian is modified to,

$$\hat{H} = \frac{1}{2m}[-i\hbar\nabla + e\mathbf{A}(\mathbf{r},t)]^2 - e\Phi(\mathbf{r},t).$$

<sup>3</sup>Note however, that doing the dipole approximation via  $e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} \simeq 1$  also deactivates the operator function of the recoil operator dipole,  $e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} = |\mathbf{p} + \hbar\mathbf{k}\rangle\langle\mathbf{k}|$ . For discussions of photonic recoil the operator character must be maintained even in the dipole approximation, which can be done by reinserting the recoil operator in the Hamiltonian after the dipole approximation has been applied.

<sup>4</sup>In the presence of several atoms  $\mathbf{d} = -e\sum_j \mathbf{r}_j$ , where the  $\mathbf{r}_j$  are the radii of the orbits of the various electrons of the atom.

where  $\mathbf{A}(\mathbf{r}, t)$  and  $\Phi(\mathbf{r}, t)$  are respectively the vector and scalar potentials of the external field. In the Coloumb gauge the vector potential satisfies the wave function,

$$\nabla^2 \mathbf{A} - \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = 0 ,$$

with solution  $\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_0 e^{i\mathbf{r} \cdot \mathbf{k} - \omega_k t} - c.c..$  For atoms  $|\mathbf{r}| \ll \lambda$ , hence over the extent of an atom the vector potential is spatially uniform  $\mathbf{A}(\mathbf{r}, t) = \mathbf{A}(t)$ , the denominated dipole approximation. In this gauge, and after some unitary transformation, the above Hamiltonian becomes,

$$\hat{H} = \frac{1}{2m} [-i\hbar \nabla + e(\mathbf{A} + \nabla \chi)]^2 - e \frac{\partial \chi}{\partial t} .$$

where we can choose the gauge function  $\chi(\mathbf{r}, t) = -\mathbf{A}(t) \cdot \mathbf{r}$ , which lead us to the following relations,

$$\nabla \chi = -\mathbf{A} \quad \text{and} \quad \frac{\partial \chi}{\partial t} = -\mathbf{r} \cdot \frac{\partial \mathbf{A}}{\partial t} = -\mathbf{r} \cdot \vec{\mathcal{E}} ,$$

and the above Hamiltonian becomes,

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 - \hat{\mathbf{d}} \cdot \vec{\mathcal{E}} .$$

### 13.2.1.1 Polarization dependence

Following Eq. (13.31) the absorption rate depends on the orientation of the dipole moment with respect to the polarization of light, which therefore plays an important role in this transition. When  $\mathbf{d}_{fi}$  between two states is zero, the transition via electric dipole radiation is prohibited. This is not to say that there is no transition, since other terms of the expansion (13.26) are not necessarily zero, and there may be transitions of higher multipolar orders. Even the matrix element  $M_{fi}^\lambda(\omega_{fi})$  being zero for transitions involving one photon, there is still the possibility of two-photon transitions.

Setting  $\theta$  as the angle between  $\hat{\mathbf{e}}$  and  $\mathbf{d}_{fi}$  we obtain,

$$W_{fi}^{(dp)} = \frac{\pi}{\varepsilon_0 \hbar^2 c} I(\omega_{fi}) |\mathbf{d}_{fi}|^2 \cos^2 \theta \delta(\omega - \omega_{fi}) . \quad (13.33)$$

In case of unpolarized (or randomly polarized) radiation we can replace the angular distribution  $\cos^2 \theta$  by its average value,

$$\overline{\cos^2 \theta} = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi \cos^2 \theta \sin \theta d\theta d\phi = \frac{1}{3} , \quad (13.34)$$

such that,

$$\boxed{W_{fi}^{(dp, no-pol)} = \frac{\pi}{3\varepsilon_0 \hbar^2 c} I(\omega_{fi}) |\mathbf{d}_{fi}|^2 \delta(\omega - \omega_{fi})} . \quad (13.35)$$

This expression also represents the stimulated emission rate in the electric dipole approximation.

The total spontaneous emission rate can be obtained from Eq. (13.25) integrating over all possible orientations,

$$\begin{aligned}
 \mathcal{W}_{fi}^{(sp)} &= \frac{\hbar e^2}{8\pi^2 \varepsilon_0 m^2 c^3} \int \sum_{\lambda=1,2} |M_{fi}^\lambda|^2 \omega_{fi} d\Omega \\
 &= 2 \frac{\hbar e^2}{8\pi^2 \varepsilon_0 m^2 c^3} \int_0^{2\pi} \int_0^\pi \left| \frac{m\omega_{fi}}{e\hbar} \hat{\varepsilon} \cdot \mathbf{d}_{fi} \right|^2 \omega_{fi} \sin\theta d\theta d\phi \\
 &= \frac{e^2}{4\pi^2 \varepsilon_0 \hbar c^3} \omega_{fi}^3 |\mathbf{r}_{fi}|^2 \int_0^{2\pi} \int_0^\pi \cos^2\theta \sin\theta d\theta d\phi = \frac{e^2}{3\pi \varepsilon_0 \hbar c^3} \omega_{fi}^3 |\mathbf{r}_{fi}|^2,
 \end{aligned} \tag{13.36}$$

such that, for non-polarized light,

$$\boxed{\mathcal{W}_{fi}^{(sp)} = \frac{4\alpha}{3c^2} \omega_{fi}^3 |\mathbf{r}_{fi}|^2 = \frac{4\alpha}{3c^2} \omega_{fi}^3 |\mathbf{r}_{fi}|^2 = \Gamma}. \tag{13.37}$$

This is the rate of spontaneous decay of an excited atomic state. It can be measured experimentally which, in turn, allows the calculation of the dipole moment,

$$d_{fi} = \sqrt{\frac{3\pi \varepsilon_0 \hbar \Gamma}{k^3}}. \tag{13.38}$$

In Exc. 13.2.6.1 we calculate the Rabi frequency from the dipole moment of an atomic transition and the electric field of a radiation field.

### 13.2.1.2 Einstein transition probabilities

Considering the problem of the transfer of energy between the electromagnetic field and a sample of atoms in thermal equilibrium, Einstein realized that the processes of absorption and stimulated emission are not sufficient to understand the radiative coupling between two energy levels, that is, the coupling is not correctly described by Fermi's Golden rule, and we need to introduce the notion of spontaneous emission.

Differently from the derivation of the preceding section, Einstein considered atoms whose populations of energy states are in thermal equilibrium with the electromagnetic field of a *black-body*. With this picture he came to the same result for the spontaneous emission rate (13.35). The famous *Einstein coefficients*  $A_{fi}$  and  $B_{fi}$  are given by,

$$A_{fi} N_f = W_{fi}^{(sp)} \quad \text{and} \quad \frac{A_{fi}}{B_{fi}} = \frac{\hbar \omega_{fi}^3}{\pi^2 c^3}, \tag{13.39}$$

where  $N_f$  is the population of the excited state. This shows that, in fact, spontaneous emission is a necessary consequence of the interaction of an atom with a *thermal bath* (also called *reservoir*).

## 13.2.2 Einstein transition probabilities

We now consider the problem of energy transfer between an electromagnetic field and a sample of atoms. The rate of *absorption* of a light field is,

$$R_{i \rightarrow f} \equiv \frac{1}{3} \dot{P}_{i \rightarrow f} = \frac{\pi}{6\hbar^2} \mathcal{E}_0^2 |d_{fi}|^2 \varrho(\omega_{fi}), \tag{13.40}$$

with  $W_0 = \mathcal{E}_0 d_{fi}$  and  $d_{fi}$  being the transition matrix element between atomic states. The factor  $\frac{1}{3}$  comes from the fact that the vector  $\vec{\mathcal{E}}$  of the electric field can have any polarization, but only polarizations along the direction of the oscillation of the dipole moment contribute.

For a single atom, the result (13.40) is symmetric with respect to an exchange of the initial and final states, that is, the rates for absorption and *induced emission* of light are the same. For a sample of atoms being in *thermal equilibrium*, the populations  $N_i$  of the ground state and  $N_f$  of the excited state are unequal according to Boltzmann's law. Therefore, as we have shown in Sec. 1.2.5,

$$N_f R_{f \rightarrow i} \neq N_i R_{i \rightarrow f} . \quad (13.41)$$

Thus, Einstein came to the conclusion that Fermi's golden rule correctly describes absorption, but does not contain all contributions of emission. The rates being related to the Einstein coefficients by the equation (1.65), we find,

$$R_{f \rightarrow i} = B_{fi} N_f u(\omega_{fi}) \quad (13.42)$$

and

$$\mathcal{S}_{f \rightarrow i} = A_{fi} N_f = \frac{\hbar \omega_{fi}^3}{\pi^2 c^3} B_{if} N_f = \frac{\hbar \omega_{fi}^3}{\pi^2 c^3} \frac{R_{i \rightarrow f}}{u(\omega_{fi})} = \frac{\omega_{fi}^3}{3\pi \epsilon_0 \hbar c^3} |d_{fi}|^2 , \quad (13.43)$$

exploiting the relation (1.70). We shall return to the subject of transitions in Sec. 13.1.

### 13.2.3 Selection rules and electronic transitions

The selection rules that determine which transitions between two sets of quantum numbers  $i \rightarrow f$  are allowed, reflect the symmetry properties of the system, e.g., the conservation of angular momentum (including the spin of the photon) or the change of parity, which can be understood by the fact that the emission of a photon in a particular direction must in some way alter the spatial isotropy of the atom. Note that symmetric oscillations of the shape of the charge distribution *do not radiate*.

Since the electronic transitions via electric dipole radiation are described by  $|\hat{\mathbf{e}} \cdot \mathbf{r}_{fi}|$ , we expect a strong dependence between the polarization state of the light and the existence of a displacement  $\mathbf{r}_{fi}$  in the transition between states. Let us express  $\hat{\mathbf{e}}$  and  $\mathbf{r}_{fi}$  in spherical coordinates, which are more adapted to the problem <sup>5</sup>,

$$x = \mathbf{r} \cdot \hat{\mathbf{e}}_x = r \sin \vartheta \cos \varphi \quad , \quad y = \mathbf{r} \cdot \hat{\mathbf{e}}_y = r \sin \vartheta \sin \varphi \quad , \quad z = \mathbf{r} \cdot \hat{\mathbf{e}}_z = r \cos \vartheta . \quad (13.44)$$

<sup>5</sup>Generally, it is useful to choose the quantization axis along the axis of a magnetic field,

$$\hat{\mathbf{e}}_0 = \frac{\vec{B}}{B} .$$

The second axis may be chosen freely, for example,

$$\hat{\mathbf{e}}_x = \frac{\hat{\mathbf{e}}_0 \times \hat{\mathbf{g}}}{|\hat{\mathbf{e}}_0 \times \hat{\mathbf{g}}|} ,$$

where  $\hat{\mathbf{g}}$  marks an arbitrary direction, for example, of gravity. The third axis must be perpendicular to the first two,

$$\hat{\mathbf{e}}_y = \frac{\hat{\mathbf{e}}_x \times \hat{\mathbf{e}}_0}{|\hat{\mathbf{e}}_x \times \hat{\mathbf{e}}_0|} .$$

Defining,

$$\hat{\mathbf{e}}_{\pm 1} \equiv -\frac{1}{\sqrt{2}}(\hat{\mathbf{e}}_x \pm i\hat{\mathbf{e}}_y) \quad , \quad \hat{\mathbf{e}}_0 \equiv \hat{\mathbf{e}}_z . \quad (13.45)$$

we obtain

$$\begin{aligned} r_{\pm 1} &\equiv \mathbf{r} \cdot \hat{\mathbf{e}}_{\pm 1} = \mathbf{r} \cdot \frac{1}{\sqrt{2}}(\mp \hat{\mathbf{e}}_x - i\hat{\mathbf{e}}_y) = \frac{1}{\sqrt{2}}(\mp x - iy) = \mp \frac{1}{\sqrt{2}}r \sin \vartheta e^{\pm i\varphi} = r\sqrt{\frac{4\pi}{3}}Y_{1,\pm 1}(\vartheta, \varphi) \\ r_0 &\equiv \mathbf{r} \cdot \hat{\mathbf{e}}_0 = \mathbf{r} \cdot \hat{\mathbf{e}}_z = z = r \cos \vartheta = r\sqrt{\frac{4\pi}{3}}Y_{1,0}(\vartheta, \varphi) . \end{aligned} \quad (13.46)$$

Similarly,

$$\epsilon_{\pm 1} \equiv \hat{\mathbf{e}} \cdot \hat{\mathbf{e}}_{\pm 1} \quad , \quad \epsilon_0 \equiv \hat{\mathbf{e}} \cdot \hat{\mathbf{e}}_0 . \quad (13.47)$$

Applying the expansion into spherical coordinates to the matrix element  $\mathbf{r}_{fi} = \langle f|\mathbf{r}|i\rangle$  with  $\hat{\mathbf{e}}_q \cdot \hat{\mathbf{e}}_{q'} = \delta_{qq'}$ , it is easy to check,

$$\hat{\mathbf{e}} \cdot \mathbf{r}_{fi} = \sum_{q=0,\pm 1} (\hat{\mathbf{e}} \cdot \hat{\mathbf{e}}_q) \hat{\mathbf{e}}_q \cdot \sum_{q=0,\pm 1} (\mathbf{r}_{fi} \cdot \hat{\mathbf{e}}_q) \hat{\mathbf{e}}_q = \sum_{q=0,\pm 1} \epsilon_q \langle f|r_q|i\rangle = \sqrt{\frac{4\pi}{3}} \sum_{q=0,\pm 1} \epsilon_q \langle f|rY_{1,q}|i\rangle . \quad (13.48)$$

The matrix elements are,

$$\begin{aligned} \langle f|r_q|i\rangle &= \sqrt{\frac{4\pi}{3}} \langle n_f \ell_f m_f | r Y_{1,q} | n_i \ell_i m_i \rangle \\ &= \sqrt{\frac{4\pi}{3}} \int_0^\infty r^3 R_{n_f, \ell_f} R_{n_i, \ell_i} dr \int Y_{\ell_f, m_f}^* Y_{1,q} Y_{\ell_i, m_i} d\Omega . \end{aligned} \quad (13.49)$$

The radial integral, called *reduced matrix element* or *irreducible matrix element* with the notation,

$$\langle n_f \ell_f || r || n_i \ell_i \rangle \equiv \int_0^\infty r^3 R_{n_f, \ell_f} R_{n_i, \ell_i} dr , \quad (13.50)$$

is always non-zero, while the angular integral is only non-zero, if the values of  $\ell_i, m_i, \ell_f, m_f$  and  $q$  satisfy certain conditions called *selection rules*. We have <sup>6</sup>,

$$\int Y_{\ell_f, m_f}^* Y_{\kappa, q} Y_{\ell_i, m_i} d\Omega = \sqrt{\frac{(2\ell_i+1)(2\ell_f+1)}{4\pi(2\kappa+1)}} \begin{pmatrix} \ell_i & \kappa & \ell_f \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_i & \kappa & \ell_f \\ m_i & q & m_f \end{pmatrix} , \quad (13.51)$$

here with  $\kappa = 1$ . Defining the electric dipole tensor operator,

$$Q_1^q(\mathbf{r}) = er_q(\mathbf{r}) = \sqrt{\frac{4\pi}{3}} Y_1^q(\vartheta, \varphi) er , \quad (13.52)$$

we can write,

$$\langle n_f \ell_f m_f | Q_1^q(\mathbf{r}) | n_i \ell_i m_i \rangle = \frac{\sqrt{(2\ell_i+1)(2\ell_f+1)}}{3} \langle n_f \ell_f || r || n_i \ell_i \rangle \begin{pmatrix} \ell_i & 1 & \ell_f \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_i & \kappa & \ell_f \\ m_i & q & m_f \end{pmatrix} . \quad (13.53)$$

<sup>6</sup>Frequently used are the  $(3j)$ -symbols connected to the Clebsch-Gordans coefficients by,

$$\langle j_i m_i, j_f m_f | J, M \rangle = (-1)^{j_i - j_f + M} \sqrt{2J+1} \begin{pmatrix} j_i & j_f & J \\ m_i & m_f & -M \end{pmatrix} ,$$

This is the *Wigner-Eckart theorem*. The electric dipole operator is a simpler example of a tensor operator  $Q_{\kappa}^q(\mathbf{r})$  characterizing the transition between atomic states. In Excs. 13.2.6.2 and 13.2.6.3 we explicitly calculate, for a hydrogen atom subjected to a magnetic field, components of the electric dipole operator.

Selection rules may be violated in higher orders, e.g., by multipolar radiation, as in the cases of *magnetic dipole transitions* or *electric quadrupole transitions*. This also is the case of the phenomenon of *phosphorescence*, which is a type of fluorescence emitted by metastable states.

### 13.2.3.1 Parity

The *parity* of a state has been defined as,

$$\mathcal{P}\psi_{n\ell m}(\mathbf{r}) = \psi_{n\ell m}(-\mathbf{r}) = (-1)^{\ell}\psi_{n\ell m}(\mathbf{r}), \quad (13.54)$$

as shown above. That is, states with  $\ell$  pair (impair) have even (odd) parity. Now the integral (13.53) only does not vanish, when  $\ell_i + \ell_f + 1 = \text{even}$ . Therefore, *dipole transitions must change the parity of the states*. F.ex., transitions  $S \rightarrow P$  would be possible, while  $S \rightarrow S$  would be prohibited.

### 13.2.3.2 Angular momentum

In the decomposition (13.53) with  $\kappa = 1$  the first Clebsch-Gordan coefficient is only non-zero, when  $|\ell_f - \ell_i| \leq 1 \leq \ell_f + \ell_i$ . That is, *dipole transitions can not change the angular momentum by more than one unit*.

### 13.2.3.3 Magnetic quantum number

In the decomposition (13.53) with  $\kappa = 1$  the second Clebsch-Gordan coefficient is only non-zero, when  $|q| \leq 1$ . That is, *dipole transitions can not change the magnetic quantum number by more than one unit*. This can also be seen from,

$$\int Y_{\ell_f, m_f}^* Y_{\kappa, q} Y_{\ell_i, m_i} d\Omega \propto \int e^{i(m_i + q - m_f)} d\Omega \propto \delta_{m_i + q, m_f}. \quad (13.55)$$

## 13.2.4 Summary of selection rules including fine structure

The fine structure is due to a coupling of the type  $\mathbf{L} + \mathbf{S} = \mathbf{J}$ . In this case,

$$\langle (L, S) J m_J | er | (L', S') J' m'_J \rangle = (-1)^{L'+L+2J'+S+m_j-1} \sqrt{2L+1} \sqrt{2L'+1} \sqrt{2J+1} \sqrt{2J'+1} \\ \delta_{S'S} \begin{Bmatrix} L & L' & 1 \\ J' & J & S \end{Bmatrix} \begin{pmatrix} L' & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L' & 1 & L \\ m' & q & -m \end{pmatrix} \langle nL || er || n'L' \rangle, \quad (13.56)$$

where the first matrix represents a so-called *{6j}-symbol*.

Electric dipolar transitions are excited by Stark-like perturbations,

$$\hat{V}_{stark} = -e\mathbf{d} \cdot \mathcal{E}, \quad (13.57)$$

where  $\mathcal{E} = \mathcal{E}_0 \cos(\mathbf{k} \cdot \mathbf{r} - \omega t)$  is the electric field of an electromagnetic oscillating wave with polarization  $\mathcal{E}_0$ . With  $\mathbf{d} = e z \hat{\mathbf{e}}_z$ , in order to determine which dipole transitions

Table 13.1: Allowed transitions: (1-3) rigorous rules, (4-5) LS-coupling, and (6) intermediate coupling ([https://en.wikipedia.org/wiki/Selection\\_rule](https://en.wikipedia.org/wiki/Selection_rule)).

	(E1)	(M1)	(E2)	(M2)	(E3)	(M3)
(1)	$\Delta J = 0, \pm 1$ ( $\Delta J = 0 \leftrightarrow 0$ )		$\Delta J = 0, \pm 1, \pm 2$ ( $\Delta J = 0 \leftrightarrow 0, 1; \frac{1}{2} \leftrightarrow \frac{1}{2}$ )		$\Delta J = 0, \pm 1, \pm 2, \pm 3$ ( $0 \leftrightarrow 0, 1, 2; \frac{1}{2} \leftrightarrow \frac{1}{2}, \frac{3}{2}; 1 \leftrightarrow 1$ )	
(2)		$\Delta M_J = 0, \pm 1$		$\Delta M_J = 0, \pm 1, \pm 2$		$\Delta M_J = 0, \pm 1, \pm 2, \pm 3$
(3)	$\mathcal{P}_f = -\mathcal{P}_i$		$\mathcal{P}_f = \mathcal{P}_i$		$\mathcal{P}_f = -\mathcal{P}_i$	$\mathcal{P}_f = \mathcal{P}_i$
(4)	one $e^-$ jump $\Delta L = \pm 1$	no $e^-$ jump $\Delta L = 0; \Delta n \neq 0$	none or one $e^-$ jump $\Delta L = 0, \pm 2$	one $e^-$ jump $\Delta L = \pm 1$	one $e^-$ jump $\Delta L = \pm 1, \pm 3$	one $e^-$ jump $\Delta L = 0, \pm 2$
(5)	if $\Delta S = 0$ $\Delta L = 0, \pm 1$ ( $L = 0 \leftrightarrow 0$ )	if $\Delta S = 0$ $\Delta L = 0$	if $\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2$ ( $L = 0 \leftrightarrow 0, 1$ )		if $\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2, \pm 3$ ( $L = 0 \leftrightarrow 0, 1, 2; 1 \leftrightarrow 1$ )	
(6)		if $\Delta S = \pm 1$ $\Delta L = 0, \pm 1, \pm 2$	if $\Delta S = \pm 1$ $\Delta L = 0, \pm 1, \pm 2, \pm 3$ ( $L = 0 \leftrightarrow 0$ )	if $\Delta S = \pm 1$ $\Delta L = 0, \pm 1$ ( $L = 0 \leftrightarrow 0$ )	if $\Delta S = \pm 1$ $\Delta L = 0, \pm 1, \pm 2, \pm 3, \pm 4$ ( $L = 0 \leftrightarrow 0, 1$ )	if $\Delta S = \pm 1$ $\Delta L = 0, \pm 1, \pm 2$ ( $L = 0 \leftrightarrow 0$ )

are possible, we must look at the matrix  $\langle J'm'_j | \hat{z} | Jm_J \rangle$ . Applying the Wigner-Eckart theorem (9.71), it is already possible to determine, between which magnetic quantum numbers  $m_J$  and  $m'_j$  transitions may occur.

We can compare the amplitudes of the various transitions between states  $|m_J\rangle$  and  $|m'_j\rangle$  via the Clebsch-Gordan coefficients (see Exc. 9.3.2.1). Transitions are only possible between states for which the corresponding Clebsch-Gordan coefficient does not zero. This is called *selection rule*. Looking at the equations (9.73), we find for dipolar transitions the following selection rules,

$$\Delta J = 0, \pm 1 \text{ but } (J = 0) \rightarrow (J = 0) \text{ is prohibited} \tag{13.58}$$

$$\Delta m_J = 0, \pm 1 \text{ but } (m_J = 0) \rightarrow (m_J = 0) \text{ is prohibited when } \Delta J = 0 .$$

In addition, we have for the  $\mathbf{L} \cdot \mathbf{S}$  coupling,

$$\Delta S = 0, \Delta L = \pm 1 \text{ and for the electron undergoing the transition } \Delta l = \pm 1 . \tag{13.59}$$

In the presence of a strong magnetic field (Paschen-Back regime) breaking up the  $\mathbf{L} \cdot \mathbf{S}$ -coupling the selection rules are,

$$\Delta m_S = 0, \Delta m_L = 0, \pm 1 . \tag{13.60}$$

For  $\mathbf{j} \cdot \mathbf{j}$ -coupling,

$$\Delta j = 0, \pm 1 \text{ for one electron and } \Delta j = 0 \text{ for all others} . \tag{13.61}$$

For all dipole transitions the parity must change between even and odd.

**Example 57 (Transitions allowed and prohibited in the dipolar approximation):** Examples of allowed transitions are  ${}^2S_{1/2} \leftrightarrow {}^2P_{1/2}$ ,  ${}^1S_0 \leftrightarrow {}^1P_0$ . Prohibited transitions are  ${}^1S_0 \leftrightarrow {}^3P_1$ ,  ${}^2S_{1/2} \leftrightarrow {}^2D_{3/2}$ ,  $(5s)^2 {}^3P_0 \leftrightarrow (5s6s) {}^3P_0$ .

### 13.2.4.1 Selection rules for emission in certain directions

As shown in Eq. (13.48), the excitation rate induced by a light field depends on the relative orientation of the laser polarization  $\hat{\epsilon}$  and the magnetic field  $\vec{B}$ . To take this

dependence into account, we decompose the polarization vector (which can be linear or elliptical) on a coordinate basis, as shown in Eq. (13.47). Thus, the relative amplitude of the transitions  $\Delta m_J = 0$  is proportional to the projection of the polarization vector onto the magnetic field axis,  $\epsilon_0 \equiv \hat{\epsilon} \cdot \hat{\mathbf{e}}_0$ . To estimate the amplitude of the transitions  $\Delta m_J = \pm 1$ , we must project onto the coordinates  $\epsilon_{\pm 1} \equiv \hat{\epsilon} \cdot \hat{\mathbf{e}}_{\pm}$ . Note that the direction of incidence of the beam, given by the wavevector  $\mathbf{k}$ , does not influence the transition probability directly (after all, the spatial dependence  $e^{i\mathbf{k}\cdot\mathbf{r}}$  was removed by the dipolar approximation (13.26)); only through the fact, that the polarization is perpendicular to the propagation vector,  $\hat{\epsilon} \perp \mathbf{k}$ .

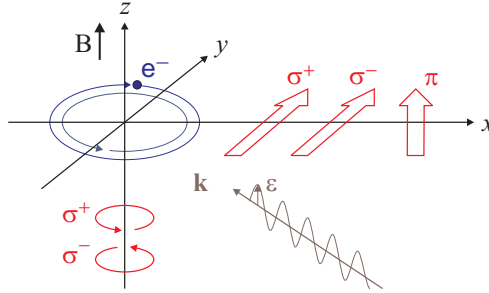


Figure 13.1: Selection rules due to polarization  $\hat{\epsilon}$  of the incident light. The projection of this vector onto the axes  $\pi = \hat{\epsilon} \cdot \hat{\mathbf{e}}_0$  and  $\sigma_{\pm} = \hat{\epsilon} \cdot \hat{\mathbf{e}}_{\pm}$  is proportional to the excitation probability (and, obviously, also to the emission probability).

## 13.2.5 Atomic transition rates

### 13.2.5.1 Irreducible tensor operators

Irreducible tensor operators are defined by their commutation relation with the angular momentum  $\mathbf{J}$ ,

$$[\mathbf{J}, \mathbb{T}_q^{(k)}] = \sum_{q'} \langle kq | \mathbf{J} | kq' \rangle T_{q'}^{(k)}. \quad (13.62)$$

Using the spherical unit vectors  $\hat{\mathbf{e}}_{\pm 1} = \frac{1}{\sqrt{2}}(\mp \hat{\mathbf{e}}_x - i \hat{\mathbf{e}}_y)$  and  $\hat{\mathbf{e}}_0 = \hat{\mathbf{e}}_z$ , we can reduce Cartesian vector operators to first-order tensor operators:

$$\vec{T} = \sum_q T_q^{(1)} \hat{\mathbf{e}}_q \quad \text{resp.} \quad T_q^{(1)} = \vec{T} \cdot \hat{\mathbf{e}}_q. \quad (13.63)$$

Examples for tensor operators are  $\mathbb{I}_0^{(0)}$ ,  $\hat{\mathbf{e}}_q^{(1)}$ ,  $\mathbf{J}_q^{(1)}$ , and  $Y_q^{(k)}$ . The most general tensor product is defined by:

$$\left( \mathbb{T}^{(k)} \times \mathbb{U}^{(k')} \right)_m^{(j)} \equiv \sum_{q, q'} \begin{pmatrix} k & k' & j \\ q & q' & -m \end{pmatrix} \mathbb{T}_q^{(k)} \mathbb{U}_{q'}^{(k')}. \quad (13.64)$$



With this product it is possible to represent scalar, vector or tensor products of higher ranks,

$$\begin{aligned}
 \left(\mathbb{T}^{(1)} \times \mathbb{U}^{(1)}\right)_0^{(0)} &= \frac{1}{\sqrt{3}} \vec{\mathbb{T}} \cdot \vec{\mathbb{U}} \\
 \left(\mathbb{T}^{(1)} \times \mathbb{U}^{(1)}\right)_m^{(1)} &= \frac{1}{\sqrt{2}} (\vec{\mathbb{T}} \times \vec{\mathbb{U}}) \cdot \hat{\mathbf{e}}_m \\
 \left(\mathbb{T}^{(1)} \times \mathbb{U}^{(1)}\right)_0^{(2)} &= -\frac{1}{\sqrt{6}} (3\mathbb{T}_z \mathbb{U}_z - \vec{\mathbb{T}} \cdot \vec{\mathbb{U}}) \\
 \left(\mathbb{T}^{(1)} \times \mathbb{U}^{(1)}\right)_{\pm 1}^{(2)} &= \pm \frac{1}{2} [(\mathbb{T}_x \mathbb{U}_z + \mathbb{T}_z \mathbb{U}_x) \pm i(\mathbb{T}_y \mathbb{U}_z + \mathbb{T}_z \mathbb{U}_y)] \\
 \left(\mathbb{T}^{(1)} \times \mathbb{U}^{(1)}\right)_{\pm 2}^{(2)} &= -\frac{1}{2} [(\mathbb{T}_x \mathbb{U}_x - \mathbb{T}_y \mathbb{U}_y) \pm i(\mathbb{T}_x \mathbb{U}_y + \mathbb{T}_y \mathbb{U}_x)].
 \end{aligned} \tag{13.65}$$

### 13.2.5.2 The Wigner-Eckart theorem

Be  $\mathbb{T}_q^{(k)}$  an irreducible tensor of rank  $k$ . Then, there exists then an irreducible matrix element  $\langle j || \mathbb{T}^{(k)} || j' \rangle$ , which does not depend on the Zeeman sublevels:

$$\langle j m | \mathbb{T}_q^{(k)} | j' m' \rangle = \begin{pmatrix} j' & k & j \\ m' & q & -m \end{pmatrix} \frac{1}{\sqrt{2j+1}} \langle j || \mathbb{T}^{(k)} || j' \rangle. \tag{13.66}$$

From the possible values for the Clebsch-Gordan coefficients follow directly the selection rules for multipolar radiation:

$$\begin{aligned}
 \langle j m | \mathbb{T}_q^{(k)} | j' m' \rangle = 0 \quad \text{else} \quad & E' - E = \hbar \omega \\
 & |j' - j| \leq k \leq j' + j \\
 & m' - m = q \\
 & \tau' \tau = T.
 \end{aligned} \tag{13.67}$$

For tensor products the reduced matrix element can be reduced:

$$\langle j || \left(\mathbb{T}^{(k)} \times \mathbb{U}^{(k')}\right)^{(l)} || j' \rangle = (-)^{j+\ell+j'} \sqrt{2\ell+1} \sum_q \begin{Bmatrix} k & k' & \ell \\ j' & j & q \end{Bmatrix} \langle j || \mathbb{T}^{(k)} || q \rangle \langle q || \mathbb{U}^{(k')} || j' \rangle. \tag{13.68}$$

In particular, it is possible to show,

$$\begin{aligned}
 \langle j || \mathbb{T}^{(0)} || j' \rangle &= \sqrt{2j+1} \delta_{jj'} \\
 \langle j || \mathbb{J}^{(1)} || j' \rangle &= \sqrt{2j+1} \sqrt{j(j+1)} \delta_{jj'} \\
 \langle j || \mathbb{Y}^{(k)} || j' \rangle &= i^{j+k+j'} \frac{\sqrt{2j+1} \sqrt{2k+1} \sqrt{2j'+1}}{4\pi} \begin{pmatrix} j & k & j' \\ 0 & 0 & 0 \end{pmatrix}.
 \end{aligned} \tag{13.69}$$

### 13.2.5.3 Matrix element for angular momentum coupling

We consider states  $|(l, s)j\rangle$ . If the factors  $\mathbb{T}$  and  $\mathbb{U}$  of the tensor product act on different angular momenta, it can be reduced as follows:

$$\langle(l, s)j|\left(\mathbb{T}^{(k)} \times \mathbb{U}^{(k')}\right)^{(l)}|(l', s')j'\rangle = \sqrt{2l+1}\sqrt{2j+1}\sqrt{2j'+1} \begin{Bmatrix} l' & s' & j' \\ k & k' & l \\ l & s & j \end{Bmatrix} \langle l|\mathbb{T}^{(k)}||l'\rangle \langle s|\mathbb{U}^{(k')}||s'\rangle. \quad (13.70)$$

Assuming, in particular,  $\mathbb{U}^{(k')} \equiv \mathbb{I}^{(0)}$ , we get, with  $\mathbb{T}^{(k)} = (\mathbb{T}^{(k)} \times \mathbb{I}^{(0)})^{(k)}$ ,

$$\langle(l, s)j|\mathbb{T}^{(k)}||l', s')j'\rangle = (-)^{l+s+j'+k} \delta_{ss'} \sqrt{2j+1}\sqrt{2j'+1} \begin{Bmatrix} l & l' & k \\ j' & j & s \end{Bmatrix} \langle l|\mathbb{T}^{(k)}||l'\rangle. \quad (13.71)$$

The last equation therefore applies when  $\mathbb{T}^{(k)}$  only acts on the angular momentum component  $l$ . If on the other hand,  $\mathbb{T}^{(k)}$  only acts on  $j$ , then we obviously have,

$$\langle(l, s)j|\mathbb{T}^{(k)}||l', s')j'\rangle = \langle j|\mathbb{T}^{(k)}||j'\rangle. \quad (13.72)$$

## 13.2.6 Exercises

### 13.2.6.1 Ex: Rabi frequency

From the expression for the dipole moment  $d$  and the relationship between the intensity  $I$  and the electric field derive the Rabi frequency  $\Omega$  produced by a laser beam of intensity  $I$  by exciting an atomic dipole transition with the wavelength  $\lambda$  and decay width  $\Gamma$ .

### 13.2.6.2 Ex: Non-stationary state

Construct a non-stationary hydrogen wavefunction with equal contributions of  $(n = 1, \ell = 0, m = 0)$  and  $(n = 2, \ell = 1, m = 1)$ . Calculate the expectation values  $\langle|\mathbf{r}|\rangle$  and  $\langle\mathbf{r}\rangle$  as a function of time.

### 13.2.6.3 Ex: Transitions between Zeeman substates

Consider a hydrogen atom immersed in a uniform magnetic field, described by the Hamiltonian  $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$ , being  $\hat{H}^{(0)} = \hat{\mathbf{p}}^2/2m + V(r)$  and  $\hat{H}^{(1)} = -(\mu_B/\hbar)\hat{\mathbf{L}} \cdot \hat{\mathbf{B}}$  despising the spin <sup>7</sup>.

a. Given the initial function,  $|\psi_m(0)\rangle = \cos \alpha|\phi_{000}\rangle + \sin \alpha|\phi_{21m}\rangle$ , determine its shape at time  $t$ .

b. Calculate the mean value  $\langle\mathbf{d}\rangle_m(t) = \langle\psi_m(t)|\mathbf{d}|\psi_m(t)\rangle$  of the electric dipole operator of the atom  $\mathbf{d} = q\mathbf{R}$ .

c. Analyze the frequencies and polarizations of the emitted radiation by the transition of the excited states  $|\phi_{21m}\rangle$  to the ground state.

<sup>7</sup>See Cohen-Tannoudji, Complemento D.VII

### 13.2.6.4 Ex: Derivation of selection rules

- Prove  $[L_k, r_m] = i\hbar r_n \epsilon_{kmn}$  for an *orbital angular momentum*.
- Using the commutator derived in (a) derive the selection rules for transitions  $\langle \alpha' L' m' | \vec{\varepsilon} \cdot \hat{\mathbf{r}} | \alpha L m \rangle$ , where  $\vec{\varepsilon}$  is the polarization vector of the radiation field chosen to be  $\hat{\mathbf{e}}_0$  or  $\hat{\mathbf{e}}_{\pm}$ .
- Prove  $[\hat{L}^2, [\hat{L}^2, \hat{\mathbf{r}}]] = 2\hbar^2(\hat{\mathbf{r}}\hat{L}^2 + \hat{L}^2\hat{\mathbf{r}})$  for an orbital angular momentum  $\hat{\mathbf{L}}$ .
- Using the commutator derived in (b) derive the selection rule for  $\hat{L}^2$ .

## 13.3 Spectral lines and lifetimes

### 13.3.1 Natural linewidth of a transition

Be  $\Gamma \equiv \sum_f \mathcal{W}_{i \rightarrow f}^{(sp)}$  the spontaneous decay rate of a state  $|i\rangle$ . This means that its population is decreasing,

$$\dot{N}_i = -\Gamma N_i. \quad (13.73)$$

Since  $N_i = \langle \psi_i | \psi_i \rangle$ , we have  $|\psi_i(t)\rangle = |\psi_i(0)\rangle e^{i\omega_{if}t - \Gamma t/2}$ . The Fourier transform is,

$$\begin{aligned} |\xi(\omega)\rangle &= \frac{1}{\sqrt{2\pi}} \int_0^\infty |\psi_i(t)\rangle e^{-i\omega t} dt = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{i\omega_{if}t - i\omega t - \Gamma t/2} dt |\psi_i(0)\rangle \\ &= \frac{1}{\sqrt{2\pi}} \lim_{t \rightarrow \infty} \frac{e^{i(\omega_{if} - \omega)t - \Gamma t/2} - 1}{i(\omega_{if} - \omega) - \Gamma/2} |\psi_i(0)\rangle = \frac{1}{\sqrt{2\pi}} \frac{1}{i(\omega - \omega_{if}) + \Gamma/2} |\psi_i(0)\rangle. \end{aligned} \quad (13.74)$$

The spectrum,

$$|\xi(\omega)|^2 = \frac{1}{2\pi} \frac{1}{(\omega - \omega_{if})^2 - \Gamma^2/4}, \quad (13.75)$$

is a *Lorentz distribution*. Note, that the natural linewidth can be blurred by line broadening effects, such as the Doppler broadening or collisions between atoms. These effects will be discussed in the Chp. 14.6.1.

Excited states can sometimes decay into various states of lower energy. In this case the linewidth is simply given by the sum of the partial decay rates, since the convolution of Lorentz distributions  $\mathcal{L}_{\Gamma_k}$  with widths  $\Gamma_k$  is again a Lorentzian with the total width  $\Gamma = \sum_k \Gamma_k$ .

### 13.3.2 Beyond perturbative treatment

We look for an equation to describe the temporal evolution of atoms interacting with a radiation field. However, to portray systems that contain excitation and relaxation processes occurring simultaneously, a theory based on Schrödinger's equation is no longer sufficient, because it is only capable of explaining stimulated processes, such as the absorption of a monochromatic wave. Dissipative process, such as spontaneous emission, require a more general approach to describe the evolution of a system. A single wavefunction is, in general, not enough to represent such a system nor to quantify the probabilities associated with each of its states, but we rather need an ensemble of wavefunctions.

A comprehensive formalism, capable of dealing with ensembles of wavefunctions and dissipative processes is the so-called density operator formalism. The dynamics

of the density operator is ruled by the *Bloch equations* [78], which provide equations of motion for the temporal evolution of populations, described by the diagonal terms of the operator, and coherences of the system, represented by the non-diagonal terms, as we shall see in the next chapter. The Bloch equations were initially developed to understand nuclear magnetic resonance (NMR) phenomena.

### 13.3.3 Line and oscillator strength

In addition to the Einstein coefficients  $A_{21}$ ,  $B_{21}$ , and  $B_{12}$ , the amplitude of the transition dipole moments  $d_{12}$  and the absorption cross-section  $\sigma_{0a}(\omega)$ , three other quantities are sometimes used to characterize atomic transitions: the oscillator strength  $f$ , the line strength  $S$ , and the spectral absorption cross section  $\sigma_\omega$ . In the following sections, we will connect these different concepts.

The line strength  $S$  is defined as the square of the transition dipole moment summed over all degeneracies of the ground and excited states,

$$S_{12} = S_{21} = \sum_{m_1, m_2} |\langle \psi_{1, m_1} | d | \psi_{2, m_2} \rangle|^2 . \quad (13.76)$$

The notion of the line strength becomes significant when working with real atoms characterized by degenerate ground and excited states. In such cases we need to extend the meaning of  $d_{12}$  and consider transitions between each of the degenerate sublevels. For a non-degenerate two-level atom, the quantities  $d_{12}$  and  $A_{21}$  are simply related by,

$$A_{21} = \frac{\omega_0^3}{3\pi\epsilon_0\hbar c^3} d_{12}^2 . \quad (13.77)$$

If the lower level would be degenerate, the spontaneous emission rate coefficient would be given by the sum of all possible deexcitation rates. In this case,  $d_{12}^2$  is defined as the sum of the elements of the transition matrix coupling the excited and the lower states,

$$d_{12}^2 = \sum_{m_1} |\langle \psi_{1, m_1} | d | \psi_2 \rangle|^2 . \quad (13.78)$$

Now, it can be shown that the spontaneous emission rate from any sublevel of a degenerate excited state toward a lower level (that is, the sum over all lower sublevels) is the same for all excited sublevels.<sup>8</sup> This statement reflects the intuitively plausible idea that spontaneous emission must be isotropic and unpolarized, if the sublevels of an excited state are uniformly populated. Therefore, the insertion of Eq. (13.78) into (13.77) should produce correct results, even when the excited state is degenerate. Comparing the sum over all upper and lower degeneracies with the line strength  $S$ ,

$$S_{12} = \sum_{m_1, m_2} |\langle \psi_{1, m_1} | d | \psi_{2, m_2} \rangle|^2 = g_2 d_{12}^2 . \quad (13.79)$$

Therefore, the insertion of Eq. (13.79) into (13.77) must be accompanied by a factor of  $1/g_2$  to correct for the fact that all excited sub-levels radiate at the same rate.

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<sup>8</sup>This applies to Zeeman sublevels (summing up  $(3j)$ -coefficients). Check for other degeneracy (also summing up  $\{6j\}$ -coefficients)!

Therefore, using the  $S_{12}$  of Eq. (13.79) the correct expression relating the transition dipole between degenerate levels to the spontaneous emission rate is,

$$S_{12} = g_2 \frac{3\pi\epsilon_0\hbar c^3}{\omega_0^3} A_{21} , \quad (13.80)$$

meaning that the line strength is proportional to the sum of the spontaneous emission rates  $A_{21}$  from each one of the  $g_2$  excited levels toward all fundamental levels.

For an atom with two levels separated by an energy  $\hbar\omega_0$  the *oscillator strength for emission* is defined as a measure for the radiative decay rate  $A_{21}$  as compared to the radiative decay rate  $\gamma_e$  of a classical electronic oscillator with frequency  $\omega_0$ :

$$f_{21} = -\frac{1}{3} \frac{A_{21}}{\gamma_e} . \quad (13.81)$$

In case of degeneracy the *oscillator strength for absorption* is consequently defined by,

$$f_{12} = -\frac{g_2}{g_1} f_{21} = \frac{g_2}{3g_1} \frac{A_{21}}{\gamma_e} . \quad (13.82)$$

The transitions  $S \longleftrightarrow P$  in real atoms behave roughly as classical oscillators, that is,  $A_{21} \simeq \gamma_e$ . The factor  $\frac{1}{3}$  in the definition compensates for the triple degeneracy of the  $P$  levels. So, a transition  $S \longleftrightarrow P$  which behaves exactly as a classical oscillator would be characterized by an oscillator strength for emission of  $f_{21} = -\frac{1}{3}$  and an oscillator strength for absorption of  $f_{12} = 1$ . The classical expression for  $\gamma_e$  derived from the *Lorentz model* is [287],

$$\gamma_e = \frac{e^2\omega_0^2}{6\pi\epsilon_0 m_e c^3} . \quad (13.83)$$

Therefore, in terms of the  $A_{21}$  coefficient and of fundamental constants, the oscillator strength for absorption is given by,

$$f_{12} = A_{21} \frac{2\pi\epsilon_0 m_e c^3}{e^2\omega_0^2} . \quad (13.84)$$

Oscillator strengths obey certain sum rules that are useful for analyzing the relative intensities of atomic spectral lines. For example, atoms with single valence electrons (which are closer to the classical situation) obey the following sum rule,

$$\sum_k f_{ik} = 1 , \quad (13.85)$$

where the sum goes over all the excited states reached from the ground state. Alkaline atoms are approximately one-electron systems, and the oscillator strength of the first transition  $S \longrightarrow P$  is typically of the order of  $f_{12} = 0.7 - 0.95$ . The sum rule tells us that most of the total transition probability for the excitation of the valence electron is concentrated in the first transition  $S \longrightarrow P$ , and that transitions to higher states will

be comparatively weaker. Another sum rule exists for the excitation and spontaneous emission from excited intermediate states  $j$ :

$$\sum_{i < j} f_{ji} + \sum_{k > j} f_{jk} = Z, \quad (13.86)$$

which is called the *Thomas-Reiche-Kuhn sum rule*. In the form of many electrons [Eq. (13.86)] this rule is very useful, when  $Z$  is the number of equivalent electrons, that is, electrons with the same quantum numbers  $n, l$ . Note also, that the numbers are intrinsically negative. Oscillator strengths are often used in astrophysics and plasma spectroscopy<sup>9</sup>. They are sometimes tabulated as  $\log gf$ , where,

$$g_1 f_{12} = -g_2 f_{21} \equiv gf. \quad (13.87)$$

### 13.3.4 Propagation of light in dielectric media

Let us now use Einstein's theory to calculate the interaction of light with a gas being so diluted that we can treat the interaction as occurring with individual atoms. We first consider the propagation of light through a continuous (non-conducting) dielectric medium. The interaction of light with such a medium allows us to introduce important quantities, such as the polarization, the susceptibility, the index of refraction, the extinction coefficient, and the absorption coefficient. We shall see later that the polarization can be considered as densities of dipole moments induced into the dielectric medium by the oscillating light field. But for the moment, we simply begin by defining the polarization  $\vec{\mathcal{P}}$  with respect to an applied electric field  $\vec{\mathcal{E}}$  as,

$$\vec{\mathcal{P}} = \varepsilon_0 \tilde{\chi}_e \vec{\mathcal{E}}. \quad (13.88)$$

The tilde  $\sim$  ornamenting the quantities means that they are complex, and that measurable quantities must be taken from the real parts.  $\chi_e$  is the linear complex *electric susceptibility*, which is an intrinsic property of the medium responding to the light field. It is related to the medium's *dielectric constant*,

$$\tilde{\varepsilon} = \varepsilon_0 (1 + \tilde{\chi}_e). \quad (13.89)$$

Near resonances, the susceptibility is a strong function of frequency and can be spatially anisotropic. It is a complex quantity with a real dispersive part,  $\chi'_e$ , and an imaginary absorptive part,  $\chi''_e$ ,

$$\tilde{\chi}_e = \chi'_e + i\chi''_e. \quad (13.90)$$

Several expressions that we already know become modified in a dielectric medium,

$$\left(\frac{kc}{\omega}\right)^2 = 1 + \tilde{\chi}_e, \quad (13.91)$$

<sup>9</sup>To find information about the atomic transition lines see 'http://www.nist.gov/pml/data/asd.cfm'.

with  $\chi_e = 0$  in free space. In a dielectric medium,  $\frac{kc}{\omega}$  becomes a complex quantity, conventionally expressed by,

$$\frac{kc}{\omega} = \eta + i\kappa, \quad (13.92)$$

where  $\eta$  is the *refraction index* and  $\kappa$  the *extinction coefficient* of the dielectric medium. The relationships between the refractive index, the extinction coefficient and the two components of the susceptibility are,

$$\eta^2 - \kappa^2 = 1 + \chi'_e \quad \text{and} \quad 2\eta\kappa = \chi''_e. \quad (13.93)$$

Note, that in a transparent dielectric medium there is no absorption, such that,  $\eta^2 = 1 + \chi'_e = \frac{\epsilon}{\epsilon_0}$ . Within a dielectric medium, we obtain the propagating wave solutions of Maxwell's equations by substituting  $k$  with the equation (13.92)

$$\vec{\mathcal{E}} = \vec{\mathcal{E}}_0 e^{i\omega(\frac{z}{c} - t) - \omega\frac{\kappa}{c}z}. \quad (13.94)$$

The relationship between the amplitudes of the electric and magnetic fields is,<sup>10</sup>

$$\mathcal{B}_0^{(\chi)} = \sqrt{\epsilon\mu}\mathcal{E}_0 = \sqrt{\epsilon_0\mu_0}\sqrt{1 + \tilde{\chi}_e}\mathcal{E}_0 = \frac{1}{c}(\eta + i\kappa)\mathcal{E}_0 = (\eta + i\kappa)\mathcal{B}_0. \quad (13.95)$$

We use the subscript ( $\chi$ ) to mark quantities within the dielectric medium. The average energy density is,

$$\bar{u}^{(\chi)} = \frac{1}{2}\epsilon_0\eta^2|\vec{\mathcal{E}}|^2 = \eta^2\bar{u}. \quad (13.96)$$

Now, the intensity of the light beam in a dielectric medium is attenuated,

$$\bar{I}^{(\chi)} = \frac{1}{\mu_0}|\vec{\mathcal{E}} \times \vec{\mathcal{B}}| = \frac{1}{2}\epsilon_0c\eta|\vec{\mathcal{E}}|^2 = \frac{1}{2}\epsilon_0c\eta\mathcal{E}_0^2 e^{-2\omega\kappa z/c} = \bar{I}_0^{(\chi)} e^{-Kz}, \quad (13.97)$$

where

$$\bar{I}_0^{(\chi)} = \frac{1}{2}\epsilon_0c\eta\mathcal{E}_0^2 \quad (13.98)$$

is the intensity at the point, where the light enters the medium, and

$$K = 2\frac{\omega\kappa}{c} = \frac{\omega}{\eta c}\chi''_e \quad (13.99)$$

is called *absorption coefficient*. Note, that the energy flow  $\bar{I}^{(\chi)}$  in the dielectric medium is always the product of energy density and propagation velocity  $c/\eta$ . Note also, since the frequency  $\omega$  of the light propagating through the dielectric remains the same, the wavelength shrinks like  $\lambda = \frac{c/\eta}{\nu}$  [440].

**Example 58 (Energy density and Poynting vector in a dielectric medium):** The energy density in vacuum,  $\bar{u} = \frac{\epsilon_0}{4}|\vec{\mathcal{E}}|^2 + \frac{1}{4\mu_0}|\vec{\mathcal{B}}|^2$ , becomes in a dielectric medium,

$$\begin{aligned} \bar{u}^{(\chi)} &= \frac{1}{4}\text{Re}(\epsilon\vec{\mathcal{E}} \cdot \vec{\mathcal{E}}^* + \frac{1}{\mu_0}\vec{\mathcal{B}} \cdot \vec{\mathcal{B}}^*) = \frac{\text{Re}\epsilon}{4}|\vec{\mathcal{E}}|^2 + \frac{1}{4\mu_0}\left|\frac{\eta + i\kappa}{c}\vec{\mathcal{E}}\right|^2 \\ &= \frac{\epsilon_0}{4}(1 + \chi'_e)\mathcal{E}_0^2 + \frac{\epsilon_0}{4}|\eta + i\kappa|^2\mathcal{E}_0^2 = (\eta^2 - \kappa^2 + \eta^2 + \kappa^2)\frac{\epsilon_0}{4}\mathcal{E}_0^2 = \frac{\epsilon_0}{2}\eta^2\mathcal{E}_0^2, \end{aligned}$$

where we only consider the real part of the susceptibility  $\chi_e$ . On the other hand, the Poynting vector is,

$$\bar{I} = \frac{1}{2\mu_0}\text{Re}[\vec{\mathcal{E}} \times \vec{\mathcal{B}}^*] = \frac{\epsilon_0c^2}{2}\mathcal{E}_0^2 \left[ e^{-2\omega\kappa z/c} \frac{\eta + i\kappa}{c} \right] = \frac{\epsilon_0c}{2}\eta\mathcal{E}_0^2 e^{-2\omega\kappa z/c}.$$

<sup>10</sup>In a dielectric medium,  $\mu \simeq \mu_0$ .

### 13.3.5 Propagation of light in dilute gases

We are often interested in the attenuation of the intensity of a beam of light traversing a dilute gas of resonant scattering atoms. The equation (13.97) describes this attenuation via the properties of the dielectric material. What we are looking for in fact is a microscopic equivalent description in terms of absorption and light emission rates. The Einstein rate equation yields the *temporal* transition rates, but does not say how they relate to the *spatial* attenuation length of the light beam. We now consider a beam propagating through a cell containing an absorptive gas and assume that, along the optical axis, absorption and emission reach a steady state. We begin with the Einstein equation (1.65), and write

$$0 = -N_1 B_{12} u(\omega) + N_2 B_{21} u(\omega) + N_2 A_{21} . \quad (13.100)$$

We now use the result (1.69) to write

$$N_2 A_{21} = u(\omega) B_{12} (N_1 - N_2 \frac{g_1}{g_2}) . \quad (13.101)$$

In steady state, the number of the excited atoms is,

$$N_2 = \frac{u(\omega) B_{12} N_1}{A_{21} + \frac{g_1}{g_2} u(\omega) B_{12}} . \quad (13.102)$$

Now, we must treat the refractive index of the dielectric medium carefully. The expression for the energy density must be modified following Eq. (13.96)

$$u(\omega) = \frac{u^{(x)}(\omega)}{\eta^2} . \quad (13.103)$$

To use the Einstein coefficients, which suppose propagation at the speed of light in the vacuum<sup>11</sup>, we must correct the energy density in the dielectric medium before using it in the equation (13.102) [440]. Therefore, we should express  $u(\omega)$  in this equation by  $u^{(x)}(\omega)/\eta^2$ ,

$$N_2 A_{21} = \frac{u^{(x)}(\omega)}{\eta^2} B_{12} (N_1 - N_2 \frac{g_1}{g_2}) . \quad (13.104)$$

Multiplying the two sides with  $\hbar\omega_0$ , we see that the left side describes the rate of energy scattered out of the beam by spontaneous emission, while the right side describes the energy loss of the beam, i.e., the difference between energy removed by absorption and energy returned to the beam by stimulated emission,

$$\frac{d\bar{U}^{(x)}}{dt} = -N_2 A_{21} \hbar\omega_0 = -\frac{u^{(x)}(\omega)}{\eta^2} B_{12} (N_1 - N_2 \frac{g_1}{g_2}) \hbar\omega_0 . \quad (13.105)$$

---

<sup>11</sup>In Einstein's model, what really matters for inducing transitions is the flux of photons, that is, the number of photons that traverse an atom per unit of time. This flux can not depend on the index of refraction. Therefore, we must use the spectral energy density calculated in the vacuum  $\bar{u}_\omega$ .



### 13.3.6 Susceptibility and polarization

Everything we have developed so far involves the coupling of a single-mode optical field with a two-level atom. For this system the Schrödinger equation would be perfectly adequate. If we want to include spontaneous emission, however, we need the density matrix formalism. The equations (6.63) do not respect the fact that the excited state is not only coupled to the incident light field (with the frequency  $\omega$ ), but also with all modes of the electromagnetic vacuum. To take spontaneous emission into account, we need to go back to Sec. 1.2.7 and recalculate the absorption coefficient  $K$  [Eqs. (13.99), (1.73)] from the relationship between susceptibility and polarization, Eq. (13.88). In order to obtain a new expression for the susceptibility, we will write the polarization in terms of an ensemble of individual transition dipoles. We will use the solutions for the coefficients of two coupled atomic levels, Eqs. (6.63). However, we will modify the expression for  $C_2$  by adding a term that reflects the spontaneous emission from the upper state. The resulting expression for the susceptibility (and hence the absorption coefficient) will reflect the finite 'natural' life time of the upper state. For the present discussion we are only concerned with the temporal dependence of the actual light wave, which we write as,

$$\vec{\mathcal{E}}(t) = \vec{\mathcal{E}}_0 \cos \omega t = \frac{1}{2} [e^{i\omega t} + e^{-i\omega t}] . \quad (13.106)$$

Then we consider how to write the polarization in terms of a susceptibility when the field contains two conjugate frequencies,  $\pm\omega$ . Substituting into Eq. (13.88), we have,

$$\vec{\mathcal{P}}(t) = \frac{1}{2} \epsilon_0 \vec{\mathcal{E}}_0 [\chi(\omega) e^{i\omega t} + \chi(-\omega) e^{-i\omega t}] . \quad (13.107)$$

The polarization can also be expressed in terms of the density of the transition dipoles in a gas of two-level atoms,

$$\vec{\mathcal{P}}(t) = \frac{N}{V} \mathbf{d}_{12}(t) \longrightarrow \frac{N}{V} \langle \mathbf{d}_{12}(t) \rangle . \quad (13.108)$$

where  $\mathbf{d}$  is the transition dipole of only one atom,  $N = V$  is the atomic density, and the quantum expectation value for the transition dipole moment is,

$$\langle \mathbf{d}_{12} \rangle = -e \int \Psi \sum_j \mathbf{r}_j \Psi d^3r . \quad (13.109)$$

Now, from Eq. (6.58),

$$\langle \mathbf{d}_{12} \rangle = -e \left[ a_1^* a_2 \langle \psi_1 | \sum_j \mathbf{r}_j | \psi_2 \rangle e^{-i\omega_0 t} + a_1 a_2^* \langle \psi_2 | \sum_j \mathbf{r}_j | \psi_1 \rangle e^{i\omega_0 t} \right] . \quad (13.110)$$

To simplify the notation we define  $\langle \mathbf{r}_{mn} \rangle \equiv \langle \psi_m | \sum_j \mathbf{r}_j | \psi_n \rangle$  and obtain,

$$\langle \mathbf{d}_{12} \rangle = -e [a_1^* a_2 \langle \mathbf{r}_{12} \rangle e^{-i\omega_0 t} + a_1 a_2^* \langle \mathbf{r}_{21} \rangle e^{i\omega_0 t}] . \quad (13.111)$$

Now, we only need to replace the solutions of the coupled equations by relating  $a_1$  and  $a_2$  of the Eqs. (6.63) in (13.111) which, in turn, can be inserted into the equation

(13.107). Thus we obtain an expression for the polarization in terms of properties of the atoms and the incident field. However, the solution for  $a_2$ , Eq. (6.79), does not consider spontaneous emission. Now, we will introduce an ad hoc modification of Eq. (6.63) by including a radiative loss constant  $\gamma$ ,

$$\Omega^* \cos \omega t e^{i\omega_0 t} a_1 - \nu \gamma a_2 = i \frac{da_2}{dt}. \quad (13.112)$$

This term does NOT EXPLAIN spontaneous emission. It simply takes into account the existence of the effect and characterizes its amplitude through  $\gamma$ : If the incident field is turned off ( $\Omega^* = 0$ )

$$-\nu \gamma a_2 = i \frac{da_2}{dt} \quad (13.113)$$

and

$$a_2(t) = a_2(0) e^{-\gamma t}. \quad (13.114)$$

Now the probability of finding an atom in the excited state (or the fraction of excited atoms in an ensemble) is,

$$N_2/N = |a_2(t)|^2 = |a_2(0)|^2 e^{-2\gamma t}. \quad (13.115)$$

Comparing this behavior with the result obtained from the Einstein rate equation, we see immediately,

$$A_{21} = 2\gamma \equiv \Gamma. \quad (13.116)$$

Now the solution for our improved  $a_2(t)$  coefficient is,

$$a_2(t) = -\frac{1}{2} \Omega^* \left[ \frac{e^{i(\omega_0 + \omega)t}}{\omega_0 + \omega - i\gamma} + \frac{e^{i(\omega_0 - \omega)t}}{\omega_0 - \omega - i\gamma} \right]. \quad (13.117)$$

Making the weak field approach,  $C_1(t) \simeq 1$ , replacing the values obtained for  $a_{1,2}$  in the transition dipole (13.111) and replacing the average of the orientations,  $|\langle r_{12} \rangle|^2 \rightarrow \frac{1}{3} |\langle r_{12} \rangle|^2$ , in the polarization (13.108), we obtain,

$$\vec{\mathcal{P}}(t) = \frac{N e^2 |\langle r_{12} \rangle|^2 \vec{\mathcal{E}}_0}{V 6\hbar} \left[ \frac{e^{i\omega t}}{\omega_0 + \omega - i\gamma} + \frac{e^{i\omega t}}{\omega_0 - \omega + i\gamma} + \frac{e^{-i\omega t}}{\omega_0 - \omega - i\gamma} + \frac{e^{-i\omega t}}{\omega_0 + \omega + i\gamma} \right]. \quad (13.118)$$

We compare this result with Eq. (13.107) and identify the susceptibility  $\chi(\omega)$  in terms of the atomic properties and the frequency of the incident field,

$$\begin{aligned} \chi(\omega) &= \frac{N e^2 |\langle r_{12} \rangle|^2}{3\epsilon_0 \hbar V} \left[ \frac{1}{\omega_0 - \omega - i\gamma} + \frac{1}{\omega_0 + \omega - i\gamma} \right] \\ &= \frac{N e^2 |\langle r_{12} \rangle|^2}{3\epsilon_0 \hbar V} \left[ \frac{\omega_0 - \omega}{(\omega_0 - \omega)^2 + \gamma^2} + \frac{\omega_0 + \omega}{(\omega_0 + \omega)^2 + \gamma^2} + \nu \gamma \left( \frac{1}{(\omega_0 - \omega)^2 + \gamma^2} + \frac{1}{(\omega_0 + \omega)^2 + \gamma^2} \right) \right]. \end{aligned} \quad (13.119)$$

In most practical situations in the laboratory  $\omega$  will not be tuned more than some 100 GHz away from  $\omega_0$ , hence  $|\omega_0 - \omega| \lesssim 10^{11}$  Hz. With optical frequencies  $\omega \simeq 10^{15}$  Hz, it is clear that the second term on the right hand side of Eq. (13.119) will be negligible compared to the first one. Therefore, we can discard the second term and write the susceptibility as,

$$\chi(\omega) \simeq \frac{N e^2 |\langle r_{12} \rangle|^2}{3\epsilon_0 \hbar V} \frac{1}{\omega_0 - \omega - i\gamma} = \frac{N d_{12}^2}{3\epsilon_0 \hbar V} \frac{-\Delta + i\Gamma/2}{\Delta^2 + (\Gamma/2)^2} = \frac{n \hbar \Omega^2}{3\epsilon_0 E_0^2} \frac{-\Delta + i\Gamma/2}{\Delta^2 + (\Gamma/2)^2}. \quad (13.120)$$

We identify the real and imaginary parts,  $\chi = \chi' + i\chi''$ , and express, starting from Eq. (13.99), the absorption coefficient as,

$$K = \frac{\omega}{c\eta} \chi''(\omega) = \frac{\pi N d_{12}^2 \omega_0}{3\epsilon_0 \hbar c V} \frac{\Gamma/2\pi}{\Delta^2 + (\Gamma/2)^2} = \frac{\pi N d_{12}^2 \omega_0}{3\epsilon_0 \hbar c V} \mathcal{L}(\omega - \omega_0) . \quad (13.121)$$

The Lorentzian profile term governs the frequency dependence of the absorption coefficient. We see that  $K$  exhibits a peak at the resonance frequency  $\omega_0$  and a width of  $\Gamma$ . The factor of  $\pi$  inserted in the numerator and denominator of the right term of Eq. (13.121) allows to normalize the profile. We have also assumed in Eq. (13.121) that the gas is sufficiently dilute for  $\eta \simeq 1$  to hold, and that the line is sufficiently narrow to be able to replace  $\omega$  with  $\omega_0$ , such that,

$$\frac{\omega}{c\eta} \longrightarrow \frac{\omega_0}{c} . \quad (13.122)$$

The absorption cross section has the same lineshape, since from Eqs. (1.73) and (13.121) we have,

$$\sigma_{0a} = \frac{\pi d_{12}^2 \omega_0}{3\epsilon_0 \hbar c V} \mathcal{L}(\omega - \omega_0) , \quad (13.123)$$

consistent with our previous expression for the frequency dependence of the absorption cross-section. We can also write the imaginary component of the susceptibility in terms of the cross section using the Eqs. (1.73) and (13.121)

$$\chi'' = \frac{cN}{\omega_0 V} \sigma_{0a} . \quad (13.124)$$

Do the Excs. 13.3.7.1 until 13.3.7.3.

### 13.3.6.1 Permittivity and permeability

The permittivity and relative permeability of a dense gas can be connected to the microscopic quantities through the *Clausius-Mossotti formula*,

$$\epsilon_r = \frac{1 + \frac{2}{3} \frac{N}{V} \alpha_{pol,e}}{1 - \frac{1}{3} \frac{N}{V} \alpha_{pol,e}} , \quad \mu_r = \frac{1 + \frac{2}{3} \frac{N}{V} \alpha_{pol,m}}{1 - \frac{1}{3} \frac{N}{V} \alpha_{pol,m}} , \quad (13.125)$$

that is, to the susceptibilities,

$$\chi_\epsilon = \epsilon_r - 1 = \frac{\frac{N}{V} \alpha_{pol,e}}{1 - \frac{1}{3} \frac{N}{V} \alpha_{pol,e}} , \quad \chi_\mu = \mu_r - 1 = \frac{\frac{N}{V} \alpha_{pol,m}}{1 - \frac{1}{3} \frac{N}{V} \alpha_{pol,m}} , \quad (13.126)$$

where the induced electric and magnetic polarizabilities are,

$$\alpha_{pol,e} = \frac{2d_{fi}}{|\vec{\mathcal{E}}_p|} \rho_{if} , \quad \alpha_{pol,m} = \frac{2m_{fi}}{|\vec{\mathcal{B}}_p|} \rho_{if} . \quad (13.127)$$

$d_{fi}$  and  $m_{fi}$  are the dipole moments for electric and magnetic transitions and  $\rho_{if}$  the coherences excited in these transitions, which can be calculated from the Bloch equations. The relative strength between magnetic and electrical transitions is,

$$\frac{2\mu_B}{cea_B} = \alpha . \quad (13.128)$$

### 13.3.7 Exercises

#### 13.3.7.1 Ex: Solution for the susceptibility

Show that the solution of Eq. (13.112) is given by the result (13.117).

#### 13.3.7.2 Ex: Width of the absorption band

The resonator of a dye laser with a large emission bandwidth additionally contains an absorbing (dense) gas. The absorption spectrum of the gas is Lorentzian with a width of 3 GHz, and the absorption coefficient has, in the middle of the absorption line (at 600 nm), the value of 0.2. What are the maximum and minimum relative spectral distances  $\Delta f/\Delta f_0$  of the axial modes within the spectral range of the absorption, compared to the distances  $\Delta f_0$  of the empty resonator?

#### 13.3.7.3 Ex: Einstein's rate equations

Show that the solution of the equations (6.63) is given by the result (13.117) using the approximation of short times,  $C_1 \simeq 1$ .

## 13.4 Further reading

M. Weissbluth, *Atoms and Molecules* [ISBN]

J. Weiner et al., *Light-matter Interaction, Fundamentals and Applications* [DOI]



# Chapter 14

## The Bloch equations

So far we mainly considered low amplitude light fields with broadband emission and incoherent phases that interact weakly with an atom or a dilute gas. The expression (6.80) allowed us to calculate the probability of finding a two-level atom exposed to a light field in the excited state. But these expressions were obtained by averaging over the spectral width of the line, ignoring any phase relationship between the incident field and the excited dipole, and basically assuming a negligible depopulation of the ground state. For the first half of the 20-th century these assumptions matched the available light sources, usually incandescent, arc or plasma discharge lamps. After the invention of the laser in 1958, single mode and pulsed lasers quickly replaced the lamps as a source for optical excitation. These new light sources initiated a revolution in optical science, the consequence of which continue to reverberate through modern sciences and applied technologies.

The characteristics of laser sources are far superior to the old lamps in all respects. They are intense, collimated, spectrally narrow and phase coherent. The laser gave rise to a multitude of new spectroscopic techniques and new disciplines, such as quantum electronics, the study of statistical properties of light in quantum optics, optical cooling and trapping of microscopic particles, the control of chemical reactivity, and new technologies for imaging and high resolution microscopy.

To tackle the problem from the base we need first to examine what happens when our two-level atom interacts with light sources, which are spectrally narrow in comparison to the natural width of optical transitions, and what happens when the states have a well-defined polarization and phase and the intensities are sufficient to significantly depopulate the ground state. We will look out for an equation that describes the temporal evolution of atoms interacting strongly with a single mode of the radiation field.

A first attempt to solve this problem could be to use the Schrödinger equation, which describes the temporal evolution of the state of any system. In fact, as long as we are only interested in stimulated processes, such as the absorption of a monochromatic wave, the Schrödinger equation would suffice. A problem arises when we want to describe relaxation processes at the same time as excitation processes, after all in most realistic situations the atom reaches a steady state, where the rate of excitation and relaxation are equal. Spontaneous emission (and any other dissipative process) must therefore be included in the physical description of the temporal evolution of our light-atom system. In this case, however, our system is no longer restricted to a single mode of the light field and the two atomic states of excitation. Spontaneous emission populates a statistical distribution of states of the light field and leaves the atom in

a superposition of many momentum states. This situation can not be described by a single wavefunction, but only by a distribution of wavefunctions, and we can only expect to calculate the probability of finding the system within this distribution. The Schrödinger equation, therefore, no longer applies, and we need to trace the time evolution of a system characterized by a density operator describing a statistical mixture of quantum states. The equations which describe the time evolution of the matrix elements of this density operator are the optical Bloch equations, and we must use them instead of the Schrödinger equation. In order to appreciate the origin and the physical content of the optical Bloch equations we begin by reviewing the rudiments of the density matrix theory.

## 14.1 Density matrix

### 14.1.1 The density operator

We define the *statistical operator* or *density operator*<sup>1</sup>,

$$\hat{\rho} \equiv \sum_k p_k \hat{P}_k \quad \text{where} \quad \hat{P}_k \equiv |\psi_k\rangle\langle\psi_k|, \quad (14.1)$$

where  $\{|\psi_k\rangle\}$  is a complete set of orthonormal states of the system under study. We have a statistical distribution of these states with  $p_k$  being the probability of finding  $|\psi_k\rangle$  in the set. Obviously,  $\sum_k p_k = 1$ . That is, the density operator acts on a member of the set  $|\psi_k\rangle$  such as to extract the probability of finding the system in  $|\psi_k\rangle$ ,

$$\hat{\rho}|\psi_m\rangle = \sum_k p_k |\psi_k\rangle\langle\psi_k|\psi_m\rangle = p_m |\psi_m\rangle. \quad (14.2)$$

If all members of the set are in the same state, for example  $|\psi_k\rangle$ , the density operator reduces to,

$$\hat{\rho} = |\psi_k\rangle\langle\psi_k|, \quad (14.3)$$

and the system is in a *pure state* with  $p_k = \delta_{kk'}$ . Each time a quantum state can be expressed by a single wave function, it is a pure state, but it does not have to be an eigenstate. Starting from the equation (14.2) we find the diagonal elements of the density matrix, which are the probabilities of finding the system in  $|\psi_m\rangle$ ,

$$\langle\psi_m|\hat{\rho}|\psi_m\rangle = p_m. \quad (14.4)$$

<sup>1</sup>In the presence of degeneracy or a continuous spectrum we can generalize the definition:

$$\hat{\rho} \equiv \sum_k p_k \hat{P}_k + \int p_\lambda \hat{P}_\lambda d\lambda \quad \text{where} \quad \hat{P}_k \equiv \sum_m |km\rangle\langle km| \quad \text{and} \quad \hat{P}_\lambda \equiv \int |\lambda\mu\rangle\langle\lambda\mu| d\mu.$$

Here,  $m$  and  $\mu$  are degenerate quantum numbers,  $m, n$  are discrete, and  $\lambda, \mu$  are continuous quantum numbers. The set of quantum numbers is complete, when

$$\sum_{k,m} |km\rangle\langle km| = \hat{1} = \int |\lambda\mu\rangle\langle\lambda\mu| d\lambda d\mu.$$

The degree of degeneracy of a state  $|k\rangle$  is  $\text{Tr} \hat{P}_k = \sum_m 1$ . The probability of finding the system in the state  $|k\rangle$  is  $\langle\hat{P}_k\rangle = p_n \sum_m 1$ .

Assuming that all  $|\psi_k\rangle$  are orthonormal, the non-diagonal elements are necessarily zero. Besides that,

$$\sum_k \langle \psi_k | \hat{\rho} | \psi_k \rangle = 1 . \tag{14.5}$$

So,  $\hat{\rho}$  contains all information about the system. When a state is unknown,  $\hat{\rho}$  describes the probability of finding the system in each state. When the state is fully known,  $\hat{\rho}$  describes a pure state, that is, a vector in the Hilbert space, which is unequivocally determined by a complete set of observables with their respective quantum numbers.

The properties of the density operator are,

$\begin{aligned} \hat{\rho} &= \hat{\rho}^\dagger \\ \langle \hat{\rho} \rangle &\geq 0 \\ \text{Tr } \hat{\rho} &= 1 \\ \text{Tr } \hat{\rho}^2 &\leq 1 \\ \det \hat{\rho} &= 0 \quad \text{for a pure state} \\ \hat{\rho} &= \hat{\rho}^2 \quad \text{for a pure state} \end{aligned}$	. \tag{14.6}
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**Example 59 (Inhomogeneous atomic clouds):** For example, a thermal atomic cloud of  $N$  two-level atoms needs in general to be described by a density operator, because the state of every atom is independent of the state of the other atoms. If we knew that all atoms behave in the same way, for instance, when exposed to a radiation field, we could restrict to calculating the evolution of a single atom and extrapolate to  $N$  atoms. However, atomic motion and interatomic interactions often influence the dynamics.

### 14.1.1.1 Entropy

In a very general sense, the *entropy* determines in what direction a reversible process will take place. It is related to the size of the available phase space on both sides of the reaction. For example, the coupling of discrete and continuous modes is governed by entropy considerations.

Entropy measures of the lack of information about a system from which we only know  $\langle \hat{H} \rangle$ ,

$$S \equiv -k_B \langle \ln \hat{\rho} \rangle = -k_B \text{Tr} (\hat{\rho} \ln \hat{\rho}) . \tag{14.7}$$

The *information entropy* (or *von Neumann entropy*) of statistically independent systems  $\hat{\rho} \equiv \hat{\rho}_1 \otimes \hat{\rho}_2$  is additive  $S = S_1 + S_2$ . We can also define absolute temperatures by  $T^{-1} \equiv \partial S / \partial \langle \hat{H} \rangle$ . The entropy of a pure state is 0. Hamiltonian processes conserve entropy, for they correspond to non-dissipative unitary transformations. On the other side, relaxation increases the entropy and the phase space volume. Another common definition is the so-called *purity* or *Renyi entropy*,

$$S_R \equiv \langle 1 - \hat{\rho} \rangle = 1 - \text{Tr} (\hat{\rho}^2) . \tag{14.8}$$

Quantum states can exhibit coherences. For example, if we express a state  $|\psi\rangle$  on a basis of eigenstates  $|1\rangle$  and  $|2\rangle$ :

$$\hat{\rho} = |\psi\rangle\langle\psi| = \begin{pmatrix} |\langle\psi|1\rangle|^2 & \langle 1|\psi\rangle\langle\psi|2\rangle \\ \langle 2|\psi\rangle\langle\psi|1\rangle & |\langle\psi|2\rangle|^2 \end{pmatrix} . \tag{14.9}$$



The evolution of such a state is described by the von Neumann equation,

$$i\hbar\partial_t\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)] . \quad (14.10)$$

The measurement process is not described by this equation. A pure state will always remain pure. If the eigenstates do not interact, the density operator will remain diagonal. The von Neumann equation conserves the properties of hermiticity,  $\hat{\rho} = \hat{\rho}^\dagger$ , completeness,  $\text{Tr } \hat{\rho} = 1$ , and purity  $\det \hat{\rho} = 0$ .

The density operator for a *statistical mixture* in a canonical ensemble (where  $S$  is maximum,  $U$  is variable, and  $N$  is fixed) follows from a variational problem with the Lagrange parameters  $\delta(S - k_B\alpha\langle\hat{1}\rangle - k_B\beta\langle\hat{H}\rangle) = 0$ , since  $\text{Tr } \hat{\rho}$  and  $\langle\hat{H}\rangle$  are fixed by boundary conditions. We find,

$$\hat{\rho} = \frac{1}{Z} e^{-\hat{H}/k_B T} \quad \text{with} \quad Z \equiv \text{Tr } e^{-\hat{H}/k_B T} . \quad (14.11)$$

We also have the expectation values,  $\langle H \rangle = -\partial \ln Z / \partial \beta$  and  $(\Delta H)^2 = -\partial \langle \hat{H} \rangle / \partial \beta$  with the abbreviation  $\beta \equiv (k_B T)^{-1}$ . All quantities are fixed, except the kinetic energy, which balances the interaction with a heat bath.  $T$  is the only equilibrium parameter. The density operator satisfies a Boltzmann distribution<sup>2</sup>,

$$U = \langle \hat{H} \rangle = \frac{p^2}{2m} = -\frac{\partial}{\partial(1/k_B T)} \ln \int e^{-p^2/2mk_B T} dp = \frac{k_B}{2} T . \quad (14.12)$$

### 14.1.2 Matrix formalism

The next step is to develop matrix representations of the density operator by expanding the state vectors  $|\psi_k\rangle$  in a complete orthonormal basis,

$$|\psi_k\rangle = \sum_n c_{nk} |n\rangle = \sum_n |n\rangle \langle n | \psi_k \rangle , \quad (14.13)$$

using the *completeness relation* (2.71), that is,  $\sum_n |n\rangle \langle n| = \mathbb{I}$ , and defining,

$$c_{nk} \equiv \langle n | \psi_k \rangle \quad (14.14)$$

as the projection of the state vector  $|\psi_k\rangle$  on the basis vector  $|n\rangle$ . Now, we can write the density operator matrix representation within the basis  $\{|n\rangle\}$  using the definition of  $\hat{\rho}$  in Eq. (14.1) and replacing the expansions of  $|\psi_k\rangle$  and  $\langle\psi_k|$  of Eq. (14.13):

$$\hat{\rho} = \sum_k p_k |\psi_k\rangle \langle\psi_k| = \sum_k p_k \sum_{m,n} |n\rangle \langle n | \psi_k \rangle \langle\psi_k | m \rangle \langle m| = \sum_k p_k \sum_{m,n} c_{nk} c_{mk}^* |n\rangle \langle m| . \quad (14.15)$$

The matrix elements of  $\hat{\rho}$  in this representation are

$$\rho_{nm} \equiv \langle n | \hat{\rho} | m \rangle = \sum_k p_k c_{nk} c_{mk}^* \quad (14.16)$$

<sup>2</sup>The von Neumann entropy  $S$  of a mixture can be expressed in terms of the eigenvalues or in terms of the trace and the logarithm of the density operator  $\hat{\rho}$ . Since  $\hat{\rho}$  is a semi-definite positive operator, its spectrum  $\lambda_i$ , given by  $\rho = \sum_i \lambda_i |\varphi_i\rangle \langle\varphi_i|$  where  $\{|\varphi_i\rangle\}$  is an orthonormal basis, satisfies  $\lambda_i > 0$  and  $\sum \lambda_i = 1$ . Then the entropy becomes  $S = -\sum_i \lambda_i \ln \lambda_i = -\text{Tr } (\rho \ln \rho)$ .

with the diagonal elements  $\langle n|\hat{\rho}|n\rangle = \sum_k p_k |c_{nk}|^2$  and,

$$\rho_{nm}^* = \langle n|\hat{\rho}|m\rangle^* = \sum_k p_k c_{nk}^* c_{mk} = \sum_k p_k \langle m|\psi_k\rangle \langle \psi_k|n\rangle = \langle m|\rho|n\rangle = \rho_{mn} , \quad (14.17)$$

which means that the operator  $\hat{\rho}$  is Hermitian.

**Example 60 (Density operator for a single atom):** For a very simple system such as a single atom with several levels, that without spontaneous emission can be described by a single wavefunction  $|\psi_1\rangle$ , we can let  $p_k = \delta_{1k}$ . That is, the equations (14.15) and (14.17) reduce to,

$$\hat{\rho} = \sum_{m,n} c_{n1} c_{m1}^* |n\rangle \langle m| \quad \text{and} \quad \langle n|\rho|m\rangle = c_{n1} c_{m1}^* . \quad (14.18)$$

### 14.1.2.1 Measurement and trace

The sum of the diagonal elements of a matrix representing an operator is called the *trace*. This quantity represents a fundamental property of the density operator, since it is invariant with respect to any unitary transformation:

$$\text{Tr } \hat{\rho} \equiv \sum_n \langle n|\hat{\rho}|n\rangle . \quad (14.19)$$

With the definition of the density operator (14.1) we can write the Eq. (14.19) as,

$$\text{Tr } \hat{\rho} \equiv \sum_{n,k} p_k \langle n|\psi_k\rangle \langle \psi_k|n\rangle . \quad (14.20)$$

Now, using the completeness relation,

$$\text{Tr } \hat{\rho} \equiv \sum_{n,k} p_k \langle \psi_k|n\rangle \langle n|\psi_k\rangle = \sum_k p_k \langle \psi_k|\psi_k\rangle = 1 , \quad (14.21)$$

which shows that the trace of the density operator representation is always 1 regardless of the basis of the matrix representation.

Expectation values of observables are expressed by,

$$\langle \hat{A} \rangle = \sum_k p_k \langle \psi_k|\hat{A}|\psi_k\rangle . \quad (14.22)$$

On the other side,

$$\hat{\rho}\hat{A} = \sum_k p_k |\psi_k\rangle \langle \psi_k|\hat{A} , \quad (14.23)$$

and in the basis  $\{|n\rangle\}$ ,

$$\langle n|\hat{\rho}\hat{A}|m\rangle = \langle n|\sum_k p_k |\psi_k\rangle \langle \psi_k|\hat{A}|m\rangle = \sum_k p_k \langle n|\psi_k\rangle \langle \psi_k|\hat{A}|m\rangle = \sum_k p_k \langle \psi_k|\hat{A}|m\rangle \langle n|\psi_k\rangle . \quad (14.24)$$

Now, along the diagonal, we have,

$$\langle n | \hat{\rho} \hat{A} | n \rangle = \sum_k p_k \langle \psi_k | n \rangle \langle n | \hat{A} | \psi_k \rangle . \quad (14.25)$$

With the closing relation in the basis  $\{|n\rangle\}$ , we now have <sup>3</sup>,

$$\boxed{\text{Tr } \hat{\rho} \hat{A} = \sum_k p_k \langle \psi_k | \hat{A} | \psi_k \rangle = \langle \hat{A} \rangle} . \quad (14.26)$$

The Eq. (14.26) says that the ensemble average of any dynamic observable  $\hat{A}$  can be calculated from the diagonal elements of the operator matrix  $\hat{\rho} \hat{A}$ : Since the trace is independent of the basis (this will be shown in Exc. 14.1.5.1), each unitary transformation taking the matrix representation from a basis  $\{|n\rangle\}$  to another one  $\{|t\rangle\}$  leaves the trace invariant. Using the definition of a unitary transformation we can easily show that the trace of a cyclic permutation of a product is invariant. For example,

$$\text{Tr } [\hat{A} \hat{B} \hat{C}] = \text{Tr } [\hat{C} \hat{A} \hat{B}] = \text{Tr } [\hat{B} \hat{A} \hat{C}] , \quad (14.27)$$

and in particular

$$\text{Tr } [\hat{\rho} \hat{A}] = \text{Tr } [\hat{A} \hat{\rho}] = \langle \hat{A} \rangle . \quad (14.28)$$

In the Excs. 14.1.5.2 and 14.1.5.3 we apply the density operator to pure and mixed states of a two-level system. In Exc. 14.1.5.4 we study thermal mixtures and Exc. 15.1.4.2 Glauber states.

### 14.1.2.2 Measurement process

If an observable  $\hat{A}$  has a spectral representation  $\hat{A} = \sum_n a_n |a_n\rangle \langle a_n| = \sum_n a_n P_n$ , with  $\hat{P}_n = |a_n\rangle \langle a_n|$ , the measurement process will transform the density operator to,

$$\hat{\rho}' = \sum_n \hat{P}_n \hat{\rho} P_n . \quad (14.29)$$

That is, after the *measurement*, the operator becomes diagonal on the basis of the eigenvalues of  $\hat{A}$  <sup>4</sup>, as explained in Sec. 2.2.7. The expression can be thought of as the mathematical formulation of von Neumann's state reduction postulate.

<sup>3</sup>In the presence of degeneracy or a continuous part of the spectrum we can generalize the definition of the expectation,

$$\langle \hat{X} \rangle \equiv \text{Tr } \hat{\rho} \hat{X} = \sum_{k,m} \langle km | \hat{\rho} \hat{X} | km \rangle .$$

<sup>4</sup>A projective measure always increases entropy. The entropy of a pure state is zero, while that of a mixture is always greater than zero. Therefore, a pure state can be converted into a mixture by a measurement, but the reverse can not happen. Thus, the action of measuring induces an irreversible change in the density matrix reminiscent of the collapse of the wavefunction. Strangely, the measurement *reduces* the amount of information by quenching the quantum interference of the compound system in a process called quantum decoherence. A subsystem can be taken from a mixed state to a pure state only at the price of increasing the von Neumann entropy elsewhere in the global system.

We note that the density operator (14.29) describes the whole ensemble after the measurement. The sub-ensemble corresponding to a particular result  $a_n$  of the measurement is described by a different density operator,

$$\hat{\rho}'_n = \frac{\hat{P}_n \hat{\rho} \hat{P}_n}{\text{Tr} [\hat{\rho} \hat{P}_n]} . \quad (14.30)$$

This is true, when  $|a_n\rangle$  is the only eigenvector with the eigenvalue  $a_n$ . If not,  $\hat{P}_n$  in the expression (14.30) should be replaced by the projection operator onto the sub-space of  $a_n$ <sup>5</sup>. In Exc. 15.1.4.3 we study the projection of Glauber states and in Exc. 14.1.5.7 of entangled states.

### 14.1.2.3 Systems and subsystems

Density operators are very useful for playing with systems and subsystems. Let us, for instance, assume that we have two quantum systems defined on the Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$ . The composite system is then the tensor product  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . We now suppose that the compound system is in a pure state,  $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ . If the state can be written in the form  $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ , this means that the state of the first subsystem is  $|\psi_1\rangle$ . However, in general,  $|\psi\rangle$  does not decompose like this. Of course, every vector in  $\mathcal{H}_1 \otimes \mathcal{H}_2$  is a linear combination of tensorial products of  $\mathcal{H}_1$  and  $\mathcal{H}_2$ . If  $|\psi\rangle$  can not be decomposed as a tensor product, we say that the two systems are *entangled*. In this case, there is no reasonable way of associating a pure state  $|\psi_1\rangle \in \mathcal{H}_1$  to the state  $\psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ . If, for example, in the case of a two particle wavefunction  $\Psi(x_1, x_2)$  there is no way to construct a wavefunction (i.e. a pure state)  $\psi_1(x_1)$  describing the state of the first particle, then  $\Psi(x_1, x_2) \neq \psi_1(x_1)\psi_2(x_2)$ .

The point of the discussion is that, even if the total system is in a pure state, the various subsystems that compose it will normally be in mixed states. On the other hand, regardless of whether the composite system is in a pure or mixed state, we can perfectly construct a density matrix that describes the state. Therefore, the use of density matrices is inevitable. Let  $\hat{\rho}$  be the density matrix of the system composed of two subsystems. Then the state in  $\mathcal{H}_2$  is described by a reduced density operator given by the partial trace of  $\hat{\rho}$  over  $\mathcal{H}_2$ . In the particular case, where the state the density matrix has the form  $\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2$ , where  $\hat{\rho}_1$  and  $\hat{\rho}_2$  are the density matrices in  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , then the partial trace is simply,  $\text{Tr}_{\mathcal{H}_2} \hat{\rho} \hat{\rho}_1$ .

### 14.1.3 Temporal evolution of the density operator

As shown in Secs. 2.4.2 to 2.4.4, the equations governing the temporal evolution of a quantum system depend on the choice of the picture, i.e. Schrödinger's (2.128), Heisenberg's (2.134), or the interaction picture (2.141). This, of course, also applies to a system represented by a density matrix.

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<sup>5</sup>In general, assuming that  $f$  is a function associating each observable  $\hat{A}$  with a number  $f(\hat{A})$  (which we may imagine as the expectation value), we can state the following: If  $f$  satisfies some natural properties (such as the one to produce positive values for positive operators), then there exists a unique density matrix  $\hat{\rho}$ , such that  $f(\hat{A}) = \text{Tr} (\hat{\rho} \hat{A})$  for all  $\hat{A}$ . That is, every reasonable 'family' of expectation values' can be represented by a density matrix, which suggests that the density matrix provides the most general description of a quantum state.

Returning to the density operator definition (14.1), we can express its temporal dependence in terms of time-dependent quantum states and of the time evolution operator (2.131),

$$\hat{\rho}(t) = \sum_k p_k |\psi_k(t)\rangle \langle \psi_k(t)| = \sum_k p_k U(t, t_0) |\psi_k(t_0)\rangle \langle \psi_k(t_0)| U^\dagger(t, t_0) . \quad (14.31)$$

Writing,

$$\hat{\rho}(t_0) = \sum_k p_k |\psi_k(t_0)\rangle \langle \psi_k(t_0)| , \quad (14.32)$$

we see immediately,

$$\hat{\rho}(t) = U(t, t_0) \hat{\rho}(t_0) U^\dagger(t, t_0) , \quad (14.33)$$

where, for the common case of a time-independent Hamiltonian,

$$U(t, t_0) = e^{-i\hat{H}(t-t_0)/\hbar} . \quad (14.34)$$

Now we find the time derivative of the density operator differentiating the two sides of (14.33) and substituting the Eqs.

$$\frac{dU}{dt} = \frac{1}{i\hbar} \hat{H}U \quad \text{and} \quad \frac{dU^\dagger}{dt} = -\frac{1}{i\hbar} U^\dagger \hat{H} \quad (14.35)$$

for the time derivatives  $U$  and  $U^\dagger$ . The result is

$$\boxed{\frac{d\hat{\rho}(t)}{dt} = \frac{i}{\hbar} [\hat{\rho}(t), \hat{H}]} . \quad (14.36)$$

The commutator itself can be considered as a *superoperator* acting, not any more on states but on operators, that is, we can write,

$$\mathcal{L}\hat{\rho}(t) \equiv \frac{i}{\hbar} [\hat{\rho}(t), \hat{H}] , \quad (14.37)$$

where  $\mathcal{L}$  is called *Liouville operator*. The equation (14.36) is called *Liouville equation* or *von Neumann equation*. The Liouville equation describes the *time evolution of the density operator* which, in turn, describes the distribution of an ensemble of quantum states. Even though the form of the Liouville equation resembles the Heisenberg equation, Eq. (14.31) shows that  $\hat{\rho}(t)$  is in the *Schrödinger picture*.

For a two-level system perturbatively interacting with a light field, the Hamiltonian can be decomposed as in (2.138) into a stationary part and a time-dependent part,

$$\hat{H} = \hat{H}_{atom} + \hat{V}(t) , \quad (14.38)$$

where  $\hat{H}_a$  is the part of the Hamiltonian describing the atomic structure and  $\hat{V}(t)$  the interaction of the dipole transition with the classical oscillating electric field. The interaction picture is the natural choice for this type of problem. In this case, we can transform the density operator into the interaction picture defined by (2.139),

$$\tilde{\rho}(t) = e^{i\hat{H}_{atom}(t-t_0)/\hbar} \hat{\rho}(t_0) e^{-i\hat{H}_{atom}(t-t_0)/\hbar} , \quad (14.39)$$

where the 'tilde' decoration (replacing the 'hat') emphasizes, that we are now in the *interaction picture*. We look for the time evolution rate of  $\tilde{\rho}(t)$  analogously to the Liouville equation. Calculating the time derivatives on both sides of (14.39) and substituting Eq. (14.36) for  $\frac{d\hat{\rho}}{dt}$  results in,

$$\boxed{\frac{d\tilde{\rho}(t)}{dt} = \frac{i}{\hbar}[\tilde{\rho}(t), \hat{V}(t)]}. \quad (14.40)$$

This equation shows that the time evolution of the density operator in the interaction picture depends only on the time-dependent part of the total Hamiltonian.

### 14.1.4 Semi-classical two-level atom in the dipolar approximation

In the following sections we will derive a ready-to-use form of the Hamiltonian governing the interaction of a weak single-mode light field with a two-level atom in the dipolar approximation.

#### 14.1.4.1 Transformation to the interaction picture

According to (14.38) the semi-classical light-atom interaction Hamiltonian comprises two terms which, in the dipolar approximation, can be written,

$$\hat{H} = \begin{pmatrix} 0 & 0 \\ 0 & \hbar\omega_0 \end{pmatrix} - \hat{\mathbf{d}} \cdot \vec{\mathcal{E}}(\mathbf{r}, t) \quad \text{where} \quad \hat{\mathbf{d}} = -e\hat{\mathbf{r}} = \begin{pmatrix} 0 & \langle 1|\mathbf{d}|2\rangle \\ \langle 2|\mathbf{d}|1\rangle & 0 \end{pmatrix} \quad (14.41)$$

is the dipole operator and

$$\vec{\mathcal{E}}(\mathbf{r}, t) = \frac{\vec{\epsilon}}{2} \left[ \mathcal{E}_0(\mathbf{r})e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + \mathcal{E}_0^*(\mathbf{r})e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \right] \quad (14.42)$$

the electric field. Note that via  $\mathcal{E}_0(\mathbf{r}) \rightarrow \iota\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\hat{a}$ , we can quantize the radiation mode, as will be shown in Sec. 15.1.2. Introducing the Rabi frequencies

$$\hbar\Omega(\mathbf{r}) \equiv -\mathcal{E}_0(\mathbf{r})\vec{\epsilon} \cdot \langle 2|\mathbf{d}|1\rangle \quad \text{and} \quad \hbar\Theta(\mathbf{r}) \equiv -\mathcal{E}_0(\mathbf{r})\vec{\epsilon} \cdot \langle 1|\mathbf{d}|2\rangle \quad (14.43)$$

as an abbreviation, we can write the Hamiltonian,

$$\hat{H} = \hbar \begin{pmatrix} 0 & \frac{\Theta(\mathbf{r})}{2}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + \frac{\Omega^*(\mathbf{r})}{2}e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \\ \frac{\Omega(\mathbf{r})}{2}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + \frac{\Theta^*(\mathbf{r})}{2}e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} & \hbar\omega_0 \end{pmatrix}. \quad (14.44)$$

As shown in Sec. 2.4.5 the transformation from the Schrödinger to Dirac's interaction picture, is done via,

$$\tilde{H} \equiv U^\dagger \hat{H} U + \hbar \dot{U}^\dagger U \quad \text{with} \quad U = e^{-i\tilde{H}_{atom}t/\hbar}. \quad (14.45)$$

Introducing the abbreviation  $\Delta = \omega - \omega_0$  we obtain,

$$\begin{aligned} \tilde{H} &= \begin{pmatrix} 0 & \frac{\hbar}{2}\Omega^*(\mathbf{r})e^{-i(\mathbf{k}\cdot\mathbf{r}-\Delta t)} \\ \frac{\hbar}{2}\Omega(\mathbf{r})e^{i(\mathbf{k}\cdot\mathbf{r}-\Delta t)} & 0 \end{pmatrix} \\ &+ \begin{pmatrix} 0 & \frac{\hbar}{2}\Theta(\mathbf{r})e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t-\omega_0 t)} \\ \frac{\hbar}{2}\Theta^*(\mathbf{r})e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t-\omega_0 t)} & 0 \end{pmatrix} \equiv \tilde{H}_{slow} + \tilde{H}_{fast}. \end{aligned} \quad (14.46)$$

### 14.1.4.2 The rotating-wave approximation

The transition amplitude in first-order time-dependent perturbation theory is,

$$\begin{aligned}
 a_{i \rightarrow f}(t) &= \frac{1}{i\hbar} \int_0^t \langle 2 | \tilde{H}(\tau) | 1 \rangle d\tau = \frac{\hbar}{2} \frac{1}{i\hbar} \int_0^t \left[ \Omega(\mathbf{r}) e^{i(\mathbf{k} \cdot \mathbf{r} - \Delta t)} + \Theta^*(\mathbf{r}) e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega t - \omega_0 t)} \right] d\tau \\
 &= \frac{\Omega(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}}{2\Delta} (e^{-i\Delta t} - 1) + \frac{\Theta^*(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}}{2(\omega + \omega_0)} \left( e^{-i(\omega + \omega_0)\Delta t} - 1 \right) \\
 &\simeq \frac{\Omega(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}}{2\Delta} (e^{-i\Delta t} - 1),
 \end{aligned} \tag{14.47}$$

where the last step corresponds to the *rotating-wave approximation*. This allows us to neglect  $\tilde{H}_{fast}$ .

### 14.1.4.3 Transformation into the rotating frame

Now, we further transform into rotating frame using,

$$H = U^\dagger \tilde{H} U + i\hbar \dot{U}^\dagger U \quad \text{with} \quad U = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\Delta t} \end{pmatrix}, \tag{14.48}$$

where the new Hamiltonian has no decoration. This yields,

$$H = \begin{pmatrix} 0 & \frac{\hbar}{2} \Omega^*(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} \\ \frac{\hbar}{2} \Omega(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} & -\hbar\Delta \end{pmatrix}. \tag{14.49}$$

We always can write the Rabi frequency as  $\Omega = |\Omega| e^{i\phi}$  and attribute the phase to the atomic position if necessary. Locating the atom in the center of the coordinate system, we finally get,

$$H = \begin{pmatrix} 0 & \frac{\hbar}{2} \Omega \\ \frac{\hbar}{2} \Omega & -\hbar\Delta \end{pmatrix}, \tag{14.50}$$

yielding the new Liouville equation,

$$\boxed{\frac{d\rho(t)}{dt} = \frac{i}{\hbar} [\rho(t), H]}. \tag{14.51}$$

The matrix representation of the Hamiltonian given in this section are given in the basis of the unperturbed states, but we still need to derive the matrix form of the Liouville equations (14.36), (14.40), and (14.40) in the various pictures. This will be the topic of the next section.

## 14.1.5 Exercises

### 14.1.5.1 Ex: Trace of an operator

The trace of an operator  $\hat{A}$  is defined by  $\text{Tr } \hat{A} = \sum_n \langle n | \hat{A} | n \rangle$ .

- Show that the trace is independent of the chosen basis!
- Show that  $\text{Tr } \hat{A}\hat{B} = \text{Tr } \hat{B}\hat{A}$ !

**14.1.5.2 Ex: Pure states and mixtures**

Consider a system of two levels coupled by a light mode. The Hamiltonian can be written ( $\hbar \equiv 1$ ),

$$\hat{H} = \begin{pmatrix} 0 & \frac{1}{2}\Omega \\ \frac{1}{2}\Omega & \omega_0 \end{pmatrix}.$$

Calculate  $\hat{\rho}$ ,  $\hat{\rho}^2$  and  $\langle \hat{H} \rangle$  for the following two cases:

- The atom is in a superposition state,  $|\psi\rangle = \alpha|1\rangle + \beta|2\rangle$  and
- The atom is a statistical mixture of eigenstates,  $\hat{\rho} = \mu|1\rangle\langle 1| + \nu|2\rangle\langle 2|$ .

**14.1.5.3 Ex: Mixture of states**

A two-level atom is initially in a superposition of two states  $|\psi\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle$ . An apparatus measures the populations of the states, but the experimenter forgot to read the indicated result.

- Describe the state the atom by the density operator.
- Now the experimenter returns to the device. Calculate with which probability he reads the state  $|1\rangle$ .

**14.1.5.4 Ex: Thermal population of a harmonic oscillator**

In thermal equilibrium the energy states of a system are populated following Boltzmann's law,

$$P_n = \frac{e^{-n\beta\hbar\omega}}{\sum_m e^{-m\beta\hbar\omega}} \quad \text{with} \quad \beta \equiv \frac{1}{k_B T}.$$

- Consider a one-dimensional harmonic oscillator characterized by the secular frequency  $\omega$  and, using the density operator, calculate the mean quantum number of the population and the mean energy.
- For an energy spacing of  $\omega/2\pi = 10$  MHz, how many levels of the harmonic oscillator are necessary at room temperature to accumulate a population of at least 50%. How many for an energy spacing of  $\omega/2\pi = 10$  GHz. Repeat the calculation for a 1  $\mu$ K cold atomic cloud.

**14.1.5.5 Ex: Density operator of a Glauber state**

Write down the density operator of a Glauber state and calculate its purity.

**14.1.5.6 Ex: Reduced density operator of a Glauber state**

Project the density operator of a Glauber state onto its two lowest Fock states using the formula (14.30). Show that the resulting density operator is pure.

**14.1.5.7 Ex: Partial measurements**

Consider the density operator describing the quantum state of two spins,  $|\psi\rangle = |\psi_a\rangle \otimes |\psi_b\rangle$ , with  $|\psi_a\rangle = a_1|\uparrow\rangle + a_2|\downarrow\rangle$  and  $|\psi_b\rangle = b_1|\rightarrow\rangle + b_2|\leftarrow\rangle$ .

- Write down the density operator for the complete system in terms of the expansion coefficients  $c_{ij} = a_i b_j$ .



b. Assume that the spin  $|\psi_b\rangle$  is measured and verify whether the new density operator describing our knowledge of the system is pure.

c. Now consider the entangled state  $|\psi_e\rangle = c_{11}|\uparrow\rangle|\rightarrow\rangle + c_{22}|\downarrow\rangle|\leftarrow\rangle$ . Write down again the density operator for the complete system, measure the spin  $|\psi_b\rangle$ , and verify whether the new density operator describing our knowledge of the system is pure.

## 14.2 Bloch equations for two-level atoms

In this section we will begin to apply the ideas and tools developed in the previous sections. Let us first make use of the density matrix to describe a two-level atom coupled to a single-mode light field without spontaneous emission. We will then introduce the atomic Bloch vector as a convenient and suggestive method to describe the time evolution of a coupled two-level atom.

The internal structure of atoms is analyzed in atomic physics, where we find that the energy levels are discrete (Bohr's axiom). The center of mass motion of the atoms and collisions with other atoms are ignored, and concerning the interaction of the atoms with light, we are only interested in the aspect, that the interaction can induce transitions between internal states via absorption or emission of photons. It is the duty of atomic physics to calculate the frequencies and strengths of transitions (by Hartree-Fock or similar methods), as well as their behavior in external electric and magnetic fields. The results of these calculations are visualized in energy level schemes called *Grotrian diagrams*. In quantum optics we do not care, how the energies of the levels were calculated, but accept them as given. That is, we assume the Hamiltonian of the unperturbed atom to be diagonalized, so that its internal structure can be written as,

$$\hat{H}_{atom} = \sum_j \hbar\omega_j |j\rangle\langle j|. \quad (14.52)$$

### 14.2.1 The matrix elements of the density operator

Since the optical Bloch equations are coupled differential equations relating the elements of the density operator matrix, we must examine the temporal dependence of these matrix elements, based on our knowledge of the operator's properties. This can be done in the Schrödinger picture using Eq. (14.36), in the interaction picture using Eq. (14.40), or directly in the co-rotating frame using Eq. (14.49). For didactic reason we will begin with the Schrödinger picture and derive the other representation once again.

So, let us begin with Liouville equation (14.36) and evaluate the elements of the matrix,

$$\begin{aligned} \langle m | \frac{d\hat{\rho}(t)}{dt} | n \rangle &= \frac{i}{\hbar} \langle m | [\hat{\rho}(t), \hat{H}] | n \rangle = \frac{i}{\hbar} \langle m | [\hat{\rho}(t), \hat{H}_{atom} + \hat{V}(t)] | n \rangle \\ &= \frac{i}{\hbar} (E_n - E_m) \langle m | \hat{\rho}(t) | n \rangle + \frac{i}{\hbar} \langle m | [\hat{\rho}(t), \hat{V}(t)] | n \rangle, \end{aligned} \quad (14.53)$$

where  $|m\rangle$  and  $|n\rangle$  are members of a complete set of vectors of a basis  $\{|k\rangle\}$  which are also eigen-kets of  $\hat{H}_A$  and span the space of  $\hat{H}$ . Now, we insert the closing expression

$\sum_k |k\rangle\langle k|$  in the commutator on the right-hand side of Eq. (14.53):

$$\langle m | [\hat{\rho}(t), \hat{V}(t)] | n \rangle = \sum_k [\langle m | \hat{\rho}(t) | k \rangle \langle k | \hat{V} | n \rangle - \langle m | \hat{V} | k \rangle \langle k | \hat{\rho}(t) | n \rangle]. \quad (14.54)$$

For our two-level atom the complete set only includes two states:  $|1(t)\rangle = |1\rangle$  and  $|2(t)\rangle = e^{-i\omega_0 t} |2\rangle$ . In addition, the matrix elements of the dipole coupling operator  $\hat{V}$  are only non-diagonal,

$$V \equiv \langle 1 | \hat{V} | 2 \rangle = \overline{\langle 2 | \hat{V} | 1 \rangle} = V^*. \quad (14.55)$$

Hence, Eq. (14.53) adopts the form,

$$\begin{array}{l} \frac{d\hat{\rho}_{11}}{dt} = \frac{i}{\hbar} [\hat{\rho}_{12} V^* - \hat{\rho}_{21} V] \\ \frac{d\hat{\rho}_{22}}{dt} = \frac{i}{\hbar} [\hat{\rho}_{21} V - \hat{\rho}_{12} V^*] = -\frac{d\hat{\rho}_{11}}{dt} \\ \frac{d\hat{\rho}_{12}}{dt} = i\omega_0 \hat{\rho}_{12} + \frac{i}{\hbar} [V(\hat{\rho}_{11} - \hat{\rho}_{22})] \\ \frac{d\hat{\rho}_{21}}{dt} = -i\omega_0 \hat{\rho}_{21} + \frac{i}{\hbar} [V^*(\hat{\rho}_{22} - \hat{\rho}_{11})] = \frac{d\hat{\rho}_{12}^*}{dt} \end{array}, \quad (14.56)$$

remembering that the dash of the diagonal terms, called *populations*, must be unitary, and that the non-diagonal terms, called *coherences*, must be complex,

$$\hat{\rho}_{11} + \hat{\rho}_{22} = 1 \quad , \quad \hat{\rho}_{12} = \hat{\rho}_{12}^*. \quad (14.57)$$

The above set of equations constitutes the *optical Bloch equations* in the *Schrödinger picture*. It does not include loss terms due to spontaneous emission. We transform the Bloch equations to the *interaction picture* by replacing the Liouville equation (14.36) by (14.40), and calculating the matrix elements. We obtain,

$$\frac{d\tilde{\rho}_{22}}{dt} = \frac{i}{\hbar} (V\tilde{\rho}_{21} - V^*\tilde{\rho}_{12}) \quad \text{and} \quad \frac{d\tilde{\rho}_{12}}{dt} = \frac{i}{\hbar} V(\tilde{\rho}_{11} - \tilde{\rho}_{22}). \quad (14.58)$$

We would also have obtained this expression via the substitution,  $\hat{\rho}_{12} = \tilde{\rho}_{12} e^{i\omega_0 t}$ . The interaction picture simplifies the expressions for the temporal dependence of the coherences by eliminating the first term on the right-hand side. Transforming to the interaction picture removes the temporal dependence of the basis vectors spanning the Hilbert space of the two-level atom.

We have derived the optical Bloch equations from the Liouville equation, which is the fundamental equation of motion of the density operator, and we have seen how a unitary transformation can be used to *represent* these equations in the Schrödinger, Heisenberg or interaction picture. So far, the Bloch equations do not include the possibility of spontaneous emission. We will learn later, how to include this phenomenon.

## 14.2.2 Rotating wave approximation

In the following, we will only consider exponentials rotating with the frequency  $\Delta \equiv \omega - \omega_0$ , and we will neglect terms rotating like  $\Delta \equiv \omega + \omega_0$ . This approximation, called

*rotating wave approximation* (RWA) is good, when the Rabi frequency is sufficiently small,  $\Omega \ll \omega$ . Otherwise, we observe an energy correction of the levels called *Bloch-Siegert shift*. The RWA can be implemented in the time dependence of the coupling operator,

$$V(t) = \hbar\Omega \cos \omega t \rightarrow \frac{\hbar}{2}\Omega e^{-i\omega t} , \quad (14.59)$$

neglecting the part  $\frac{1}{2}\hbar\Omega e^{i\omega t}$ .

Once the RWA made, we can transform to the rotating system by the prescription,

$$\boxed{\rho_{12} \equiv \hat{\rho}_{12} e^{-i\omega t} \quad , \quad \rho_{22} \equiv \hat{\rho}_{22}} , \quad (14.60)$$

which, applied to the Bloch equations in the *Schrödinger picture* Eq. (14.56), yields,

$$\frac{d\rho_{22}}{dt} = \frac{i\Omega}{2}\rho_{21} - \frac{i\Omega^*}{2}\rho_{12} \quad , \quad \frac{d\rho_{12}}{dt} = -i\Delta\rho_{12} + \frac{i\Omega}{2}(\rho_{11} - \rho_{22}) . \quad (14.61)$$

In Exc. 14.2.6.1 we derive the Bloch equations from the equations of motion for the population amplitudes  $a_1$  and  $a_2$ .

For arbitrary starting conditions, the solution of these equations is not simple. To solve the problem we write the equations in a matrix form,

$$\boxed{\vec{\rho} \equiv \begin{pmatrix} \rho_{11} \\ \rho_{22} \\ \rho_{12} \\ \rho_{21} \end{pmatrix} \quad , \quad \mathcal{M} \equiv \begin{pmatrix} 0 & 0 & \frac{i}{2}\Omega^* & -\frac{i}{2}\Omega \\ 0 & 0 & -\frac{i}{2}\Omega^* & \frac{i}{2}\Omega \\ \frac{i}{2}\Omega & -\frac{i}{2}\Omega & -i\Delta & 0 \\ -\frac{i}{2}\Omega^* & \frac{i}{2}\Omega^* & 0 & i\Delta \end{pmatrix} \quad , \quad \dot{\vec{\rho}} = \mathcal{M}\vec{\rho}} . \quad (14.62)$$

To solve this system of differential equations, we calculate the eigenvalues of the matrix,

$$\det(\mathcal{M} - \lambda\mathbb{I}_4) = \lambda^2(\Delta^2 + |\Omega|^2) + \lambda^4 = 0 \quad (14.63)$$

$$\lambda = 0, \pm iG ,$$

with the *generalized Rabi frequency*  $G \equiv \sqrt{\Delta^2 + |\Omega|^2}$ . Therefore, the general solution is,

$$\rho_{22}(t) = \rho_{22}^{(1)} + \rho_{22}^{(2)} e^{iGt} + \rho_{22}^{(3)} e^{-iGt} \quad (14.64)$$

$$\rho_{12}(t) = \rho_{12}^{(1)} + \rho_{12}^{(2)} e^{iGt} + \rho_{12}^{(3)} e^{-iGt} .$$

The coefficients follow from the Bloch equations with particular starting conditions. With a little algebra we get

$$\begin{aligned} \rho_{22}^{(1)} &= \rho_{22}(0) + \frac{1}{2G^2} [|\Omega|^2(1 - 2\rho_{22}(0)) - \Delta(\Omega\rho_{12}^*(0) + \Omega^*\rho_{12}(0))] \\ \rho_{22}^{(2)} &= \frac{1}{4G^2} [-|\Omega|^2(1 - 2\rho_{22}(0)) + (\Delta + G)\Omega\rho_{12}^*(0) + (\Delta - G)\Omega^*\rho_{12}(0)] \\ \rho_{22}^{(3)} &= \frac{1}{4G^2} [-|\Omega|^2(1 - 2\rho_{22}(0)) + (\Delta - G)\Omega\rho_{12}^*(0) + (\Delta + G)\Omega^*\rho_{12}(0)] \\ \rho_{12}^{(1)} &= \frac{1}{2G^2} [\Delta\Omega(1 - 2\rho_{22}(0)) + \Omega(\Omega\rho_{12}^*(0) + \Omega^*\rho_{12}(0))] \\ \rho_{12}^{(2)} &= \frac{\Delta - G}{4G^2} [-\Omega(1 - 2\rho_{22}(0)) + (\Delta + G)\frac{\Omega}{\Omega^*}\rho_{12}^*(0) + (\Delta - G)\rho_{12}(0)] \\ \rho_{12}^{(3)} &= \frac{\Delta + G}{4G^2} [-\Omega(1 - 2\rho_{22}(0)) + (\Delta - G)\frac{\Omega}{\Omega^*}\rho_{12}^*(0) + (\Delta + G)\rho_{12}(0)] . \end{aligned} \quad (14.65)$$

We derive this solution in Exc. 14.2.6.2.

To begin the discussion of this solution, let us consider a sample of atoms initially in the ground state when the light field is switched on at time  $t = 0$ ,

$$\rho_{11}(0) = 1 = 1 - \rho_{22}(0) \quad , \quad \rho_{12}(0) = 0 = \rho_{21}(0) . \quad (14.66)$$

In this case, the conditions (14.65) simplify to,

$$\begin{aligned} \rho_{22}^{(1)} &= \frac{|\Omega|^2}{2G^2} \quad , \quad \rho_{12}^{(1)} = \frac{1}{2G^2} \Delta \Omega \\ \rho_{22}^{(2)} &= \frac{-|\Omega|^2}{4G^2} \quad , \quad \rho_{12}^{(2)} = \frac{G-\Delta}{4G^2} \Omega \\ \rho_{22}^{(3)} &= \frac{-|\Omega|^2}{4G^2} \quad , \quad \rho_{12}^{(3)} = \frac{-G-\Delta}{4G^2} \Omega , \end{aligned} \quad (14.67)$$

such that,

$$\begin{aligned} \rho_{22} &= \rho_{22}^{(1)} + \rho_{22}^{(2)} e^{iGt} + \rho_{22}^{(3)} e^{-iGt} = \frac{|\Omega|^2}{4G^2} (2 - e^{iGt} - e^{-iGt}) \\ \rho_{12} &= \rho_{12}^{(1)} + \rho_{12}^{(2)} e^{iGt} + \rho_{12}^{(3)} e^{-iGt} = \frac{\Delta \Omega}{2G^2} - \frac{\Delta - G}{4G^2} \Omega e^{iGt} - \frac{\Delta + G}{4G^2} \Omega e^{-iGt} \\ &= \frac{2\Omega}{4G^2} (\Delta - \Delta \cos Gt + iG \sin Gt) . \end{aligned} \quad (14.68)$$

Using  $\cos x = 1 - 2 \sin^2 \frac{x}{2}$  and  $\sin x = 2 \sin \frac{x}{2} \cos \frac{x}{2}$ , we finally obtain,

$$\boxed{\rho_{22} = \frac{|\Omega|^2}{G^2} \sin^2 \frac{Gt}{2} \quad , \quad \rho_{12} = \frac{\Omega}{G^2} \sin \frac{Gt}{2} \left( \Delta \sin \frac{Gt}{2} + iG \cos \frac{Gt}{2} \right)} . \quad (14.69)$$

And comparing with the solutions of the Schrödinger equation for a coupled two-level atom 2.4.7.1 and (6.93), we verify,

$$\begin{aligned} \rho_{22} &= \left| \frac{i\Omega}{G} e^{-it\Delta/2} \sin \frac{Gt}{2} \right|^2 = |a_2|^2 \\ \rho_{12} &= -e^{-it\Delta/2} \left[ \cos \frac{Gt}{2} - i \frac{\Delta}{G} \sin \frac{Gt}{2} \right] \frac{-i\Omega}{G} e^{it\Delta/2} \sin \frac{Gt}{2} = a_1 a_2^* . \end{aligned} \quad (14.70)$$

### 14.2.3 Pauli matrices and the atomic Bloch vector

Let us come back to the unperturbed atomic Hamiltonian (14.52). The electronic states are orthonormal  $\langle i|j \rangle = \delta_{ij}$ , and we define the transition operators by

$$\hat{\sigma}_{ij} |k \rangle = \delta_{jk} |i \rangle , \quad (14.71)$$

and  $\hat{\sigma}_{ij}^\dagger = \hat{\sigma}_{ji}$  satisfying the commutation relation,

$$[\hat{\sigma}_{ij}, \hat{\sigma}_{lk}] = \delta_{jl} \hat{\sigma}_{ik} - \delta_{ik} \hat{\sigma}_{lj} . \quad (14.72)$$

Many times we will restrict ourselves to atoms of two or three levels. For a two-level system we obtain the *Pauli spin matrix* defined in (2.45). Every  $2 \times 2$  matrix can be

expanded on a Pauli matrix basis (see Exc. 14.2.6.3),

$$\begin{aligned}
 \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} &= |1\rangle\rho_{11}\langle 1| + |1\rangle\rho_{12}\langle 2| + |2\rangle\rho_{21}\langle 1| + |2\rangle\rho_{22}\langle 2| \\
 &= \rho_{11}\left(\frac{1}{2} + \frac{1}{2}\hat{\sigma}_z\right) + \rho_{12}\hat{\sigma}^- + \rho_{21}\hat{\sigma}^+ + \rho_{22}\left(\frac{1}{2} - \frac{1}{2}\hat{\sigma}_z\right) \\
 &= \rho_{11}\hat{\sigma}^+\hat{\sigma}^- + \rho_{12}\hat{\sigma}^- + \rho_{21}\hat{\sigma}^+ + \rho_{22}\hat{\sigma}^-\hat{\sigma}^+ = \begin{pmatrix} \langle\hat{\sigma}^-\hat{\sigma}^+\rangle & \langle\hat{\sigma}^-\rangle \\ \langle\hat{\sigma}^+\rangle & \langle\hat{\sigma}^+\hat{\sigma}^-\rangle \end{pmatrix}.
 \end{aligned} \tag{14.73}$$

For the two-level case it is useful to introduce an alternative notation based on the *Bloch vector* defined in (2.47),

$$\langle\hat{\sigma}\rangle \equiv \begin{pmatrix} 2 \operatorname{Re} \rho_{12} \\ 2 \operatorname{Im} \rho_{12} \\ \rho_{11} - \rho_{22} \end{pmatrix} = \begin{pmatrix} \langle\hat{\sigma}^+\rangle + \langle\hat{\sigma}^-\rangle \\ i(\langle\hat{\sigma}^+\rangle - \langle\hat{\sigma}^-\rangle) \\ \langle\hat{\sigma}^-\hat{\sigma}^+\rangle - \langle\hat{\sigma}^+\hat{\sigma}^-\rangle \end{pmatrix} = \begin{pmatrix} \langle\hat{\sigma}_x\rangle \\ \langle\hat{\sigma}_y\rangle \\ \langle\hat{\sigma}_z\rangle \end{pmatrix}. \tag{14.74}$$

We also define the torque vector,

$$\mathbf{G} \equiv \begin{pmatrix} \operatorname{Re} \Omega \\ \operatorname{Im} \Omega \\ \Delta \end{pmatrix} \quad \text{with} \quad \|\mathbf{G}\| = G = \sqrt{|\Omega|^2 + \Delta^2}, \tag{14.75}$$

the length of which is simply the generalized Rabi frequency. Note that here we allow for the possibility of complex Rabi frequency.

Now, using  $\hat{\sigma}_z = [\hat{\sigma}^-, \hat{\sigma}^+]$ , we may write the Hamiltonian of an unperturbed two-level system,

$$\hat{H}_0 = -\hbar\Delta\hat{\sigma}^+\hat{\sigma}^- = \frac{\hbar}{2}\Delta(\hat{\sigma}_z - \mathbb{I}_2) = \frac{\hbar}{2}\Delta\hat{\sigma}_z + \text{offset}. \tag{14.76}$$

For the perturbed system,

$$\hat{H} = \hat{\mathbf{s}} \cdot \mathbf{G} = \frac{\hbar}{2}\mathbf{G} \cdot \hat{\sigma} = \frac{\hbar}{2}\Delta\hat{\sigma}_z + \frac{\hbar}{2}\hat{\sigma}_x \operatorname{Re} \Omega + \frac{\hbar}{2}\hat{\sigma}_y \operatorname{Im} \Omega = \begin{pmatrix} \frac{\hbar}{2}\Delta & \frac{\hbar}{2}\Omega^* \\ \frac{\hbar}{2}\Omega & -\frac{\hbar}{2}\Delta \end{pmatrix}. \tag{14.77}$$

The Bloch equations (14.76) then follow as the Heisenberg equation with the Hamiltonian (14.78) using  $[\hat{\sigma}_k, \hat{\sigma}_m] = 2i\epsilon_{klm}\hat{\sigma}_m$ ,

$$\begin{aligned}
 \frac{d\hat{\sigma}}{dt} &= \frac{i}{\hbar}[\hat{H}, \hat{\sigma}] = \frac{i}{2}[\mathbf{G} \cdot \hat{\sigma}, \hat{\sigma}] \\
 &= \frac{iG_x}{2}[\hat{\sigma}_x, \hat{\sigma}] + \frac{iG_y}{2}[\hat{\sigma}_y, \hat{\sigma}] + \frac{iG_z}{2}[\hat{\sigma}_z, \hat{\sigma}] = \begin{pmatrix} G_y\hat{\sigma}_z - G_z\hat{\sigma}_y \\ G_z\hat{\sigma}_x - G_x\hat{\sigma}_z \\ G_x\hat{\sigma}_y - G_y\hat{\sigma}_x \end{pmatrix} = \mathbf{G} \times \hat{\sigma}.
 \end{aligned} \tag{14.78}$$

For graphical illustrations we generally prefer to represent the population inversion as a positive number, which can be achieved by plotting the negative Bloch vector,  $\vec{\varrho} \equiv -\langle\hat{\sigma}\rangle$ ,

$$\frac{d\vec{\varrho}}{dt} = \mathbf{G} \times \vec{\varrho}. \tag{14.79}$$

As will be shown in Exc. 14.2.6.4, these equations are identical to the Liouville equations (14.62).  $\rho_{12}$  describes the polarization and  $\rho_{22} - \rho_{11}$  the *population inversion* of the atom. The equation is analogous to the equation of motion for a *rigid rotor* or *spinning top* (for example, a dipole in a homogeneous field). It displays phenomena such as *precession* and *nutation*. The physical content and usefulness of the Bloch vector will become clearer when we use the formalism to analyze electric and magnetic couplings. In Exc. 14.2.6.5 we verify that the Bloch vector is normalized (as long as spontaneous emission is not considered).

### 14.2.4 State manipulations by sequences of radiation pulses

The temporal dependence of the three components of the atomic Bloch vector provides a useful illustration of the atom-field interaction. Resonant coupling,  $\Delta = 0$  and  $G = \Omega$ , puts the solutions (14.69) into the form,

$$\rho_{22}(t) = \frac{1}{2}(1 - \cos \Omega t) \quad , \quad \rho_{12}(t) = \frac{i}{2} \sin \Omega t \quad , \quad (14.80)$$

that is,

$$\vec{\varrho}(t) = \begin{pmatrix} 0 \\ \sin \Omega t \\ -\cos \Omega t \end{pmatrix} . \quad (14.81)$$

That is, a resonant pulse rotates a Bloch vector initially pointing in the direction  $-z$  within the plane  $z$ - $y$ , until it arrives, at time  $t = \frac{\pi}{2\Omega}$ , at the  $+y$  direction and at time  $t = \frac{\pi}{\Omega}$  at the  $+z$  direction. This means that the entire population has been transferred to the excited state. The Bloch vector continues to rotate (the movement is called *nutation*) around the torque vector  $\mathbf{G}$  which, as can be seen from Eq. (14.76), points at the  $+x$  direction when  $\Delta = 0$ . The nutation frequency is proportional to the force  $\Omega$  of the atom-field interaction. With the Eq. (14.69) we see that the population oscillates between the ground and excited state with the frequency  $\Omega$ . This means that the energy  $\hbar\omega$  is periodically exchanged between the atom and the field. A pulse of resonant light of duration such that  $\tau = \pi/2\Omega$  is called a  $\pi/2$ -pulse. The nutation is illustrated in Fig. 14.1(a).

Once the coherence has been excited by a detuned radiation,  $\Delta \neq 0$ , the Bloch vector does not stand still, even after the radiation has been switched off. To see this, we consider again the general solution (14.65) now entering  $\Omega = 0$ . If the Bloch vector is initially at a point in the unitary circle of the plane  $z$ - $y$ , it will rotate according to the formula,

$$\rho_{22}(t) = \rho_{22}(0) \quad , \quad \rho_{12}(t) = \rho_{12}(0)e^{-i\Delta t} \quad , \quad (14.82)$$

that is,

$$\vec{\varrho}(t) = \begin{pmatrix} \rho_{12}(0) \sin \Delta t \\ \rho_{12}(0) \cos \Delta t \\ 2\rho_{22}(0) - 1 \end{pmatrix} . \quad (14.83)$$

That is, the Bloch vector performs a motion of *precession* around the symmetry axis. The precession is illustrated in Fig. 14.1(b).

The evolution of the Bloch vector on the surface of the Bloch sphere under the influence of radiation fields can be considered a coherent trajectory of the wavefunction

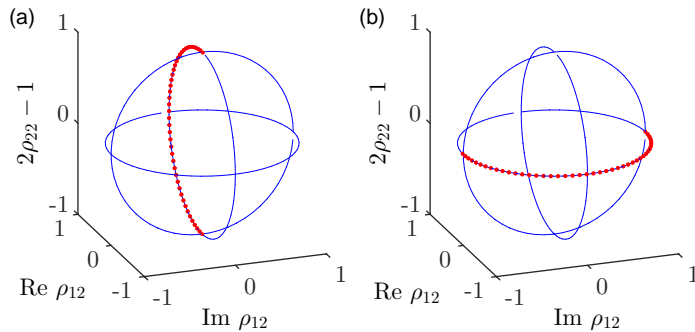


Figure 14.1: (code) (a) Nutation of the Bloch vector. The red circles show the evolution of the Bloch vector on the Bloch sphere for a resonant  $\pi$ -pulse. (b) Precession of the Bloch vector.

of the atomic state, which is therefore subject to interference phenomena [347]. Interferometers can be realized by sequences of consecutive pulses splitting populations, exciting coherences, and remixing populations.

Sensors based on interferometry of atomic excitation are nowadays among the most accurate and most sensitive. We will discuss the method of radiation pulse sequences in several exercises: In the Excs. 14.2.6.6, 14.2.6.7, and 14.2.6.8 the *Ramsey method*.

#### 14.2.4.1 Atomic ensembles

While it is technically challenging to observe the dynamics of single atoms, it is relatively easy monitor the dynamics of ensembles of atoms, provided that they react synchronously to incident radiation. The concentration of a sufficient number of atoms in a small volume can, however, introduce additional (desirable or undesirable) effects. Collisions, for instance, induce (irreversible) decoherence. On the other hand, if the ensemble is sufficiently dense that the mean distance between atoms is less than a resonant wavelength, then the transition dipoles of the individual atoms will couple to produce a collective dipole moment and generate effects known as superradiance.

Thermal motion of the atoms is another undesired effect, because every atom will interact with the radiation on a different Doppler-shifted frequency. This leads to diffusion of the individual atomic Bloch vectors in the  $x$ - $y$ -plane, which in turn limits the resolution of interferometric applications. We will discuss in Exc. 14.2.6.9 the *photon echo method*, which allows to circumvent this problem.

### 14.2.5 Nuclear magnetic resonance

*Nuclear magnetic resonance* (NMR) is a physical phenomenon in which nuclei in a strong constant magnetic field (up to 20 T) are perturbed by a weak oscillating magnetic field (in the near field) and respond by producing an electromagnetic signal with a frequency characteristic of the magnetic field at the nucleus. This process occurs near resonance, when the oscillation frequency (typically 60..1000 MHz) matches the intrinsic frequency of the nuclei, which depends on the strength of the static magnetic field, the chemical environment, and the magnetic properties of the isotope involved.

NMR spectroscopy is widely used to determine the structure of organic molecules in solution and in advanced medical imaging techniques, such as in magnetic resonance imaging (MRI). The most commonly used nuclei are  $^1\text{H}$  and  $^{13}\text{C}$ .

NMR transitions can be excited, when the electron spins do not participate in the interaction, e.g. because they are paired (see Eq. (9.41)), and when the nucleus has an intrinsic nuclear magnetic moment  $\hat{\mu}_I$  and hence an angular momentum  $\hat{\mathbf{I}}$ . This is the case for an odd number of protons and/or neutrons. Nuclides with even numbers of both have a total spin of zero and are therefore NMR-inactive.

The principle of NMR usually involves three sequential steps: (i) The alignment of the magnetic nuclear spins in an applied, constant magnetic field  $\vec{\mathcal{B}}_0$ . (ii) The perturbation of this alignment of the nuclear spins by a weak oscillating magnetic field  $\vec{\mathcal{B}}_1(t)$  called rf-pulse. (iii) The detection of the NMR signal during or after the rf-pulse via the voltage induced in a detection coil due to the precession of the nuclear spins around  $\vec{\mathcal{B}}_0$ . After an rf-pulse, the nuclear dipole moment precesses at the nuclei's intrinsic Larmor frequency without involving transitions between spin states. Choosing the two magnetic fields perpendicular to each other, one maximizes the NMR signal strength,

$$\vec{\mathcal{B}}(t) = \mathcal{B}_{rf}(t)\hat{\mathbf{e}}_x + \mathcal{B}_0\hat{\mathbf{e}}_z, \quad (14.84)$$

where, because of  $|\mathcal{B}_{rf}(t)| \ll \mathcal{B}_0$ , we choose the  $z$ -axis as the quantization axis and the rf-field as a perturbation along the  $x$ -axis.

The energy of a nuclear magnetic dipole moment placed in a magnetic field is [198],

$$\hat{H} = -\hat{\mu} \cdot \vec{\mathcal{B}} = -\gamma_I \hat{\mathbf{I}} \cdot \vec{\mathcal{B}}, \quad (14.85)$$

where  $\gamma_I$  is the *gyromagnetic ratio* of the specific nucleus and  $\hat{\mathbf{I}}$  the nuclear spin satisfying the usual commutation relation  $[\hat{I}_m, \hat{I}_n] = i\hbar\epsilon_{kmn}\hat{I}_k$ . Hence, as shown in Exc. 14.2.6.10, we can derive from the Heisenberg equation,

$$i\hbar \frac{d\hat{\mu}}{dt} = [\hat{\mu}, \hat{H}], \quad (14.86)$$

the Bloch equations,

$$\frac{d\hat{\mu}}{dt} = \gamma_I \hat{\mu} \times \vec{\mathcal{B}}. \quad (14.87)$$

Now, let us restrict to a two-level system,  $I = \frac{1}{2}$  such that  $\hat{I}_z = \frac{\hbar}{2}\hat{\sigma}_z$ . In thermal equilibrium, without time-dependent perturbation,

$$\hat{H}_0 = -\hat{\mu} \cdot \vec{\mathcal{B}}_0 = -\hat{\mu}_z \mathcal{B}_0 = -\gamma_I \hat{I}_z \mathcal{B}_0 \equiv -\omega_L \hat{I}_z. \quad (14.88)$$

where we introduced the *Larmor frequency*  $\omega_L$ . We expect energy levels,

$$E = -\hbar\gamma_I m \mathcal{B}_0, \quad (14.89)$$

with  $m = \pm\frac{1}{2}$ . The energy difference between the two states,  $\Delta E = \gamma_I \hbar \mathcal{B}_0$ , results in a small population bias favoring the lower energy state in thermal equilibrium and,



hence, in a net spin magnetization  $\vec{\mathcal{M}} = \frac{1}{V} \sum_i \langle \vec{\mu}_i \rangle$  along the magnetic field  $\vec{\mathcal{B}}_0$ . For a thermal statistical mixture, as shown in (14.11), we write the density operator <sup>6</sup>,

$$\hat{\rho} = \frac{e^{-\hat{H}_0/k_B T}}{Z} = \frac{e^{-\frac{1}{2}\beta\hbar\omega_L\hat{\sigma}_z}}{Z} = \sum_{m=\pm 1/2} |I, m\rangle \frac{e^{-\beta\hbar\omega_L m}}{Z} \langle I, m|, \quad (14.90)$$

with the partition function,

$$Z \equiv \text{Tr} e^{-\hat{H}_0/k_B T} = \sum_{m=\pm 1/2} e^{-\beta\hbar\omega_L m}. \quad (14.91)$$

Now, as shown in (14.39), we can express the time-evolution of the density operator as,

$$\hat{\rho}(t) = e^{-i\hat{H}_0 t} \hat{\rho}(0) e^{i\hat{H}_0 t} = e^{-i\beta\hbar\omega_L \hat{I}_z t} \hat{\rho}(0) e^{i\beta\hbar\omega_L \hat{I}_z t}. \quad (14.92)$$

Then, as shown in Exc. 14.2.6.11,

$$\langle \hat{\mathbf{I}}(t) \rangle = \begin{pmatrix} \cos \omega_L t & -\sin \omega_L t & 0 \\ \sin \omega_L t & \cos \omega_L t & 0 \\ 0 & 0 & 1 \end{pmatrix} \langle \hat{\mathbf{I}}(0) \rangle, \quad (14.93)$$

which corroborates the result (14.87). Apparently, the nuclear magnetic dipole moment (and hence the spin magnetization) precesses around the magnetic field with the Larmor frequency leaving the populations of the energy levels unaffected.

A perturbation of nuclear spin orientations from equilibrium will occur when an oscillating magnetic field is applied whose frequency  $\omega_{rf}$  sufficiently closely matches the Larmor precession frequency  $\omega_L$ . The populations of the spin-up and -down energy levels then undergo Rabi oscillations. The stronger the oscillating field, the faster the Rabi oscillations or the precession around the effective field in the rotating frame. After a certain time (typically on the order of 2..1000  $\mu\text{s}$ ), a resonant rf- $\pi/2$ -pulse flips the spin magnetization to the transverse plane, while after a twice longer time, the initial magnetization is inverted ( $\pi$ -pulse). It is the transverse magnetization generated by a resonant oscillating field which is usually detected in NMR.

The most important perturbation of the NMR frequency for applications of NMR is the 'shielding' effect of the surrounding shells of electrons. Electrons, similar to the nucleus, are also charged and rotate with a spin to produce a magnetic field opposite to the applied magnetic field. In general, this electronic shielding reduces the magnetic field at the nucleus. The corresponding shift in the NMR frequency due to the electronic molecular orbital coupling to the external magnetic field is called chemical shift, and it explains why NMR is able to probe the chemical structure of molecules, which depends on the electron density distribution in the corresponding molecular orbitals.

<sup>6</sup>Note that at high temperatures we get,  $Z \simeq 1$  and may approximate,

$$\hat{\rho} - 1 \simeq \beta\hbar\omega_L \hat{I}_z.$$

After perturbation the nuclear spins return to thermodynamic equilibrium due to relaxation processes. These are phenomenological included in the Bloch equations via decay time constants  $T_i$ ,

$$\frac{d\hat{\mu}}{dt} = \gamma_I \hat{\mu} \times \vec{B} - \frac{\hat{\mu}_z}{T_1} \hat{e}_z - \frac{\hat{\mu}_x}{T_2} \hat{e}_x . \quad (14.94)$$

$T_1 = \Gamma^{-1}$  is the time constant for 'longitudinal magnetic' relaxation and refers to the mean time for an individual nucleus to return to its thermal equilibrium state of the spins. The precessing nuclei can also fall out of alignment with each other and gradually stop producing a signal. This is called  $T_2$  or transverse relaxation, where  $T_2 = 2\gamma^{-1}$ . Because of the difference in the actual relaxation mechanisms involved (for example, intermolecular versus intramolecular magnetic dipole-dipole interactions),  $T_1$  is usually longer than  $T_2$ , which, in practice, also depends on significant static magnetic field inhomogeneities.

## 14.2.6 Exercises

### 14.2.6.1 Ex: Derivation of Bloch equations

Derive the Bloch equations explicitly based on the temporal evolutions of the coefficients  $a_{1,2}$  (6.63) knowing that  $\rho_{ij} = a_i^* a_j$ .

### 14.2.6.2 Ex: General solution of Bloch equations

Derive the solution (14.65) of the Bloch equations (14.62).

### 14.2.6.3 Ex: Expansion in Pauli matrices

Show explicitly  $\text{Tr } \hat{\rho} \hat{\sigma}^- \hat{\sigma}^+ = \rho_{11}$ .

### 14.2.6.4 Ex: Bloch vector and Bloch equations

Show that Eq. (14.76) is equivalent to the Bloch equations (14.62).

### 14.2.6.5 Ex: Normalization of the Bloch vector

Verify  $\|\vec{\rho}\| = 1$ .

### 14.2.6.6 Ex: Sequence of Ramsey pulses

Many atomic clocks work according to the Ramsey spectroscopy method: The two-level atom is resonantly excited by a microwave  $\pi/2$ -pulse. Then, the phase of atomic coherence precesses freely over a period of time  $T$  accumulating an angle  $\phi$ . Finally, a second  $\pi/2$ -pulse is applied and the population of the upper-level is measured. Calculate this population as a function of the angle  $\phi$ . Neglect spontaneous emission.

**14.2.6.7 Ex: Analytical treatment of the Ramsey experiment**

Derive the analytic formula for the final population  $\rho_{22}$  for the Rabi and Ramsey experiments. Derive and compare the line widths of the 'interference fringes' in these two experiments.

**14.2.6.8 Ex: Atomic clocks by the Ramsey method with spontaneous emission**

In this exercise we study the Ramsey method used in atomic clocks. For this, we will consider a two-level system  $|1\rangle$  and  $|2\rangle$  excited by a microwave radiation field characterized by the Rabi frequency  $\Omega_{12}$ , and we will compare two cases: without and with spontaneous emission:

- Write down the Hamiltonian of the system, propose a sequence of pulses allowing the observation of the Ramsey fringes, do a numerical simulation of the Schrödinger equation (based on the prescription (14.172)), and prepare a graph of the type Fig. 14.1 illustrating the temporal evolution of the Bloch vector during the sequence.
- Calculate numerically from the Schrödinger equation the population  $\rho_{22}$  immediately after the pulse sequence as a function of the detuning  $\Delta_{12}$  of the radiation field, and prepare a graph of the spectrum. Also, assuming a decay rate of  $\Gamma_{12} = 0.1\Omega_{12}$ , calculate the population  $\rho_{22}$  as a function of detuning  $\Delta_{12}$  from the Bloch equations (making sequences of type (14.172)), prepare a new graph, and compare it with the previous graph obtained by the Schrödinger equation.
- What happens to the width of the fringes, when the free precession time  $\tau$  between the Ramsey pulses is increased? Prepare a graph of the inversion  $2\rho_{22} - 1$  as a function of  $\Delta_{12}$  and  $\tau$  and interpret the results.

**14.2.6.9 Ex: Photon echo**

'Photon echo' is a powerful spectroscopic technique that allows circumvention of certain dephasing processes, for example, the Doppler shift due to the atomic motion in a thermal sample of atoms. The technique resembles the Ramsey method with the difference, that between the two Ramsey  $\pi/2$ -pulses, that is, during the free precession time, we apply an additional  $\pi$ -pulse, which inverts the imaginary part of the coherence. We will study this method by numerical simulation of the Schrödinger equation and the Bloch equations for a two-level system with and without spontaneous emission:

- Write down the Hamiltonian of the system and do a numerical simulation of the Schrödinger equation (concatenating the pulses as explained in Eq. (14.172)) for the following temporal pulse sequence:
  - resonant  $\pi/2$ -pulse ( $\Delta_{12} = 0$ ) choosing  $\Omega_{12} = 2$ ,
  - evolution for a time  $T$  without radiation ( $\Omega_{12} = 0$ ),
  - resonant  $\pi/2$ -pulse using the same parameters as in (i),
  - evolution for a time  $T$  without radiation, and
  - resonant  $\pi/2$ -pulse identical to the first pulse.

Prepare a graph of type Fig. 14.1 illustrating the temporal evolution of the Bloch vector during the sequence. Now, repeat the sequence taking into account a possible Doppler shift leading to  $\Delta_{12} \neq 0$ .

b. Repeat the calculation of (a), now numerically solving the Bloch equations, which allow the occurrence of spontaneous emission ( $\Gamma_{12} = 0.03\Omega_{12}$ ). Interpret the results.

#### 14.2.6.10 Ex: Time-evolution of NMR spin components

Derive the coherent part of the Bloch equations (14.86) from the Heisenberg equation (14.85).

#### 14.2.6.11 Ex: Precession of the nuclear spin in a magnetic field

Show for  $\hat{H}_0 = -\frac{\hbar\omega_L}{2}\hat{\sigma}_z$  that,

$$\langle \hat{\sigma}(t) \rangle = \begin{pmatrix} \cos \omega_L t & -\sin \omega_L t & 0 \\ \sin \omega_L t & \cos \omega_L t & 0 \\ 0 & 0 & 1 \end{pmatrix} \langle \hat{\sigma}(0) \rangle .$$

## 14.3 Bloch equations with spontaneous emission

In this section we will introduce spontaneous emission and the important concepts of polarization and susceptibility emanating from an excited sample of oscillating dipoles. Optical Bloch equations including spontaneous emission will be given and their stationary solutions will be discussed. Dissipative processes always broaden transition lines, and thus we will discuss various broadening mechanisms.

### 14.3.1 Phenomenological inclusion of spontaneous emission

To find the Bloch equations including spontaneous emission, we insert the phenomenological term  $-\nu\gamma a_2$  into the Eqs. (6.63), as we have already done for Eq. (13.112),

$$\Omega^* \cos \omega t e^{i\omega_0 t} a_1 - \nu\gamma a_2 = i \frac{da_2}{dt} , \quad (14.95)$$

that is, the equations of motion can be corrected by simply replacing,

$$\frac{da_2}{dt} \rightsquigarrow \left( \frac{d}{dt} + \gamma \right) a_2 . \quad (14.96)$$

Knowing  $\rho_{mn} = a_m^* a_n$ , it is easy to check,

$$\frac{d\rho_{22}}{dt} \rightsquigarrow \left( \frac{d}{dt} + \Gamma \right) \rho_{22} \quad \text{and} \quad \frac{d\rho_{12}}{dt} \rightsquigarrow \left( \frac{d}{dt} + \gamma \right) \rho_{12} , \quad (14.97)$$

with  $\gamma = \Gamma/2$ , such that the Bloch equations become,

$$\frac{d}{dt} \begin{pmatrix} \rho_{11} \\ \rho_{22} \\ \rho_{12} \\ \rho_{21} \end{pmatrix} = \begin{pmatrix} 0 & \Gamma & \frac{i}{2}\Omega & -\frac{i}{2}\Omega \\ 0 & -\Gamma & -\frac{i}{2}\Omega & \frac{i}{2}\Omega \\ \frac{i}{2}\Omega & -\frac{i}{2}\Omega & -i\Delta - \gamma & 0 \\ -\frac{i}{2}\Omega & \frac{i}{2}\Omega & 0 & i\Delta - \gamma \end{pmatrix} \begin{pmatrix} \rho_{11} \\ \rho_{22} \\ \rho_{12} \\ \rho_{21} \end{pmatrix} . \quad (14.98)$$

**Example 61 (Langevin equation):** The *Heisenberg equation* for the evolution of the internal degrees of freedom, including the phenomenologically introduced decay, is also called *Langevin equation*. It can be written as,

$$i\frac{d\hat{\sigma}^-}{dt} = \frac{1}{\hbar}[\hat{\sigma}^-, \hat{H}] - \frac{i}{2}\Gamma\hat{\sigma}^- ,$$

and analogously for  $\hat{\sigma}_z$ . With the Hamiltonian  $\hat{H} = \hbar\Delta\hat{\sigma}^+\hat{\sigma}^- + \frac{1}{2}\hbar\Omega(e^{i\omega t}\hat{\sigma}^- + h.c.)$  we obtain, using the Pauli spin matrices, exactly the Bloch equations,

$$\begin{aligned} i\dot{\hat{\sigma}}^- &= \Delta[\hat{\sigma}^-, \hat{\sigma}^+\hat{\sigma}^-] + \frac{1}{2}\Omega e^{-i\omega t}[\hat{\sigma}^-, \hat{\sigma}^+] - \frac{i}{2}\Gamma\hat{\sigma}^- = \Delta\hat{\sigma}^- - \frac{1}{2}\Omega e^{-i\omega t}\hat{\sigma}_z - \frac{i}{2}\Gamma\hat{\sigma}^- \\ i\dot{\hat{\sigma}}_z &= \Delta[\hat{\sigma}_z, \hat{\sigma}^+\hat{\sigma}^-] + \frac{1}{2}\Omega e^{-i\omega t}[\hat{\sigma}_z, \hat{\sigma}^+] + \frac{1}{2}\Omega e^{i\omega t}[\hat{\sigma}_z, \hat{\sigma}^-] - \frac{i}{2}\Gamma\hat{\sigma}_z = \Omega(\hat{\sigma}^- - \hat{\sigma}^+) - \frac{i}{2}\Gamma\hat{\sigma}_z . \end{aligned}$$

### 14.3.1.1 Stationary solution of the Bloch equations

The dissipation introduced by the spontaneous emission allows the system to reach a steady state. Letting the time derivatives be 0, we obtain the stationary solutions,

$$\boxed{\rho_{22}(\infty) = \frac{\frac{1}{4}|\Omega|^2}{\Delta^2 + \frac{1}{2}|\Omega|^2 + \frac{1}{4}\Gamma^2} \quad \text{and} \quad \rho_{12}(\infty) = e^{i\Delta t} \frac{\frac{1}{2}\Omega(\Delta - \frac{i}{2}\Gamma)}{\Delta^2 + \frac{1}{2}|\Omega|^2 + \frac{1}{4}\Gamma^2}} . \quad (14.99)$$

This will be shown in Exc. 14.3.5.1. We see that the populations and coherences both have a frequency dependence, which is similar but not identical to the one already found for the susceptibility  $\chi$ , the absorption coefficient  $K$ , and the absorption cross section  $\sigma_{0a}$  in the Eqs. (13.120), (13.121), and (1.73). But here the denominators have an extra term  $\frac{1}{2}\Omega^2$  contributing to an *effective* widths of  $\rho_{22}$  and  $\rho_{12}$ ,

$$\Gamma_{\text{eff}} = \sqrt{2|\Omega|^2 + \Gamma^2} . \quad (14.100)$$

This effect, called *power broadening* or *saturation broadening*, has already been discussed in (1.102). The phase factor  $e^{i\Delta t}$  describes the optical precession of the Bloch vector.

By introducing the *saturation parameter*,

$$s \equiv \frac{2|\Omega|^2}{4\Delta^2 + \Gamma^2} , \quad (14.101)$$

we can rewrite the stationary dipole moment and the excited state population (14.99) as,

$$\boxed{\rho_{22}(\infty) = \frac{s/2}{1+s} \quad , \quad \rho_{12}(\infty) = e^{i\Delta t} \frac{\Delta - i\Gamma/2}{\Omega} \frac{s}{1+s}} . \quad (14.102)$$

and

$$|\rho_{12}(\infty)|^2 = \frac{s/2}{(1+s)^2} . \quad (14.103)$$

Fig. 14.2(a) shows the Rabi oscillations damped by spontaneous emission. For long times the population of the excited state  $\rho_{22}$  converges to the asymptote (14.102). Fig. 14.2(b) shows the temporal evolution of the Bloch vector subject to spontaneous emission. In Exc. 14.3.5.2 we see the behavior of the phase of the dipole moment  $\rho_{12}$  with respect to the driving field.

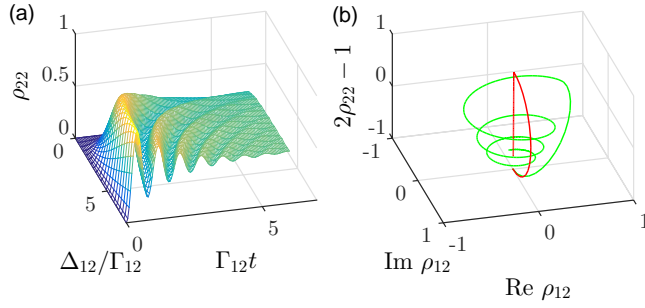


Figure 14.2: (code) (a) Rabi oscillations damped by spontaneous emission for Rabi frequencies between  $\Omega/\Gamma = 0.2, \dots, 5$ . (b) Evolution of the Bloch vector subject to spontaneous emission ( $\Gamma_{12} = 0.05\Omega_{12}$ ) after application of a resonant  $\pi$ -pulse (red) and after a  $\pi$ -pulse with detuning  $\Delta_{12} = \Omega_{12}/2$  (green).

**Example 62 (Resonant excitation and weak excitation):** A case where the Bloch equations can be analytically treated is under resonant excitation,  $\Delta = 0$ . In this case, for the initial conditions,  $\rho_{12}(0) = \rho_{22}(0) = 0$ , the solution including decay is,

$$\rho_{22}(t) = \frac{\Omega^2}{2|\Omega|^2 + \Gamma^2} \left[ 1 - e^{-3\Gamma t/4} \left( \cos \lambda t + \frac{3\Gamma}{4\lambda} \sin \lambda t \right) \right] \quad \text{and} \quad \rho_{12}(t) = 0, \quad (14.104)$$

where  $\lambda \equiv \sqrt{\Omega^2 - \Gamma^2}$ . This solution (which will be derived in Exc. 14.3.5.3), describes the optical nutation of the Bloch vector along the  $\rho_z$  axis. We note here that, due to spontaneous emission, the norm of the Bloch vector is NOT conserved, i.e., the Bloch vector evolves to the interior of the Bloch sphere.

Another case that can be solved analytically is the weakly excited atom,  $|\Omega| \ll \gamma$ ,

$$\begin{aligned} \rho_{22} &\simeq \frac{\Omega^2}{4\Gamma^2} \left( 1 + e^{-2\Gamma t} - 2 \cos \Delta t \right) \\ \text{and} \quad \rho_{12}(t) &\simeq \frac{-i\Omega}{2i\Delta + 2\Gamma} \left( e^{-(i\Delta + \Gamma)t} - 1 \right) + \rho_{12}(0)e^{-(i\Delta + \Gamma)t}. \end{aligned} \quad (14.105)$$

### 14.3.2 Susceptibility and nonlinear optics

The frequency-dependent linear *susceptibility* completely describes the linear propagation of an electromagnetic wave within a medium. It is related to the index of refraction and the absorption coefficient. Nonlinear processes should be described by higher order susceptibilities. Electric fields  $\vec{\mathcal{E}} = \vec{\mathcal{E}}_0 e^{i\omega t} + c.c.$  induce in media characterized by a given susceptibility  $\chi$  the polarization  $\vec{\mathcal{P}} = \chi \vec{\mathcal{E}}$ . The polarization is the sum of the dipole moments of the individual atoms,  $\vec{\mathcal{P}} = n \langle \mathbf{d} \rangle$ , where  $n = N/V$  is the atomic density. The susceptibility can therefore be expressed by the Hamiltonian interaction  $\hat{H} = -\mathbf{d} \cdot \vec{\mathcal{E}}$ ,

$$\chi = -\frac{n}{|\mathbf{E}|^2} \langle \hat{H} \rangle. \quad (14.106)$$

Using the two-level Hamiltonian (13.119) we obtain,

$$\chi = -n \frac{\hbar\Omega}{2|\vec{\mathcal{E}}|^2} \rho_{12} e^{i\Delta t} + c.c. \quad (14.107)$$

for the polarization,

$$\vec{\mathcal{P}} = n \mathbf{d}\rho_{12} + c.c. \quad (14.108)$$

and for the susceptibility,

$$\chi(\omega) = \frac{2nd^2}{3\epsilon_0\hbar} \frac{\Delta + i\Gamma}{4\Delta^2 + 2|\Omega|^2 + \Gamma^2} \quad \text{with} \quad d = \sqrt{\frac{3\pi\epsilon_0\hbar\Gamma}{k^3}}. \quad (14.109)$$

We can insert the new expression (14.99) for  $\rho_{12}$  into our previous expression for  $\langle d_{12} \rangle$  (13.111) and get new expressions for the polarization  $\vec{\mathcal{P}}(t)$ , (13.108) and (13.118), and the susceptibility  $\chi$  (13.120). The modified expression for the susceptibility is,

$$\chi = \frac{Nd_{12}^2}{3\epsilon_0\hbar V} \frac{-\Delta + \frac{1}{2}\Gamma}{\Delta^2 + \frac{1}{2}|\Omega|^2 + \frac{1}{4}\Gamma^2}. \quad (14.110)$$

In the imaginary component we obtain the new absorption coefficient,

$$K = \frac{\omega}{c\eta} \chi''(\omega) = \frac{\pi N e^2 |\langle \mathbf{r}_{12} \rangle|^2 \omega_0}{3\epsilon_0 \hbar c V} \frac{\Gamma/2\pi}{\Delta^2 + \frac{1}{2}\Omega^2 + \frac{1}{4}\Gamma^2}, \quad (14.111)$$

and the absorption cross-section,

$$\sigma_{0a} = \frac{\pi e^2 |\langle \mathbf{r}_{12} \rangle|^2 \omega_0}{3\epsilon_0 \hbar c} \frac{\Gamma/2\pi}{\Delta^2 + \frac{1}{2}\Omega^2 + \frac{1}{4}\Gamma^2}. \quad (14.112)$$

The important new property is the effective width  $\Gamma_{\text{eff}}$ , which appears in  $\chi$ ,  $K$ , and  $\sigma_{0a}$ . In Exc. 14.3.5.4 and 14.3.5.5 we calculate the impact of the spontaneous emission on the determinant of the density operator. Solve the Excs. 14.3.5.6, 14.3.5.7, 14.3.5.8, and 14.3.5.9.

### 14.3.2.1 Nonlinearity of the Bloch equations

Because the Bloch equation go beyond perturbation theory they contain nonlinear optics. We can see this by the simple fact that strong radiation field can saturate atomic transitions. For example, expanding the population and coherence (14.99) by the incident electric field amplitude  $\mathcal{E} \propto \Omega$ ,

$$\begin{aligned} \rho_{22}(\infty) &\simeq \frac{1}{4\Delta^2 + \Gamma^2} \Omega^2 - \frac{2}{(4\Delta^2 + \Gamma^2)^2} \Omega^4 + \dots \\ \rho_{12}(\infty) &\simeq e^{i\Delta t} \frac{2\Delta - i\Gamma}{4\Delta^2 + \Gamma^2} \Omega - 2e^{i\Delta t} \frac{2\Delta - i\Gamma}{(4\Delta^2 + \Gamma^2)^2} \Omega^3 + \dots \end{aligned} \quad (14.113)$$

The theory of nonlinear optics will be developed in Sec. 15.5.2 and Chp. ??.

### 14.3.3 Liouville equation for two levels

In this chapter we chose to include spontaneous emission in the Bloch equations by phenomenological arguments. We will show more ahead, that dissipation can be treated from general principles. This treatment, named after *Weisskopf-Wigner*, derives from a Liouville type equation (14.36), but which holds for a total density operator  $\rho_{atom\&field}$  describing the atom and the electromagnetic modes, an equation for the density operator of only the atom. The price to pay for this simplification is an additional term appearing in the equation now called *master equation*,

$$\begin{aligned} \dot{\hat{\rho}}(t) &= (\mathcal{L}_0 + \mathcal{L}_{sp})\hat{\rho}(t) \quad \text{with} \\ \mathcal{L}_0\hat{\rho}(t) &\equiv \frac{i}{\hbar}[\hat{\rho}(t), \hat{H}] \quad \text{and} \quad \mathcal{L}_{sp} = \frac{\Gamma}{2}(2\hat{\sigma}^-\hat{\rho}^-\hat{\sigma}^+ - \hat{\sigma}^+\hat{\sigma}^-\hat{\rho} - \hat{\rho}\hat{\sigma}^+\hat{\sigma}^-) \end{aligned} \quad (14.114)$$

where  $\hat{\sigma}^\pm$  are the Pauli matrices. We show in Exc. 14.3.5.10, that the known Bloch equations can be derived from the master equation.

### 14.3.4 Saturation effects by the effective Hamiltonian

The eigenvalues of the effective Hamiltonian of a two-level system excited by radiation,

$$\hat{H} = \begin{pmatrix} 0 & \frac{1}{2}\Omega \\ \frac{1}{2}\Omega & \Delta - \frac{i}{2}\Gamma \end{pmatrix}, \quad (14.115)$$

describe possible effects of line broadening and/or displacement due to coupling,

$$\frac{1}{2} \left( \Delta - \frac{i}{2}\Gamma \right) \pm \frac{1}{2} \sqrt{\left( \Delta - \frac{i}{2}\Gamma \right)^2 + \Omega^2}. \quad (14.116)$$

The real parts of the eigenvalues  $\text{Re } E$  describe shifts and/or splittings of the transition line. The imaginary parts  $\text{Im } E$  describe broadening effects of the lines.

In the simplest case,  $\Delta = 0$  and  $\Gamma > 4\Omega$ , we find the *saturation broadening* already discussed in (14.100), and we will deepen it in Exc. 14.3.5.11. For the case  $\Gamma < 4\Omega$ , we observe a splitting of the line called *Autler-Townes splitting*, which will be studied in Exc. 14.3.5.12. If  $\Omega \neq 0$ , the spectrum becomes asymmetrical. In the case of weak excitation,  $\Gamma \gg 4\Omega$ , we observe a shift of the transition line with dispersive dependence (near the resonance) on the frequency of the incident radiation. This is the *dynamic Stark shift* (or *light shift*). In the case of strong excitation,  $\Gamma \ll 4\Omega$ , we observe again at the split spectrum, but now the two lines exhibit an *avoided crossing*-type dependence on the radiation frequency. We study these effects in Exc. 14.3.5.14.

Obviously, these effects can be studied by the Bloch equation formalism containing the terms of spontaneous relaxation.

### 14.3.5 Exercises

#### 14.3.5.1 Ex: Stationary solution of the Bloch equations

Derive the stationary solution of the Bloch equations including spontaneous emission.



**14.3.5.2 Ex: Detuning-dependent phase-shift of the dipole moment**

Calculate the phase-shift of the dipole moment with respect to the driving field across resonance.

**14.3.5.3 Ex: Solution of the Bloch equations for resonant excitation**

Derive the solution (14.104) of the Bloch equations with spontaneous emission for resonant excitation.

**14.3.5.4 Ex: Determinant of the Bloch matrix**

In Sec. 14.1.1 we already saw that  $\det \hat{\rho} = 0$  for conservative systems. Now, show explicitly for the Bloch matrix of a two-level system, that  $\det \hat{\rho} = 0$  only holds in the absence of spontaneous emission.

**14.3.5.5 Ex: Density operator with dissipation**

Discuss the phenomenon of dissipation in the example of

- a thermal sample of two-level systems  $|i\rangle = |1\rangle, |2\rangle$  characterized by the density operator  $\hat{\rho} = |i\rangle\langle i| \otimes |v\rangle\langle v|$ , where  $|v\rangle$  is the velocity state of the atom and
- a two-level atom coupled to a radiation field,  $\hat{\rho} = |i\rangle\langle i| \otimes |n\rangle\langle n|$ , where  $|n\rangle$  is the number of photons inside the mode.

**14.3.5.6 Ex: Bloch vector**

A two-level atom with decay rate  $\Gamma = 2\pi \times 6$  MHz be excited by a light field detuned by  $\Delta = 2\Gamma$  and whose intensity is a quarter of the saturation intensity. Write down the Bloch vector for  $t \rightarrow \infty$ .

**14.3.5.7 Ex: Purity of two-level atoms with spontaneous emission**

Calculate for a driven two-level atom in the stationary limit  $\text{Tr } \hat{\rho}$  and  $\text{Tr } \hat{\rho}^2$ .

**14.3.5.8 Ex: Bloch sphere**

Check the temporal evolution of the norm of the Bloch vector defined by  $\vec{\rho} \equiv (2 \text{Re } \sigma_+, 2 \text{Im } \sigma_-, \sigma_z)$ , where the  $\sigma_k$  are the Pauli matrices, for a resonantly excited two-level system with and without spontaneous emission.

**14.3.5.9 Ex: Atomic beam**

An atomic beam is illuminated perpendicular to its propagation direction by (quasi-)monochromatic, collimated laser pulses having the intensity  $I = 1 \text{ W/cm}^2$ , the wavelength  $\lambda = 780 \text{ nm}$ , and the duration 200 ns. The laser is tuned to the center of an atomic resonance line ( $\Gamma/2\pi = 6 \text{ MHz}$ ).

- How does the population of the upper atomic state develop?
- How does the dynamics change, when the light is detuned by 100 MHz?

**14.3.5.10 Ex: General form of the master equation**

Show that the general form of the master equation:  $\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] - \frac{\Gamma}{2}(2\hat{\sigma}\hat{\rho}\hat{\sigma}^+ - \hat{\sigma}^+\hat{\sigma}\hat{\rho} - \hat{\rho}\hat{\sigma}^+\hat{\sigma})$ , reproduces the Bloch equations including spontaneous emission.

**14.3.5.11 Ex: Quantum Zeno effect and saturation broadening**

In this exercise we study saturation broadening effect in a three-level system  $|1\rangle$ ,  $|2\rangle$ , and  $|3\rangle$  in  $V$ -configuration, as shown in Fig. 14.6(b), excited by two resonant lasers with the Rabi frequencies  $\Omega_{12}$  and  $\Omega_{23}$ .

a. From the eigenvalues  $E_{1,2}$  of the effective Hamiltonian (14.115) of the system, describe the behavior of the real part (energy shift) and the imaginary part (linewidth) as a function of the Rabi frequency. Prepare diagrams  $\Omega_{12}$  versus  $\text{Re } E_{1,2}$  and versus  $\text{Im } E_{1,2}$  and discuss the limits  $\Omega_{12} > \frac{1}{2}\Gamma_{12}$  and  $\Omega_{12} < \frac{1}{2}\Gamma_{12}$ .

Saturation broadening can be measured experimentally in a three-level system in  $V$ -configuration. To reproduce the experiment by numerical simulations of the Bloch equations (14.164),

b. write down the Liouville matrix  $\mathcal{L}$  of the system and calculate the time evolution of the Bloch vector via equation (14.168) varying the Rabi frequency  $\Omega_{23}$ . Choosing the parameters  $\Gamma_{23} = \Gamma_{12}$ ,  $\Gamma_{13} = 0.001\Gamma_{12}$ ,  $\Omega_{12} = 0.2\Gamma_{12}$ , and  $\Delta_{12} = 0 = \Delta_{23}$ , prepare a 3D curve (similar to Fig. 14.2(a)) of the population  $\rho_{33}(t)$ .

c. Interpret the results in terms of broadening by saturation. The broadening can also be understood in terms of the quantum Zeno effect, where the transition  $|1\rangle$ - $|2\rangle$  plays the role of the 'observed system' and the transition  $|2\rangle$ - $|3\rangle$  the role of the measuring device or 'meter' (for example, we can observe the light scattered on the 'meter transition' to infer the evolution of the 'system transition').

**14.3.5.12 Ex: Saturation broadening and Autler-Townes splitting**

In this exercise we study the Autler-Townes effect in a two-level system  $|1\rangle$  and  $|2\rangle$  resonantly excited ( $\Delta_{12} = 0$ ) by a laser with the Rabi frequency  $\Omega_{12}$ :

a. From the eigenvalues  $E_{1,2}$  of the effective Hamiltonian (14.115) of the system, describe the behavior of the real part (energy shift) and the imaginary part (linewidth) as a function of the Rabi frequency. Prepare diagrams  $\Omega_{12}$  versus  $\text{Re } E_{1,2}$  and versus  $\text{Im } E_{1,2}$  and discuss the limits  $\Omega_{12} > \frac{1}{2}\Gamma_{12}$  and  $\Omega_{12} < \frac{1}{2}\Gamma_{12}$ .

The Autler-Townes effect can be measured experimentally by probing the population of level  $|2\rangle$  via excitation of a third (higher) level by a second laser with the Rabi frequency  $\Omega_{23}$ . Thus, we obtain a three-level system in cascade configuration, as shown in Fig. 14.6(c). In order to reproduce the experiment by numerical simulations of the Bloch equations (14.164),

b. write down the Liouville matrix  $\mathcal{M}_{red}$  reduced by the trace condition (14.169) and

c. compute the stationary Bloch vector from equation (14.171) varying the detuning of the probe laser  $\Delta_{23}$  and the Rabi frequency  $\Omega_{12}$  of the system under study ( $|1\rangle$  and  $|2\rangle$ ). Choosing the parameters  $\Gamma_{23} = 0.5\Gamma_{12}$ ,  $\Gamma_{13} = 0.01\Gamma_{12}$ ,  $\Omega_{23} = 0.1\Gamma_{12}$ , prepare a 3D curve (similar to Fig. 14.2(a)) of the stationary population  $\rho_{22}(\infty)$ . Interpret the results.

**14.3.5.13 Ex: Light-shift**

Calculate the light-shift in a driven two-level system from the *effective Hamiltonian*,

$$\hat{H}_{eff} = \begin{pmatrix} 0 & \frac{1}{2}\Omega \\ \frac{1}{2}\Omega & \Delta - \frac{i}{2}\Gamma \end{pmatrix}.$$

Prepare spectra of the eigenvalues for  $\Gamma/\Omega = 0, 0.5, \text{ and } 2$ .

**14.3.5.14 Ex: Light-shift**

In this exercise we study the effect of the dynamic Stark shift (or light shift) of the energy levels of a two-level system  $|1\rangle$  and  $|2\rangle$  excited by a laser with the Rabi frequency  $\Omega_{12}$  and the detuning  $\Delta_{12}$ :

a. From the eigenvalues  $E_{1,2}$  of the effective Hamiltonian (14.115) system, find approximations for weak coupling ( $\Omega_{12} \ll \Gamma_{12}$ ) and strong coupling ( $\Omega_{12} \gg \Gamma_{12}$ ). Prepare a graph showing the eigenvalue spectrum (separating the parts  $\text{Re } E_{1,2}$  and  $\text{Im } E_{1,2}$ ) as a function of detuning  $\Delta_{12}$  for various values of  $\Omega_{12}$ . Also search for approximations valid for large detunings  $\Delta_{12} \gg \Gamma_{12}, \Omega_{12}$  and add them to the graph.

The light shift can be experimentally measured in a three-level system in  $\Lambda$ -configuration, as illustrated in Fig. 14.6(a). To reproduce the experiment by numerical simulations of the Bloch equations (14.164),

b. write the Liouville matrix  $\mathcal{M}_{red}$  reduced by the condition to the trace (14.169) and calculate the stationary Bloch vector from equation (14.171) varying the detunings of the two lasers  $\Delta_{12}$  and  $\Delta_{23}$ . Choosing the parameters  $\Gamma_{23} = \Gamma_{12}$ ,  $\Gamma_{13} = 0.01\Gamma_{12}$ ,  $\Omega_{12} = 2\Gamma_{12}$ , and  $\Omega_{23} = 0.2\Gamma_{12}$ , prepare a 3D curve (similar to Fig. 14.2(a)) of the stationary population  $\rho_{22}(\infty)$ . Interpret the results.

**14.4 Line broadening mechanisms**

The resolution of atomic spectroscopy is generally limited by several perturbative effects, many of them originating in the atomic motion. They manifest themselves as broadening and/or shifts of atomic resonances. Free atoms, as well as atoms confined in potentials, have kinetic energy and evolve on extended phase space trajectories. If the spatial localization is less than the effective cross section of the exciting laser beam, then the interaction time is limited and the resonance lines are broadened by the Fourier effect in a process called *transit time broadening*, and the efficiency of fluorescence collection is reduced. The same happens with the *Doppler effect*: Only those atoms that have a specific velocity along the optical axis defined by the laser beam can interact. Free as well as confined atoms can only scatter when they are in specific cells of the phase space.

There are two different fundamental types of broadening. The so-called *homogeneous broadening* affects all atoms in the same way regardless of their positions or velocities. It usually give rise to Lorentzian line profiles and can be included in the Bloch equations. It correspond to an acceleration of the relaxation. Examples are the natural linewidth, saturation broadening, and collision broadening.

The so-called *inhomogeneous broadening* is due to a displacement of atomic levels, which may be different for each atom. Averaging over a large sample of atoms,

the displacements generate an *effective* broadening usually with a Gaussian line profile. It *can not* be included in the Bloch equations, but only as an average over all trajectories of all atoms. It does not correspond to an accelerated relaxation. Inhomogeneous broadening is often due to external perturbations, e.g., Doppler broadening and broadening due to temporal fluctuations or spatial inhomogeneities of external electric or magnetic fields. In Exc. 14.4.6.1 we calculate the optical density of atomic clouds. In Exc. 14.4.6.2 we present a spectroscopic technique bypassing the Doppler broadening called *Doppler-free spectroscopy* and calculate the *Lamb-dip* profile. Finally, in Exc. 14.4.6.3, we discuss a cooling technique allowing for the reduction of Doppler broadening, called *Zeeman slower*.

### 14.4.1 Saturation broadening

Eq. (14.100) shows that when the power of the incident light increases, the population of the excited state saturates at a limit value of  $\rho_{22} = \frac{1}{2}$ . The *saturation parameter* defined in (14.101) measures the degree of saturation. When the narrowband light source is tuned to resonance, the saturation parameter is basically a measure for the ratio between the stimulated population transfer rate  $\Omega$  and the spontaneous decay rate  $A_{21}$ . We can rewrite the stationary population of the excited level as in (14.102). In resonance and with the saturation parameter  $s = 1$ , we obtain

$$\Omega = \frac{1}{\sqrt{2}}\Gamma . \quad (14.117)$$

We can use equation (14.117) to define the *saturation intensity*  $I_{sat}$  for an atom with the transition dipole  $d_{12}$ . From Eq. (1.41) we have,

$$E_0 = \sqrt{\frac{2\bar{I}}{\epsilon_0 c}} . \quad (14.118)$$

Therefore, using the definition of the Rabi frequency,  $\hbar\Omega = d_{12}E_0$ , and the relationship between  $d_{12}$  and  $\Gamma$  given by Eq. (13.38), we have <sup>7</sup>,

$$\boxed{I_{sat} = \frac{g_1}{g_2} \frac{2\pi^2 c \hbar}{3\lambda_0^3} \Gamma} , \quad (14.119)$$

taking into account the degeneracies  $g_j$  of the levels. In Exc. 14.4.6.4 we calculate the *saturation intensity* of popular atomic transitions.

### 14.4.2 Collision broadening

The theory of atomic collisions covers a large area of research, including elastic and inelastic, reactive and ionizing processes. In low-pressure gases at room temperature or hotter we need only consider the simpler processes: long-range van der Waals interactions that result in *elastic collisions*. The 'low pressure' criterion requires that the average free path between collisions be greater than any linear dimension of the gas volume. Under these conditions, collisions can be modeled with straight trajectories,

<sup>7</sup>Some authors define the saturation for  $s = 2$ , as happens when  $\Omega = \Gamma$ .

along which the interaction time is short and the time between collisions is long in comparison with the radiative lifetime of the excited atomic state. Then, the impact of a collision on the emission of a radiating atom causes a loss of coherence due to a phase interruption of the excited state atomic wavefunction. The term 'elastic' means that the collision does not disturb the populations of the internal states, so we only need to consider the off-diagonal elements of the density matrix,

$$\frac{d\rho_{12}}{dt} = i\frac{\Omega_0}{2}e^{i(\omega-\omega_0)t}(\rho_{11} - \rho_{22}) - \gamma'\rho_{12} , \quad (14.120)$$

where  $\gamma'$  is the sum of the spontaneous emission  $\gamma$  and the collision rate  $\gamma_{col}$ ,

$$\boxed{\gamma' = \gamma + \gamma_{col}} . \quad (14.121)$$

The inverse of the collision rate is simply the time between phase interruptions or the time between collisions. Now, for collisions between hard cores of atoms of mass  $m$  (with reduced mass  $m_{red} = m/2$ ) and with radius  $\rho$  in a gas with density  $n$  consisting of a single species, a standard analysis based on the kinetic theory of dilute gases shows that the time between collisions is given by the *collision rate*,

$$\gamma_{col} = \tau_{col}^{-1} = \sigma n \bar{v} , \quad (14.122)$$

where  $\bar{v} = \sqrt{\frac{8k_B T}{\pi m_{red}}}$  is the average collision velocity in a homogeneous gas at the temperature  $T$  and  $\sigma = \sqrt{8}\pi\rho^2$  the collision cross section. Thereby,

$$\boxed{\gamma_{col} = \frac{8\rho^2 n}{\sqrt{m_{red}/\pi k_B T}}} . \quad (14.123)$$

We can now relate this simple result of gas kinetics to the phase interruption rate by reinterpreting the meaning of the *collision radius*. When an excited atom propagating through space suffers a collision, the long-range interaction will produce a time-dependent perturbation of the energy levels of the radiating atom and a phase shift in the radiation,

$$\eta = \int_{-\infty}^{\infty} [\omega(t) - \omega_0] dt = \int_{-\infty}^{\infty} \Delta\omega(t) dt . \quad (14.124)$$

The long-range van der Waals interaction is expressed by,

$$\Delta E = \hbar\omega = \frac{C_n}{[b^2 + (vt)^2]^{n/2}} , \quad (14.125)$$

where  $b$  is the impact parameter of the collision trajectory and  $v$  the collision velocity. The phase shift is then

$$\eta = \frac{1}{\hbar} \int_{-\infty}^{\infty} \frac{C_n}{[b^2 + (vt)^2]^{n/2}} dt . \quad (14.126)$$

The integral is easily assessed for the two most frequent cases: non-resonant van der Waals interactions  $n = 6$  and resonant van der Waals interactions  $n = 3$ . The phase shifts are,

$$\eta_6(b) = \frac{2\pi}{3\hbar} \frac{C_6}{b_6^5 v} \quad \text{and} \quad \eta_3(b) = \frac{4\pi}{3\sqrt{3}\hbar} \frac{C_3}{b_3^2 v} . \quad (14.127)$$

Now, if instead of using the *hard core approximation*, we define a collision as an encounter causing a phase shift of at least 1 radians, we have a new condition for the collision radius,

$$b_6 = \left( \frac{2\pi C_6}{3\hbar v} \right)^{1/5} \quad \text{and} \quad b_3 = \left( \frac{4\pi C_3}{3\sqrt{3}\hbar v} \right)^{1/2}. \quad (14.128)$$

Replacing these collision radiuses for the radius  $\rho$  in Eq. (14.123) and inserting the average collision velocity, we find the collision rate,

$$\gamma_{c6} = 4n \left( \frac{\sqrt{2}\pi^2 C_6}{3\hbar} \right)^{2/5} \left( \frac{4\pi k_B T}{\mu} \right) \quad \text{and} \quad \gamma_{c3} = 4n \left( \frac{2}{3} \right)^{3/2} \left( \frac{\pi^2 C_3}{\hbar} \right)^{3/10}. \quad (14.129)$$

Substituting the generalized  $\gamma'$  of (14.121) for  $\gamma$  in the Bloch equations (14.99), we find the stationary solutions,

$$\rho_{22} = \frac{\frac{1}{4} \frac{\gamma'}{\gamma} |\Omega|^2}{\Delta^2 + \frac{1}{2} \frac{\gamma'}{\gamma} |\Omega|^2 + \gamma'^2} \quad \text{and} \quad \rho_{12} = e^{i(\omega - \omega_0)t} \frac{\frac{1}{2} \Omega (\Delta - i\gamma')}{\Delta^2 + \frac{1}{2} \frac{\gamma'}{\gamma} |\Omega|^2 + \gamma'^2}. \quad (14.130)$$

The effective linewidth (radiative and collisions) is,

$$\Gamma'_{\text{eff}} = 2\sqrt{\gamma'^2 + \frac{1}{2} \frac{\gamma'}{\gamma} |\Omega|^2}. \quad (14.131)$$

When the excitation is sufficiently weak, so that power broadening can be neglected in comparison to collision broadening, the second term can be discarded,

$$\Gamma'_{\text{eff}} = 2(\gamma + \gamma_{col}). \quad (14.132)$$

The equations (14.100) and (14.132) express the linewidths in the limits of dominating power and collision broadening, respectively. Note that the susceptibility, absorption coefficient, and absorption cross-section retain their Lorentzian profile, but with a larger width due to collisions. Since each atom is subject to the same broadening mechanism, the broadening is homogeneous. Solve Excs. 14.4.6.5.

### 14.4.3 Doppler broadening

The *Doppler broadening* is simply the apparent frequency distribution of a sample of radiating atoms at temperature  $T$ . The contribution of each atom to the radiation appears detuned by the *Doppler shift* because of its velocity. The frequency shift for a non-relativistically moving particle is  $\omega = \omega_0 / (1 - \frac{v}{c})$ , such that,

$$\Delta \equiv \omega - \omega_0 \simeq \omega_0 \frac{v}{c} = \mathbf{k} \cdot \mathbf{v} = kv_z, \quad (14.133)$$

where  $\mathbf{k}$  is the wavevector of the light and  $\mathbf{v}$  is the velocity of the atom. This distribution of Doppler shifts of a gaseous sample in thermal equilibrium follows the probability distribution of velocities,

$$P(v_z) dv_z \propto e^{-mv_z^2/2k_B T} dv_z = e^{-mc^2 \Delta^2 / 2\omega_0^2 k_B T} \frac{c}{\omega_0} d\omega. \quad (14.134)$$

This frequency distribution is a Gaussian centered at  $\omega = \omega_0$  and with the width,

$$\text{FWHM} = 2\omega_0 \left( \frac{2k_B T \ln 2}{mc^2} \right)^2. \quad (14.135)$$

A measure of the width is also the *standard deviation*,

$$2\sigma = \frac{2\omega_0}{c} \sqrt{\frac{k_B T}{m}} = \frac{\text{FWHM}}{1.177}. \quad (14.136)$$

From Eq. (14.134) we can see that the line profile is,

$$\mathcal{D}(\omega - \omega_0) \equiv \frac{1}{\sqrt{2\pi}} \frac{m}{k_B T} e^{-(\omega - \omega_0)^2 / 2\sigma^2} d\omega. \quad (14.137)$$

The profile compares with the Lorentzian profile Eq. (1.74) associated with natural, power, or collision broadening. Doppler broadening is a property of the atomic ensemble, each atom suffering a unique but different displacement than the other atoms. Hence, it is called *inhomogeneous broadening*.

The Liouville equation (14.51) used to derive the Bloch equations assumes immobile atoms. However, we can easily apply the Galilei transformation to a system, where the atoms move with the given velocity  $\mathbf{v}$ ,

$$(\partial_t + \mathbf{v} \cdot \nabla) \hat{\rho}(\mathbf{r}, t) = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}(\mathbf{r}, t)]. \quad (14.138)$$

Since the light fields propagate as  $e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})}$ , the solution of the above equation simply follows from the immobile solution with the substitution  $\Delta \rightarrow \Delta - \mathbf{k} \cdot \mathbf{v}$ . For a cloud obeying Maxwell's velocity distribution,  $P(v) \sim e^{-mv^2/k_B T}$ ,

$$\bar{\rho}(\Delta) = \frac{1}{\sqrt{2\pi}\delta} \int_{\mathbb{R}} e^{-(\mathbf{k} \cdot \mathbf{v})^2 / 2\delta^2} \hat{\rho}(\Delta - \mathbf{k} \cdot \mathbf{v}) d(\mathbf{k} \cdot \mathbf{v}). \quad (14.139)$$

The average of the density operator over all velocities,  $\bar{\rho}$ , therefore follows as the convolution of the density operator  $\rho$  (obtained as the solution of the Bloch equation) and the Gaussian function  $G(\Delta) = (2\pi\delta^2)^{-1/2} e^{-\Delta^2/2\delta^2}$ ,

$$\boxed{\bar{\rho}(\Delta) = (G \star \hat{\rho})(\Delta)}. \quad (14.140)$$

#### 14.4.4 Voigt profile

It is clear that in many practical circumstances homogeneous and inhomogeneous processes simultaneously contribute to the broadening of lines. In these cases, we can consider that the radiation of each atom, homogeneously broadened by phase-interruption processes (such as spontaneous emission or collisions), is displaced by the Doppler effect within the Maxwell-Boltzmann distribution corresponding to the temperature  $T$ . The profile of the gaseous sample, therefore, is a convolution of homogeneous and inhomogeneous profiles. The resulting profile is called *Voigt profile*:

$$\begin{aligned} V(\omega - \omega_0) &= \int_{-\infty}^{\infty} \mathcal{L}(\omega - \omega_0 - \omega') \mathcal{D}(\omega - \omega_0) d\omega' \\ &= \frac{\gamma}{2\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{-(\omega - \omega_0)^2 / 2\sigma^2}}{(\omega - \omega_0 - \omega')^2 + (\gamma/2)^2} d\omega'. \end{aligned} \quad (14.141)$$

This integral has no analytical solution, but it is easy to solve numerically. Resolve Excs. 14.4.6.6 and 14.4.6.7.

### 14.4.5 Bloch equations with phase modulation

In some situations, the atom vibrates thus producing an oscillating Doppler shift. Also, external magnetic fields or oscillating laser frequencies can produce this effect. We incorporate this temporal modulation (frequency  $\Omega_a$ ) of the light frequency shifts, induced by the Doppler effect, into the optical Bloch equations via the substitution [620],

$$\Delta_{ij} \rightarrow \Delta_{ij} + \mathbf{k}_{ij} \cdot \mathbf{v} \cos \Omega_a t . \quad (14.142)$$

The Bloch equations can then be brought into the form,

$$\dot{\hat{\rho}} = (\mathbf{L} + 2\mathbf{X} \cos \Omega_a t)\hat{\rho} + \mathbf{b} , \quad (14.143)$$

where the matrix  $\mathbf{X}$  contains the modulation index of the atomic motion  $\mathbf{k}_{ij}\mathbf{v}$ . The stationary solution of the differential equation, averaged over the time of an oscillation period, can be expressed as an infinite continuous fraction:

$$\hat{\rho}(\infty) = -(\mathbf{L} + \mathbf{S}^+ + \mathbf{S}^-)^{-1}\mathbf{b} \quad (14.144)$$

where  $\mathbf{S}^\pm = -\mathbf{X} \frac{1}{\mathbf{L} \pm i\Omega_a \mathbf{1} - \mathbf{X} \frac{1}{\mathbf{L} \pm i\Omega_a \mathbf{1} - \mathbf{X} \dots \mathbf{X}}}$  .

This solution replicates the correct excitation spectra even for a multilevel system.

Let us be more specific for a two-level system. Its Hamiltonian is,  $\hat{H}_{int} = \frac{1}{2}\hbar\Omega e^{-i[\omega t - \mathbf{k}\cdot\mathbf{v}/\Omega_a \sin \Omega_a t]}$ , such that the Bloch equation is,

$$\frac{d}{dt} \begin{pmatrix} \rho_{22} \\ \rho_{12} \\ \rho_{21} \end{pmatrix} = \left[ \begin{pmatrix} -\Gamma & -\frac{i}{2}\Omega & \frac{i}{2}\Omega \\ -\frac{i}{2}\Omega & -\Lambda & 0 \\ \frac{i}{2}\Omega & 0 & -\Lambda^* \end{pmatrix} + 2 \cos \Omega_a t \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\frac{i}{2}kv & 0 \\ 0 & 0 & \frac{i}{2}kv \end{pmatrix} \right] \begin{pmatrix} \rho_{22} \\ \rho_{12} \\ \rho_{21} \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{i}{2}\Omega \\ -\frac{i}{2}\Omega \end{pmatrix} . \quad (14.145)$$

We look for the stationary solution by expanding  $\hat{\rho} = \sum_{n=-\infty}^{\infty} \hat{\rho}_n e^{-in\Omega_a t}$ , letting  $\dot{\hat{\rho}}_n = 0$ , and projecting on  $e^{-in\Omega_a t}$  via,

$$(\mathbf{L} + in\Omega_a \mathbf{1})\hat{\rho}_n + \mathbf{X}(\hat{\rho}_{n+1} + \hat{\rho}_{n-1}) + \mathbf{b}\delta_{n0} = 0 . \quad (14.146)$$

Now we define  $\hat{\rho}_{n\pm 1} = \mathbf{S}^\pm \hat{\rho}_n$  for  $n \gtrless 0$ . Then, equation (14.146) becomes,

$$\begin{aligned} \hat{\rho}_0 &= -[\mathbf{L} + \mathbf{X}(\mathbf{S}_0^+ + \mathbf{S}_0^-)]^{-1}\mathbf{b} \quad \text{for } n = 0, \\ \mathbf{S}_{n\mp 1}^\pm &= -[\mathbf{L} + in\Omega_a \mathbf{1} + \mathbf{X}\mathbf{S}_n^\pm]^{-1}\mathbf{b} \quad \text{for } n \gtrless 0 . \end{aligned} \quad (14.147)$$

Substituting the equation below into the equation above,

$$\hat{\rho}_0 = - \left[ \mathbf{L} + \left( \frac{-\mathbf{X}}{|\mathbf{L} + i\Omega_a} + \frac{-\mathbf{X}}{|\mathbf{L} + 2i\Omega_a} + \dots \right) + \left( \frac{-\mathbf{X}}{|\mathbf{L} + i\Omega_a} + \frac{-\mathbf{X}}{|\mathbf{L} + 2i\Omega_a} + \dots \right) \right]^{-1} \mathbf{b} . \quad (14.148)$$



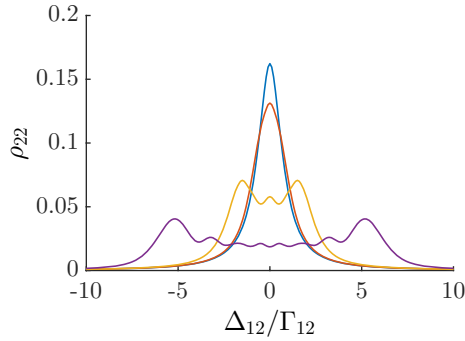


Figure 14.3: (code) Spectral broadening due to the periodic movement of the atom.

## 14.4.6 Exercises

### 14.4.6.1 Ex: Optical density of a cold cloud

The cross section of an atom with the resonant frequency  $\omega_0$  moving with velocity  $v$  and irradiated by a laser beam of frequency  $\omega$  is,

$$\sigma(v) = \frac{6\pi}{k^2} \frac{\Gamma^2}{4(\omega - \omega_0 - kv)^2 + \Gamma^2} .$$

The normalized one-dimensional Maxwell distribution,

$$\rho(v)dv = \sqrt{\frac{m}{2\pi k_B T}} e^{-mv^2/2k_B T} dv .$$

- Calculate the absorption profile of the resonance line at 461 nm ( $\Gamma_{461} = (2\pi) 30.5$  MHz) of a strontium gas cooled to the Doppler limit ( $k_B T_D = \hbar\Gamma$ ) of this transition.
- Calculate the absorption profile of the resonance line at 689 nm ( $\Gamma_{689} = (2\pi) 7.6$  kHz) of a strontium gas cooled to the Doppler limit of the transition at 461 nm.
- Compare the optical densities in case of resonance.

**Help:** To evaluate the convolution integral approximate the narrower distribution by a  $\delta$ -function maintaining the integral over the distribution normalized.

### 14.4.6.2 Ex: Saturated absorption spectroscopy

Saturated absorption spectroscopy is a technique to avoid Doppler broadening. The setup, shown in Fig. 14.4, consists of a cell filled with a rubidium gas (resonance frequency  $\omega_0 = ck = 2\pi c/780$  nm, decay rate  $\Gamma = (2\pi) 6$  MHz) and two laser beams with the same frequency  $\omega$  but counterpropagating, one called saturation and another called probe. The one-dimensional and normalized Maxwell velocity distribution is,

$$\rho(v)dv = \sqrt{\frac{m}{2\pi k_B T}} e^{-mv^2/2k_B T} dv .$$

The gas is at  $T = 300$  K, where the partial pressure of rubidium is around  $P = 10^{-1}$  mbar. The length of the cell is  $L = 10$  cm. The probe laser has an intensity

below the saturation limit, such that the cross section of an atom moving at velocity  $v$  is,

$$\sigma(v) = \frac{6\pi}{k^2} \frac{\Gamma^2}{4(\omega - \omega_0 - kv)^2 + \Gamma^2} .$$

The saturation laser has high intensity. We suppose here,  $\Omega \equiv 10\Gamma$ , where  $\Omega$  is the frequency of Rabi caused by the saturation beam. In this way it creates a population  $N_e$  of atoms in the excited state. As this population lacks in the ground state,  $N_g = N - N_e$ , the absorption of the probe beam is decreased by the factor,

$$\frac{N_e}{N} = \frac{\Omega^2}{4(\omega - \omega_0 + kv)^2 + 2\Omega^2 + \Gamma^2} .$$

To obtain the laser probe transmission spectrum, first calculate the optical density,  $OD(\omega) = Ln \int_{-\infty}^{\infty} \frac{N_g - N_e}{N} \sigma(v) \rho(v) dv$  where  $n$  is the gas density, and then the intensity of light transmitted through the cell using the Lambert-Beer law  $\frac{I}{I_0} = e^{-OD}$ .

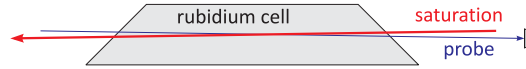


Figure 14.4: Scheme of saturation spectroscopy.

**14.4.6.3 Ex: The Zeeman slower**

Consider a tube through which passes a collimated beam of atoms, all having the same initial velocity  $v = v_0$ . In the opposite direction to the atomic motion travels a collimated and monochromatic light beam with frequency  $\omega = kc$ . The absorption rate for photons by an atom has a Lorentzian profile, which can be written as:

$$W(v) = \frac{W_0}{2\pi} \frac{\Gamma^2}{(\omega - \omega_0 + kv)^2 + (\Gamma/2)^2} ,$$

where  $\Gamma$  is the natural width of the spectral line at  $\omega_0$ , and  $W_0$  is a constant. The frequency of the light is tuned in order to compensate for the Doppler effect at the beginning of the tube,  $\delta = \omega - \omega_0 = -kv_0$  (the light is tuned to the red of the resonance). As the atoms are decelerated, they cease to be resonant with the light beam and fail to absorb photons. This can be avoided by employing the so-called Zeeman-slowng technique, which compensates for the effect using the Zeeman-shift induced by magnetic fields. In this exercise, we will study what happens if this technique is not used.

- a. For an atom with velocity  $v$ , write an expression for the mean travel distance

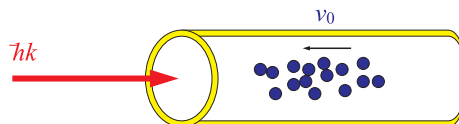


Figure 14.5: Zeeman slower scheme.

$\Delta s(v)$  before it absorbs a photon as a function of the parameters  $\Gamma$ ,  $v_0$ ,  $k$ , and  $W_0$ . (The mean time it takes to absorb a photon is  $W(v)^{-1}$ ).

b. The velocity of the atom as a function of the number of absorbed photons is  $v_n = v_0 - n \frac{hk}{m}$ , the second term being the recoil due to the absorption of a single photon. The average total distance traveled by an atom after absorbing  $N$  photons is estimated by:

$$S = \sum_{n=0}^N \Delta s(v_n) \simeq \int_0^N \Delta s(v_n) dn .$$

Calculate the average distance required for the atoms to be slowed down to  $v = 0$  (ignoring the Doppler limit). Write the expression as a function of  $\Gamma$ ,  $v_0$ ,  $k$ , and  $W_0$ .

**Help:** Do the following change of variables to simplify the evaluation of the integral:  $n \rightarrow v$ .

c. Typically, the detuning of the light,  $|\delta| = kv_0$ , is much larger than the natural width  $\Gamma$  of the transition. What happens to  $S$  in the limit when  $kv_0 \gg \Gamma$ ? Interpret this result, justifying the need for the Zeeman-slowing technique.

#### 14.4.6.4 Ex: Saturation intensity

Calculate the saturation intensity for the sodium transition  $3s \ ^2S_{1/2}, F = 2 \longleftrightarrow 3p \ ^2P_{3/2}, F' = 3$ . The natural width of the transition is  $\Gamma/2\pi = 9.89$  MHz and the wavelength  $\lambda = 590$  nm.

#### 14.4.6.5 Ex: Pressure broadening

At what pressure the collision broadening [given by the expression (14.123)] between sodium atoms in the ground state dominates the width of the D2-transition at ambient temperature. The natural width of the D2-line is  $\Gamma/2\pi = 6$  MHz.

#### 14.4.6.6 Ex: Optical density of a hot cloud

Calculate and draw the effective Lorentz profile, Gauss profile and Voigt profile for the resonance line at 461 nm ( $\Gamma = (2\pi) 32$  MHz) of a strontium gas heated to the temperature 400 C and the pressure  $P = 10^{-4}$  mbar inside a 15 cm long cell.

#### 14.4.6.7 Ex: Rate equations as a limiting case of Bloch equations

We show in this exercise that, in the limit  $\Gamma \gg \Omega$ , we can derive, from the Bloch equations, the Einstein rate equations. Proceed as follows:

a. Apply the condition  $\dot{\rho}_{12} = 0$  to the Bloch equations for a two-level system (14.99), determine  $\rho_{12}(\infty)$ , and replace this stationary value in the equations for the populations  $\rho_{kk}(t)$  using, as an abbreviation, the transition rate  $R \equiv \gamma s$ , where  $s$  is the saturation parameter (14.101).

b. Integrate the rate equations over the entire spectrum, i.e.  $\Delta \in [-\infty, \infty]$ , and derive Einstein's equations using the relations (13.7), (13.38), and (13.39).

**14.4.6.8 Ex: Lorentzian versus Gaussian line profile**

Beyond what detuning is a Doppler-broadened transition dominated by the Lorentzian profile of the transition?

## 14.5 Multi-level systems

The two-level system represents an idealization of the real atom, since at least one of the levels is usually degenerate. Many important phenomena in quantum optics are not found in this system, but conditioned to the existence of a third level. Examples are optical pumping (essential for laser operation), quantum jumps or dark resonances [which are at the basis of the phenomenon of electromagnetically induced transparency (EIT)].

To derive the Bloch equations for atoms with several levels excited by several lasers and coupled to free space (i.e. without external cavity), we can use the same master equation (14.114), but with a generalized Hamiltonian in the semiclassical approximation <sup>8</sup> and a Lindblad operator,

$$\begin{aligned} \hat{H}_{atom} &= \sum_i \hbar\omega_i \hat{\sigma}_{ji} \hat{\sigma}_{ij} = \sum_i |i\rangle \hbar\omega_i \langle i| & (14.149) \\ \hat{H}_{atom:field} &= \frac{\hbar}{2} \Omega_{ij} (e^{-i\omega_{ij}t} \hat{\sigma}_{ij} + e^{i\omega_{ij}t} \hat{\sigma}_{ji}) = \sum_{i<j} |i\rangle \frac{\hbar}{2} \Omega_{ij} \langle j| e^{i\omega_{ij}t} + c.c. \\ \mathcal{L}_{decay} \hat{\rho} &= \sum_{i,j} \begin{aligned} &\Gamma_{ij} ([\hat{\sigma}_{ij}, \hat{\rho} \hat{\sigma}_{ij}^+] + [\hat{\sigma}_{ij} \hat{\rho}, \hat{\sigma}_{ij}^+]) \\ &+ R_{ij} ([\hat{\sigma}_{ij}^+, \hat{\rho} \hat{\sigma}_{ij}] + [\hat{\sigma}_{ij}^+ \hat{\rho}, \hat{\sigma}_{ij}]) \\ &+ 2\beta_{ij} ([\hat{\sigma}_{ij} \hat{\sigma}_{ij}^+, \hat{\rho} \hat{\sigma}_{ij} \hat{\sigma}_{ij}^+] + [\hat{\sigma}_{ij} \hat{\sigma}_{ij}^+ \hat{\rho}, \hat{\sigma}_{ij} \hat{\sigma}_{ij}^+]) \end{aligned} . \end{aligned}$$

Here,  $\hat{\sigma}_{ij} \equiv |i\rangle \langle j| = \hat{\sigma}_{ji}^\dagger$ . The constants  $R_{ij}$  are eventual incoherent pump rates due to optical pumping,  $\beta_{ij}$  take account of homogeneous broadening, e.g. due to finite laser linewidths. The levels have the energy  $\hbar\omega_i$  above the ground level. The Rabi frequency  $\Omega_{ij}$  is a measure for the force at which the levels  $|i\rangle$  and  $|j\rangle$  are coupled by the resonantly irradiated light field. The master equation can be simplified by applying the rotating wave approximation and transforming to the coordinate system which rotates with the light frequencies  $\omega_{ij}$ :

$$\rho_{ij} \rightarrow \hat{\rho}_{ij} e^{i\omega_{ij}t} \quad , \quad \hat{H}_{atom:field} \rightarrow e^{-i\hat{H}t/\hbar} \hat{H}_{atom:field} e^{i\hat{H}t/\hbar} . \quad (14.150)$$

### 14.5.1 Liouville equation for many levels

The indices for the atomic levels are joined to a single index, such that the master equation takes a simpler form after having introduced a *Liouville operator*:

$$\begin{aligned} \hat{\rho} &= (\dots \rho_k \dots) \equiv \sum_{i,j} |i\rangle \rho_{ij} \langle j| , & (14.151) \\ \dot{\hat{\rho}} &= \mathcal{L} \hat{\rho} , \\ \hat{\rho} &= e^{\mathcal{L}_{atom} t} \hat{\rho}_0 . \end{aligned}$$

---

<sup>8</sup>That is, the atom is quantized and consists of several levels  $|i\rangle$  with energies  $\hbar\omega_i$ , while the light fields are described by factors  $e^{i\omega_{ij}t}$ , with frequencies  $\omega_{ij}$  tuned near the transitions  $|i\rangle - |j\rangle$ .

The relation with the *von Neumann equation* with  $\hat{H} = \sum_{i,j} |i\rangle H_{ij} \langle j|$  and  $\hat{\rho} = \sum_{k,l} |k\rangle \rho_{kl} \langle l|$  and  $\hat{\sigma}_{ij} = |i\rangle \langle j|$  is:

$$\mathcal{L}_{atom} \hat{\rho} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] = -i \sum_{k,l,j} H_{kl} \rho_{lj} |k\rangle \langle j| + i \sum_{k,l,j} H_{lj} \rho_{kl} |k\rangle \langle j|. \quad (14.152)$$

For example, for the two-level system with the definition of the external product (2.113):

$$\mathcal{L}_{atom} = -i \hat{H} \otimes \mathbb{I} + i \mathbb{I} \otimes \hat{\rho}. \quad (14.153)$$

The relaxation terms are,

$$\begin{aligned} \mathcal{L}_{decay} \hat{\rho} &= \sum_{i,j} \gamma_{ij} (2\hat{\sigma}_{ji} \hat{\rho} \hat{\sigma}_{ij} - \hat{\sigma}_{ij} \hat{\sigma}_{ji} \hat{\rho} - \hat{\rho} \hat{\sigma}_{ij} \hat{\sigma}_{ji}) \\ &= \sum_{i,j,k} (2\gamma_{ji} \delta_{kj} \rho_{ii} - \gamma_{ij} \rho_{kj} - \gamma_{ik} \rho_{kj}) |k\rangle \langle j|. \end{aligned} \quad (14.154)$$

**Example 63 (Liouville equation for two levels):** For example, for the two-level system,

$$\mathcal{L}_{atom} = \begin{pmatrix} 2\gamma_{11} & 0 & 0 & 2\gamma_{21} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 2\gamma_{12} & 0 & 0 & 2\gamma_{22} \end{pmatrix} - \begin{pmatrix} 2(\gamma_{11} + \gamma_{12}) & 0 & 0 & 0 \\ 0 & \sum_{(kj)} \gamma_{(kj)} & 0 & 0 \\ 0 & 0 & \sum_{(kj)} \gamma_{(kj)} & 0 \\ 0 & 0 & 0 & 2(\gamma_{22} + \gamma_{21}) \end{pmatrix}.$$

Here, we consider  $(kj) = (11 \ 12 \ 21 \ 22)$  as a single index.

### 14.5.1.1 Derivation of the multilevel Bloch equation

Now, starting from the Hamiltonian in the RWA,

$$\hat{H} = \hat{H}_{atom} + \hat{H}_{atom:field} = \sum_i \hbar \omega_i |i\rangle \langle i| + \frac{\hbar}{2} \sum_{i<j} \Omega_{ij} \hat{\sigma}_{ij} + h.c., \quad (14.155)$$

with the von Neumann equation,

$$\dot{\hat{\rho}} = \frac{i}{\hbar} [\hat{\rho}, \hat{H}] + \mathcal{L}_d \hat{\rho} \quad (14.156)$$

with

$$\mathcal{L}_d \hat{\rho} \equiv \sum_{i,j} \gamma_{ij} (2\hat{\sigma}_{ij} \hat{\rho} \hat{\sigma}_{ji} - \hat{\sigma}_{ji} \hat{\sigma}_{ij} \hat{\rho} - \hat{\rho} \hat{\sigma}_{ji} \hat{\sigma}_{ij}), \quad (14.157)$$

and  $\rho_{jk} = \langle j | \hat{\rho} | k \rangle$ , we derive the multilevel master equation,

$$\dot{\rho}_{jk} = \frac{i}{\hbar} \langle j | [\hat{\rho}, \hat{H}] | k \rangle + \langle j | \mathcal{L}_d \hat{\rho} | k \rangle. \quad (14.158)$$

First we calculate the unperturbed Hamiltonian part,

$$\begin{aligned} \langle k | [\hat{\rho}, \hat{H}_{atom}] | m \rangle &= \hbar \langle k | \hat{\rho} \sum_a |a\rangle \langle a| \sum_i \omega_i |i\rangle \langle i| m \rangle - \hbar \langle k | \sum_i \omega_i |i\rangle \langle i| \sum_a |a\rangle \langle a| \hat{\rho} | m \rangle \\ &= \hbar (\omega_m - \omega_k) \rho_{km}. \end{aligned} \quad (14.159)$$

For the interaction part we get,

$$\begin{aligned}
& \langle k | [\hat{\rho}, \hat{H}_{atom-field}] | m \rangle \\
&= \frac{\hbar}{2} \sum_a \sum_{i < j} [\langle k | \hat{\rho} | a \rangle \langle a | (\Omega_{ij} | i \rangle \langle j | + \Omega_{ij}^* | j \rangle \langle i |) | m \rangle - \langle k | (\Omega_{ij} | i \rangle \langle j | + \Omega_{ij}^* | j \rangle \langle i |) | a \rangle \langle a | \hat{\rho} | m \rangle] \\
&= \frac{\hbar}{2} \sum_{i < j} (\Omega_{ij} \rho_{ki} \delta_{jm} + \Omega_{ij}^* \rho_{kj} \delta_{im} - \Omega_{ij} \rho_{jm} \delta_{ki} - \Omega_{ij}^* \rho_{im} \delta_{kj}) ,
\end{aligned} \tag{14.160}$$

and for the dissipative part,

$$\begin{aligned}
\langle k | \mathcal{L}_d \hat{\rho} | m \rangle &= \langle k | \sum_{i,j} \gamma_{ij} (2 | i \rangle \langle j | \hat{\rho} | j \rangle \langle i | - | j \rangle \langle i | \langle j | \hat{\rho} - \hat{\rho} | j \rangle \langle i |) | m \rangle \\
&= \sum_j 2 \gamma_{mj} \delta_{km} \rho_{jj} - \sum_i (\gamma_{ik} + \gamma_{im}) \rho_{km} .
\end{aligned} \tag{14.161}$$

So all in all,

$$\boxed{
\begin{aligned}
\dot{\rho}_{km} &= 2 \sum_j \gamma_{mj} \rho_{jj} \delta_{km} - \left[ \sum_i (\gamma_{ik} + \gamma_{im}) + i(\omega_k - \omega_m) \right] \rho_{km} \\
&+ \frac{\hbar}{2} \sum_{i < j} (\Omega_{ij} \rho_{ki} \delta_{jm} + \Omega_{ij}^* \rho_{kj} \delta_{im} - \Omega_{ij} \rho_{jm} \delta_{ki} - \Omega_{ij}^* \rho_{im} \delta_{kj})
\end{aligned}
}, \tag{14.162}$$

where the index  $j$  runs over all levels  $|j\rangle$  into which a population  $\rho_{kk}$  can decay and the index  $i$  runs over all levels  $|i\rangle$  into which the levels  $|k\rangle$  and  $|m\rangle$  of a dipole moment  $\rho_{km}$  can decay. In Exc. 14.5.5.1 we will apply this formula to three-level systems.

Finally, the master equation can be reformulated by introducing a *generalized Bloch vector*  $\vec{\rho}$ , and the matrix representation of the Liouville superoperator  $\mathcal{L}$  as a linear system of  $n^2$  coupled differential equations,

$$\frac{d}{dt} \vec{\rho} = \mathcal{M} \vec{\rho} \quad , \quad \vec{\rho} = (\rho_{11} \quad \dots \quad \rho_{nn} \quad \rho_{12} \quad \rho_{21} \quad \dots \quad \rho_{n-1} \quad n \quad \rho_n \quad n-1) , \tag{14.163}$$

where the Bloch matrix  $\mathcal{M}$  is obtained from the Liouvillean  $\mathcal{L}$  simply by rearranging the matrix elements.

Alternatively to the complex formulation, the differential equations can be written for the real and imaginary part of the Bloch vector. The components  $\rho_{ii}$  correspond to the population probabilities of the levels  $|i\rangle$ , the non-diagonal elements  $\rho_{ij}$  describe the coherences between  $|i\rangle$  and  $|j\rangle$ . Now, we must insert the Hamiltonian (14.149) and the density operator  $\rho_{ij}$  into the Liouville equation (14.36) in order to derive the generalized Bloch equations. In practice, these calculations are simple but heavy. Therefore, we describe in Sec. 14.5.4 a simplified recipe for compiling Bloch equations for arbitrary level systems for real atoms.

## 14.5.2 Bloch equations for three levels

In principle, three-level system can exist in three possible configurations, shown in Fig. 14.6. Note that it is not possible to describe a three-level system with all levels pairwise coupled by three lasers within the formalism of Bloch's equations<sup>9</sup>.

<sup>9</sup>For the same reason that the three-body problem has no general analytic solution.

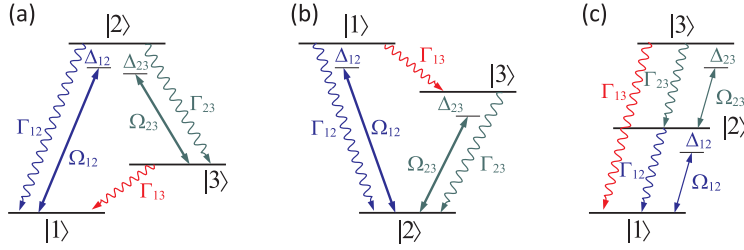


Figure 14.6: Three level system (a) in  $\Lambda$ -configuration, (b) in  $V$ -configuration, and (c) in cascade configuration.

Defining the Bloch vector by  $\vec{\rho}$ , the Bloch equation matrix for three levels in Raman configuration (that is, in  $\Lambda$ -configuration) using the labeling of Fig. 14.6(a), is,

$$\dot{\vec{\rho}} = \mathcal{M}\vec{\rho} = \quad (14.164)$$

$$\begin{pmatrix} 0 & \Gamma_{12} & \Gamma_{13} \\ 0 & -\Gamma_{12} - \Gamma_{23} & 0 \\ 0 & \Gamma_{23} & -\Gamma_{13} \\ \frac{1}{2}\Omega_{12} & -\frac{1}{2}\Omega_{12} & 0 \\ -\frac{1}{2}\Omega_{12} & \frac{1}{2}\Omega_{12} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \frac{1}{2}\Omega_{23} & -\frac{1}{2}\Omega_{23} \\ 0 & -\frac{1}{2}\Omega_{23} & \frac{1}{2}\Omega_{23} \end{pmatrix} \begin{pmatrix} \frac{1}{2}\Omega_{12} & -\frac{1}{2}\Omega_{12} & 0 \\ -\frac{1}{2}\Omega_{12} & \frac{1}{2}\Omega_{12} & 0 \\ 0 & 0 & 0 \\ -\Lambda_{12} & 0 & \frac{1}{2}\Omega_{23} \\ 0 & -\Lambda_{12}^* & 0 \\ \frac{1}{2}\Omega_{23} & 0 & -\Lambda_{13} \\ 0 & -\frac{1}{2}\Omega_{23} & 0 \\ -\Lambda_{13}^* & 0 & \frac{1}{2}\Omega_{12} \\ 0 & -\Lambda_{23} & 0 \\ \frac{1}{2}\Omega_{12} & 0 & -\Lambda_{23}^* \end{pmatrix} \begin{pmatrix} \rho_{11} \\ \rho_{22} \\ \rho_{33} \\ \rho_{12} \\ \rho_{21} \\ \rho_{13} \\ \rho_{31} \\ \rho_{23} \\ \rho_{32} \end{pmatrix}$$

with  $\Lambda_{mn} = i\Delta_{mn} + \gamma_{mn}$  and,

$$\begin{aligned} \Delta_{13} &= \Delta_{12} - \Delta_{23} \\ \gamma_{12} &= \frac{1}{2}(\Gamma_{12} + \Gamma_{23}) \quad , \quad \gamma_{23} = \frac{1}{2}(\Gamma_{12} + \Gamma_{23} + \Gamma_{13}) \quad , \quad \gamma_{13} = \frac{1}{2}\Gamma_{13} . \end{aligned} \quad (14.165)$$

In Exc. 14.5.5.2 we will derive the matrix (14.164).

The coherent terms of the same matrix can be used for the  $V$ - and the cascade configurations shown in Figs. 14.6(b,c). Obviously, the incoherent terms, that is, the submatrix  $3 \times 3$  separated in the matrix (14.164) containing the population decay rates must be adjusted, as well as the decay rates of the coherences on the diagonal. Finally, the definition of the Raman detuning  $\Delta_{13}$  must be adjusted. For the system in  $V$ -configuration we have,

$$\begin{aligned} \mathcal{M}_{incoh} &= \begin{pmatrix} -\Gamma_{12} - \Gamma_{13} & 0 & 0 \\ \Gamma_{12} & 0 & \Gamma_{23} \\ \Gamma_{13} & 0 & -\Gamma_{23} \end{pmatrix} \quad , \quad \Delta_{13} = \Delta_{12} - \Delta_{23} \\ \gamma_{12} &= \frac{1}{2}(\Gamma_{12} + \Gamma_{13}) \quad , \quad \gamma_{23} = \frac{1}{2}\Gamma_{13} \quad , \quad \gamma_{13} = \frac{1}{2}(\Gamma_{12} + \Gamma_{13} + \Gamma_{23}) . \end{aligned} \quad (14.166)$$

For the cascade system we have,

$$\mathcal{M}_{incoh} = \begin{pmatrix} 0 & \Gamma_{12} & \Gamma_{13} \\ 0 & -\Gamma_{12} & \Gamma_{23} \\ 0 & 0 & -\Gamma_{13} - \Gamma_{23} \end{pmatrix} \quad , \quad \Delta_{13} = \Delta_{12} - \Delta_{23} \quad (14.167)$$

$$\gamma_{12} = \frac{1}{2}\Gamma_{12} \quad , \quad \gamma_{23} = \frac{1}{2}(\Gamma_{12} + \Gamma_{23} + \Gamma_{13}) \quad , \quad \gamma_{13} = \frac{1}{2}(\Gamma_{13} + \Gamma_{23}) .$$

These matrices serve to calculate, among others, the phenomena of *Autler-Townes splitting* treated in Exc. 14.3.5.12, of the *light shift* treated in Excs. 14.3.5.13 and 14.3.5.14, the *dark resonances* treated in Exc. 14.5.5.4, the *STIRAP* method treated in Exc. 14.5.5.5, *adiabatic sweeps* treated in Exc. 14.5.5.6, the dispersive interaction between atoms and light treated in Exc. 14.5.5.7, *Fano resonance*-type line profiles of dark resonances treated in Exc. 14.5.5.8, and the *quantum jumps*, which will be studied in later chapters. In Excs. 14.5.5.9 and 14.5.5.10 we will show, that an atomic gas may have *negative permittivity* and *negative permeability* and, consequently, properties usually only found in artificial metamaterials, as for example, a *negative refractive index*.

### 14.5.3 Numerical treatment of Bloch equations

Since the differential Bloch equations are linear, they can be easily solved. For example, the prescription

$$\boxed{\vec{\rho}(t) = e^{\mathcal{M}t} \vec{\rho}(0)} \quad (14.168)$$

propagates the Bloch vector to later times.

The matrix  $\mathcal{M}$  is not invertible, but by applying the condition  $\text{Tr } \rho = 1$ , a component of the density matrix can be eliminated, for example by letting,

$$\rho_{11} = 1 - \sum_k \rho_{kk} . \quad (14.169)$$

The resulting state vector,  $\vec{\rho}_{red}$ , has the length  $n^2 - 1$ , and from  $\mathcal{M}$  we obtain the (trace-)reduced, now invertible matrix  $\mathcal{M}_{red}$  and the inhomogeneity vector  $\mathbf{b}$ . The differential equation is now,

$$\frac{d}{dt} \vec{\rho}_{red} = \mathcal{M}_{red} \vec{\rho}_{red} + \mathbf{b} , \quad (14.170)$$

with the stationary and time-dependent solutions,

$$\boxed{\vec{\rho}_{red}(\infty) = -\mathcal{M}_{red}^{-1} \mathbf{b} \quad , \quad \vec{\rho}_{red}(t) = e^{\mathcal{M}_{red}t} \vec{\rho}_{red}(0) + (1 - e^{\mathcal{M}_{red}t}) \vec{\rho}_{red}(\infty)} .} \quad (14.171)$$

Once the matrix  $\mathcal{M}$  or the matrix  $\mathcal{M}_{red}$  and the inhomogeneity vector  $\mathbf{b}$  are determined for a system, the state of the atom can be calculated at any time, as well as the populations and coherences. The system's free parameters are the natural transition linewidths and the detunings, as well as the intensities and emission bandwidths of the incident light fields.



### 14.5.3.1 Simulation of the Schrödinger and Bloch equation

Once we have written the solution of the Schrödinger equation in the form (??) with a time-independent Hamiltonian  $\hat{H}$ , or of the Bloch equations in the form (14.168) or (14.171) with a time-independent Liouvillian  $\mathcal{M}$ , we can easily simulate temporal evolutions of quantum systems. If the Hamiltonian or Liouvillian depend on time, for example, when the Rabi frequencies are pulsed or the detunings are ramped, we must solve the equations iteratively. That is, we chose time intervals  $\Delta t$  sufficiently short, so that the Hamiltonian (or the Liouvillian) can be considered constant during this interval, and we propagate the wavefunction (or the Bloch vector) to later times via:

$$|\psi(t + \Delta t)\rangle = e^{i\hat{H}(t)\Delta t}|\psi(t)\rangle \quad \text{or} \quad \vec{\rho}(t + \Delta t) = e^{\mathcal{M}(t)\Delta t}\vec{\rho}(t) , \quad (14.172)$$

and insert the solution obtained again into equations (14.172) with the Hamiltonian  $\hat{H}(t + \Delta t)$  (or the Liouvillian  $\mathcal{M}(t + \Delta t)$ ) adjusted to the new time.

**Example 64 (Electromagnetically induced transparency):** In some special cases, the three-level Bloch equations can be solved analytically. The system in  $\Lambda$ -configuration schematized in Fig. 14.6(a), where the two lasers satisfy the condition  $\Delta_{12} = \Delta_{23}$  can exhibit a *dark resonance* leading to the phenomena of *electromagnetically induced transparency (EIT)* and *electromagnetically induced absorption*. In these resonances a dramatic change of the refractive index is observed despite the fact that the atom becomes transparent,  $\text{Re } \chi \gg 0$  and  $|\text{Im } \chi| \ll \text{Re } \chi$ :

$$\text{Re } n = \sqrt{1 + \text{Re } \chi} \gg 0 ,$$

resulting in a high group velocity,

$$v_g = \frac{c}{n + \omega \frac{dn}{d\omega}} .$$

EIT is usually studied in  $\Lambda$ -type systems, but similar phenomena can be found in cascade-type systems [747, 736], which will be studied here. Disregarding the decay rate  $\Gamma_{13}$ , the Bloch equations (14.164) and (14.167) give the coherences,

$$\begin{aligned} \dot{\rho}_{12} &= -\Lambda_{12}\rho_{12} + \frac{i\Omega_{12}}{2}(\rho_{11} - \rho_{22}) - \frac{i\Omega_{23}}{2}\rho_{13} \\ \dot{\rho}_{13} &= -\Lambda_{13}^*\rho_{13} - \frac{i\Omega_{12}}{2}\rho_{23} - \frac{i\Omega_{23}}{2}\rho_{12} \\ \dot{\rho}_{23} &= -\Lambda_{23}\rho_{23} + \frac{i\Omega_{23}}{2}(\rho_{22} - \rho_{33}) - \frac{i\Omega_{12}}{2}\rho_{13} . \end{aligned}$$

Assuming stationarity and negligible depletion of the ground state,  $\rho_{11} = 1$ ,

$$\begin{aligned} 0 &= -\Lambda_{12}\rho_{12} + \frac{i\Omega_{12}}{2} - \frac{i\Omega_{23}}{2}\rho_{13} \\ 0 &= -\Lambda_{13}^*\rho_{13} - \frac{i\Omega_{12}}{2}\rho_{23} - \frac{i\Omega_{23}}{2}\rho_{12} \\ 0 &= -\Lambda_{23}\rho_{23} - \frac{i\Omega_{12}}{2}\rho_{13} . \end{aligned}$$

Substituting the third into the first equation,

$$\begin{aligned} 0 &= -\Lambda_{12}\rho_{12} + \frac{i\Omega_{12}}{2} - \frac{i\Omega_{23}}{2}\rho_{13} \\ 0 &= -\Lambda_{13}^*\rho_{13} - \frac{\Omega_{12}^2}{4\Lambda_{23}}\rho_{13} - \frac{i\Omega_{23}}{2}\rho_{12} . \end{aligned}$$

and finally,

$$\rho_{12} = \frac{i\Omega_{12}}{2} \frac{4\Lambda_{13}^*\Lambda_{23} + \Omega_{12}^2}{\Lambda_{12}(4\Lambda_{13}^*\Lambda_{23} + \Omega_{12}^2) + \Omega_{23}^2\Lambda_{23}} .$$

The macroscopic polarization is now  $\mathcal{P} = \frac{N}{V} d_{12} \rho_{21}$ , with the number of atoms  $N$ . In the limit of weak probes, the *dressed* susceptibility follows from  $\mathcal{P} = \varepsilon_0 \chi \mathcal{E}_{12} = \frac{N}{V} d_{12} \rho_{21}$ ,

$$\chi = \frac{N d_{12}}{V \varepsilon_0 \mathcal{E}_{12}} \rho_{21} = \frac{N |d_{12}|^2}{V \varepsilon_0 \hbar \Omega_{12}} \rho_{21} .$$

For a resonant probe laser,  $\Delta_{23} = 0$  and with  $\Gamma_{13} \simeq 0$ , we have  $\Lambda_{13} = \frac{1}{2} \Gamma_{23} + i \Delta_{12}$  and  $\Lambda_{23} = \frac{1}{2} (\Gamma_{23} + \Gamma_{12})$ . The susceptibility in the probe transition is now, using  $\Theta \equiv \Gamma_{23} + \frac{\Omega_{12}^2}{2\Lambda_{23}}$ ,

$$\begin{aligned} \chi &= \frac{N |d_{12}|^2}{V \varepsilon_0 \hbar \Omega_{12}} i \Omega_{12} \frac{\Gamma_{23} + \frac{\Omega_{12}^2}{2\Lambda_{23}} - 2i \Delta_{12}}{\left( \Gamma_{23} + \frac{\Omega_{12}^2}{2\Lambda_{23}} - 2i \Delta_{12} \right) (\Gamma_{12} + 2i \Delta_{12}) + \Omega_{23}^2} \\ &= \frac{N |d_{12}|^2}{V \varepsilon_0 \hbar \Omega_{12}} i \Omega_{12} \frac{\Theta - 2i \Delta_{12}}{(\Theta - 2i \Delta_{12})(\Gamma_{12} + 2i \Delta_{12}) + \Omega_{23}^2} = \chi' + i \chi'' . \end{aligned}$$

We consider, for example, the intercombination line of atomic strontium  $^1S_0$ - $^3P_1$  ( $\lambda_{12} = 689$  nm and  $\Gamma_{12} = (2\pi) 7.6$  kHz) be the 'dressing' transition  $^3P_1$ - $(5s4d)^3D_1$  ( $\lambda_{23} = 2700$  nm and  $\Gamma_{23} = (2\pi) 90.3$  kHz), be the 'dressing' transition  $^3P_1$ - $(5s5d)^3D_1$  ( $\lambda_{23} = 497$  nm and  $\Gamma_{23} = (2\pi) 2.3$  MHz), both characterized by  $\Gamma_{23} \gg \Omega_{12}, \Gamma_{12}, |\Delta_{12}|$ , such that  $\Theta \simeq \Gamma_{23}$ . Hence,

$$\chi' + i \chi'' = \frac{N |d_{12}|^2}{V \varepsilon_0 \hbar} \frac{2\Delta_{12} + i \Gamma_{23}}{\Omega_{23}} .$$

The refraction index follows with,

$$n = \sqrt{1 + \chi} \simeq 1 + \frac{1}{2} \chi .$$

Its imaginary part originates from the decay term of the atom: it is here responsible for the absorbing nature of the cloud. EIT is characterized by a pronounced dispersion and a small concomitant absorption.

#### 14.5.4 General rules for setting up multilevel Bloch equations

The canonical way of deriving multi-level Bloch equations starts from a von Neumann equation for the total density operator for the atom embedded in the electromagnetic mode structure of the environment including incident laser beams. After tracing over the degrees of freedom of the electromagnetic vacuum and using the Markov and the Born approximations, one arrives at a master equation of the form [257],

$$\dot{\hat{\rho}} = -\frac{i}{\hbar} [H, \hat{\rho}] + \mathcal{L}_\Gamma \hat{\rho} + \mathcal{L}_\beta \hat{\rho} . \quad (14.173)$$

Here  $H$  is the Hamiltonian of coupled atom-laser system. The Liouville superoperators,

$$\begin{aligned} \mathcal{L}_\Gamma \hat{\rho} &= \sum_{k,l} \Gamma_{kl} \left( [\sigma_{kl}, \rho \sigma_{kl}^\dagger] + [\sigma_{kl} \rho, \sigma_{kl}^\dagger] \right) \\ \mathcal{L}_\beta \hat{\rho} &= \sum_{k,l} \beta_{kl} \left( [\sigma_{kl} \sigma_{kl}^\dagger, \hat{\rho} \sigma_{kl} \sigma_{kl}^\dagger] + [\sigma_{kl} \sigma_{kl}^\dagger \hat{\rho}, \sigma_{kl} \sigma_{kl}^\dagger] \right) , \end{aligned} \quad (14.174)$$

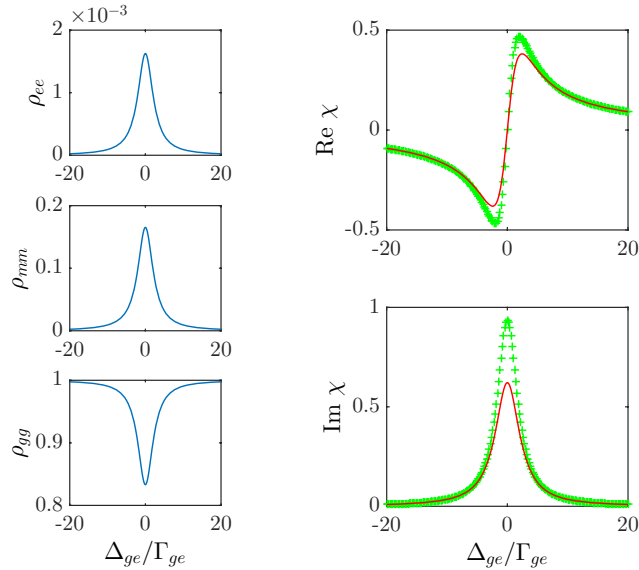


Figure 14.7: (code) EIT signal for the cascade system of strontium with the transitions at 689 nm and 497 nm with  $\Omega_{12} = \Gamma_{12}$ ,  $\Omega_{23} = \Gamma_{23}$  and  $\Delta_{23} = 0$ . The red lines are calculated by numerical integration of the Bloch equations. The dotted lines are obtained from analytical formulas based on the assumptions of weak ground state depletion (which is not really correct in the chosen parameter regime).

describe dissipation through spontaneous emission from the various excited states and decoherence due to phase fluctuations of the laser fields, respectively. The operators  $\sigma_{kl} = |k\rangle\langle l|$  describe the transition between two states.  $\Gamma_{kl}$  is the spontaneous decay of level  $|k\rangle$  into  $|l\rangle$ , and  $\beta_{kl}$  is the emission bandwidth of the laser coupling the two levels. Simple but tedious algebraic transformations of the master equation lead, in the rotating wave approximation, to a set of linear first-order differential equations in the populations of the atomic excitation levels and the coherences between them. The equations are called the optical Bloch equations.

Alternatively, the Bloch equations may be found by breaking down the multi-level scheme into a set of three-level systems. Respecting a few symmetry considerations, the multi-level Bloch equations can then be reassembled from the three-level Bloch equations corresponding to every possible combination of three levels. Based on such considerations, we provide in the following a simple recipe for setting up Bloch matrices for arbitrary level schemes. A movie showing a simulation of multi-level Bloch equations for Li atoms can be watched under the following link: [\(watch movie\)](#).

Let us regard a  $n$ -level atom. Its internal state is fully described by the populations  $\rho_{kk}$  and the (complex) coherences  $\rho_{kl}$ , with  $k, l = 1, \dots, n$ . In this work we describe the coherences by their real and imaginary parts. The labeling is such that the levels are sorted according to their excitation energy,  $E_k < E_l$  for  $k < l$ . We define the Bloch

vector,

$$\begin{aligned} \vec{\rho} \equiv & (\rho_{11} \dots \rho_{nn} \operatorname{Im} \rho_{12} \operatorname{Re} \rho_{12} \operatorname{Im} \rho_{13} \operatorname{Re} \rho_{13} \dots \\ & \dots \operatorname{Im} \rho_{1n} \operatorname{Re} \rho_{1n} \operatorname{Im} \rho_{23} \operatorname{Re} \rho_{23} \dots \\ & \dots \operatorname{Im} \rho_{n-1,n} \operatorname{Re} \rho_{n-1,n}) . \end{aligned} \quad (14.175)$$

The Bloch equations then formally read,

$$\dot{\vec{\rho}} = \mathcal{M} \vec{\rho}, \quad (14.176)$$

where in the given Bloch vector basis the matrix  $\mathcal{M}$  has the following structure,

$$\mathcal{M} = \begin{pmatrix} (A) & (B_1) \\ (B_2) & \begin{pmatrix} (C) & (D) \\ (D) & (C) \end{pmatrix} \end{pmatrix}. \quad (14.177)$$

The different blocks of the matrix have the following significations. Block  $A$  handles the transfer of populations by spontaneous decay. Its rank corresponds to the number of levels  $n$ . The diagonal elements of this block are the decay rates  $\Gamma$  of the excited states. The off-diagonal elements  $\Gamma_{kl}$  denote the gain of level  $k$  from a decaying level  $l$ . Conservation of energy thus requires that the sum of the transition rates cancels for every column of matrix  $A$ ,  $\Gamma = \sum_k \Gamma_{kl}$ , as it is the case for the two-level Bloch matrix. If the levels are sublevels of a Zeeman and/or hyperfine split multiplet, the rates have to be weighted with Wigner's  $\{3j\}$  and  $\{6j\}$  symbols,  $\Gamma_{kl} = \Gamma S_{kl}$ . The relative oscillator strengths  $S_{kl}$  are given in Sec. 14.5.4.2.

The blocks  $B_k$  treat the interdependence of the populations and the coherences.  $B_1$  describes how the coherence between any pair of states driven by a light field generating a Rabi frequency  $\Omega_{kl}$  influences the populations. The block consists of convoluted  $2 \times 2$  matrices of the form,

$$\begin{pmatrix} \dot{\rho}_{kk} \\ \dot{\rho}_{ll} \end{pmatrix} \sim \begin{pmatrix} -\Omega_{kl} & 0 \\ \Omega_{kl} & 0 \end{pmatrix} \begin{pmatrix} \operatorname{Im} \rho_{kl} \\ \operatorname{Re} \rho_{kl} \end{pmatrix}. \quad (14.178)$$

$B_2$  describes how the populations in turn influence the coherences,

$$\begin{pmatrix} \operatorname{Im} \dot{\rho}_{kl} \\ \operatorname{Re} \dot{\rho}_{kl} \end{pmatrix} \sim \begin{pmatrix} \frac{1}{2} \Omega_{kl} & -\frac{1}{2} \Omega_{kl} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \rho_{kk} \\ \rho_{ll} \end{pmatrix}. \quad (14.179)$$

The Rabi frequencies have to be weighted not only with the relative oscillator strength  $S_{kl}$ , but also with the projection  $H_{kl}$  of the laser polarization onto the orientation of the magnetic field and the laser polarization,  $\Omega_{kl} = \Omega_x S_{kl} H_{kl}$ . Here  $\Omega_x$  is the Rabi frequency generated by a laser on a transition, whose oscillator strength is 1. The projection is calculated in Sec. 14.5.4.3 for the three possible laser polarizations, i.e. for  $\sigma^\pm$  and for  $\pi$  light.

The matrix  $C$  rules the influence of the decays of the coherences, of the detunings  $\Delta_{kl} = \omega_x - \omega_{atom}$ , and the laser linewidths  $\beta_{kl}$ . Note that the detuning of the laser frequency  $\omega_x$  is negative for red-detuned light. In the chosen basis it breaks down into an array  $2 \times 2$  matrices aligned along the diagonal of  $\mathcal{M}$ . Their shape is,

$$\begin{pmatrix} \operatorname{Im} \dot{\rho}_{kl} \\ \operatorname{Re} \dot{\rho}_{kl} \end{pmatrix} \sim \begin{pmatrix} -\frac{\gamma_{kl}}{2} & -\Delta_{kl} \\ \Delta_{kl} & -\frac{\gamma_{kl}}{2} \end{pmatrix} \begin{pmatrix} \operatorname{Im} \rho_{kl} \\ \operatorname{Re} \rho_{kl} \end{pmatrix}. \quad (14.180)$$

where  $\gamma_{kl} = \sum_{m, E_m < E_k, E_l} (\Gamma_{km} + \Gamma_{lm}) + 2\beta_{kl}$ . Often the levels are sublevels of a Zeeman and/or hyperfine split multiplets. In this case the frequency shift  $Z_{kl}$  of the level is added to the detuning  $\Delta_{kl}$ . The shift is calculated in Sec. 14.5.4.4 for the example of the  ${}^6\text{Li } D_2$  line.

The block  $D$  governs the interdependences of all laser-driven coherences of the atom. The block contains  $2 \times 2$  submatrices at any place of the matrix  $\mathcal{M}$ , where the row index pair  $(mn)$  and the column index pair  $(kl)$  have one index in common provided the two different indices correspond to the Rabi frequency of an incident laser:

$$\begin{pmatrix} \text{Im } \dot{\rho}_{mn} \\ \text{Re } \dot{\rho}_{mn} \end{pmatrix} \sim \begin{pmatrix} 0 & \pm \frac{1}{2} \Omega_{kl} \\ \pm \frac{1}{2} \Omega_{kl} & 0 \end{pmatrix} \begin{pmatrix} \text{Im } \rho_{pq} \\ \text{Re } \rho_{pq} \end{pmatrix}. \quad (14.181)$$

The submatrix elements indexed by column  $(pq)$  and row  $(mn)$  are non-zero if one of the indices  $p$  or  $q$  is equal to one of the indices  $m$  or  $n$  and the unequal indices correspond to a laser-driven transition. In order to find the correct signs of the submatrix elements, we distinguish four cases: 1. For  $m = p$ ,  $n = k$ , and  $q = l$  the signs are:  $(- \ +)$ ; 2. for  $n = q$ ,  $m = k$ , and  $p = l$  the signs are:  $(+ \ -)$ ; 3. for  $m = q$ ,  $n = k$ , and  $p = l$  the signs are:  $(+ \ +)$ ; and 4. for  $n = p$ ,  $m = k$ , and  $q = l$  the signs are:  $(- \ -)$ . A proper parametrization is proposed in the next section.

#### 14.5.4.1 Recipe for $D$ transitions in alkalines

In order to give a simple algorithm we parametrize the particular choice of sorting the components of the vector, we define a new index  $\mu$  running from 1 to  $n^2$  by setting  $(\varrho_\mu) \equiv (\rho_{kl})$ , where,

$$\begin{aligned} \mu(k, k) &= k \\ \mu(k, l) &= 2nk - n - k^2 - k + 2l - 1, \end{aligned} \quad (14.182)$$

so that,

$$\begin{aligned} \varrho_{\mu(k,k)} &= \rho_{kk} \\ \varrho_{\mu(k,l)} &= \text{Im } \rho_{kl} \\ \varrho_{\mu(k,l)+1} &= \text{Re } \rho_{kl}. \end{aligned} \quad (14.183)$$

The Bloch equations then formally read,

$$\dot{\varrho}_\mu = \mathcal{M}_{\mu\nu} \varrho_\nu. \quad (14.184)$$

We illustrate the procedure by considering the case of the  ${}^6\text{Li } D_2$  line with 6 ground states  $k \in G \equiv \{1, \dots, 6\}$  belonging to the  ${}^2S_{1/2}$  hyperfine levels  $F = \frac{1}{2}, \frac{3}{2}$  and 12 excited states  $k \in E \equiv \{7, \dots, 18\}$  belonging to the  ${}^2P_{3/2}$  hyperfine levels  $F = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$ .

According to the parametrization (14.176) the block  $A$  of the matrix  $\mathcal{M}$  is filled with the following components,

$$\begin{aligned} \mathcal{M}_{\mu(kk), \mu(kk)} &= -\Gamma \quad \text{for } k \in E \\ \mathcal{M}_{\mu(kk), \nu(ll)} &= \Gamma S_{kl} \quad \text{for } k \in G \quad \text{and } l \in E, \end{aligned} \quad (14.185)$$

where the relative oscillator strength  $S_{kl}$  is given by Eq. (14.192).

The blocks  $B_k$  of the matrix  $\mathcal{M}$  are filled with the components,

$$\begin{aligned}\mathcal{M}_{\mu(k,k),\nu(k,l)} &= -\mathcal{M}_{\mu(l,l),\nu(k,l)} \\ &= -2\mathcal{M}_{\mu(k,l),\nu(k,k)} = 2\mathcal{M}_{\mu(k,l),\nu(l,l)} \\ &= -\Omega_{kl}S_{kl}H_{kl} \ ,\end{aligned}\tag{14.186}$$

for  $k \in G$  and  $l \in E$ . The projection onto the quantization axis  $H_{kl} = H_{kl} \left( \frac{\hat{\epsilon}_{kl}}{|\hat{\epsilon}_{kl}|}, \vec{B}, m_l - m_k \right)$  is given by Eq. (14.195).

The block  $C$  contains the components,

$$\begin{aligned}\mathcal{M}_{\mu(k,l),\mu(k,l)} &= \mathcal{M}_{\mu(k,l)+1,\mu(k,l)+1} \\ &= -\frac{\Gamma}{2} - \frac{\Gamma}{2}\delta_{k \geq 7} - \beta_{pb}\delta_{2 < k < 7} - \beta_{rp}\delta_{k \leq 2}\end{aligned}\tag{14.187}$$

for  $k \in G \cup E$  and  $l \in E$  and ,

$$\begin{aligned}\mathcal{M}_{\mu(k,l),\mu(k,l)+1} &= -\mathcal{M}_{\mu(k,l)+1,\mu(k,l)} \\ &= -\Delta_{pb}\delta_{k > 2} - \Delta_{rp}\delta_{k < 3} + Z_{kl}(B)\end{aligned}\tag{14.188}$$

for  $k \in G$  and  $l \in E$ ,

$$\begin{aligned}\mathcal{M}_{\mu(k,f),\mu(k,f)+1} &= -\mathcal{M}_{\mu(k,f)+1,\mu(k,f)} \\ &= -\Delta_{pb} + \Delta_{rp} + Z_{k,10}(B) - Z_{f,10}(B)\end{aligned}\tag{14.189}$$

for  $k \in \{1, 2\}$  and  $f \in \{3, \dots, 6\}$ . The Zeeman shift  $Z_{kl}$  is given by Eq. (14.196).

Finally, the block  $D$  is filled with the components,

$$\begin{aligned}\mathcal{M}_{\mu(k,f),\mu(f,l)+1} &= (\delta_{f < k} - \frac{1}{2})\Omega_{kl}S_{kl}H_{kl} \\ \mathcal{M}_{\mu(k,f)+1,\mu(f,l)} &= (\delta_{l < f} - \frac{1}{2})\Omega_{kl}S_{kl}H_{kl} \\ \mathcal{M}_{\mu(l,f),\mu(f,k)+1} &= (\delta_{l < f} - \frac{1}{2})\Omega_{kl}S_{kl}H_{kl} \\ \mathcal{M}_{\mu(l,f)+1,\mu(f,k)} &= (\delta_{f < k} - \frac{1}{2})\Omega_{kl}S_{kl}H_{kl} \ ,\end{aligned}\tag{14.190}$$

where,

$$\begin{aligned}\Omega_{kl} &\equiv (\Omega_{rp}\delta_{k \leq 2} + \Omega_{pb}\delta_{k \geq 3})\delta_{l \geq 7} \\ \hat{\epsilon}_{kl} &\equiv (\hat{\epsilon}_{rp}\delta_{k \leq 2} + \hat{\epsilon}_{pb}\delta_{k \geq 3})\delta_{l \geq 7} \ .\end{aligned}\tag{14.191}$$

for  $k \in G \cup E$  and  $l \in E$  and  $f \in G \cup E$  but  $f \neq k, l$ . The projection onto the quantization axis  $H_{kl} = H_{kl} \left( \frac{\hat{\epsilon}_{kl}}{|\hat{\epsilon}_{kl}|}, \vec{B}, m_l - m_k \right)$  is given by Eq. (14.195).

The Eqs. (14.185)-(14.190) form together an algorithm to generate the matrix allowing one to numerically solve the Bloch equations (14.184), as has been done in the main text.

#### 14.5.4.2 Relative forces of oscillators

Spontaneous transitions between hyperfine- and Zeeman split levels have to be weighted according to the Wigner-Eckardt theorem using Clebsch-Gordan ( $3j$ ) and Wigner

$\{6j\}$  symbols. Consider the transition  $|(J_k, I)F_k, m_k\rangle \leftrightarrow |(J_l, I)F_l, m_l\rangle$ . The relative oscillator strength is,

$$S_{kl} = \left( \begin{array}{ccc} F_k & \kappa & F_l \\ m_k & \text{sign}(m_l - m_k) & -m_l \end{array} \right)^2 \quad (14.192)$$

$$\left\{ \begin{array}{ccc} J_l & J_k & \kappa \\ F_k & F_l & I \end{array} \right\}^2 \frac{(2F_k + 1)(2J_l + 1)(2\kappa + 1)}{2I + 1}.$$

#### 14.5.4.3 Elliptical laser polarization

The transition rates additionally depend on the relative orientation of the laser polarizations and the magnetic field direction. This dependence is accounted for by decomposing the polarization vector into the,

$$\hat{\mathbf{e}}_3 = \frac{\vec{\mathcal{B}}}{B}, \quad \hat{\mathbf{e}}_2 = \frac{\hat{\mathbf{e}}_3 \times \hat{\mathbf{g}}}{|\hat{\mathbf{e}}_3 \times \hat{\mathbf{g}}|}, \quad \hat{\mathbf{e}}_1 = \frac{\hat{\mathbf{e}}_2 \times \hat{\mathbf{e}}_3}{|\hat{\mathbf{e}}_2 \times \hat{\mathbf{e}}_3|}, \quad (14.193)$$

where  $\hat{\mathbf{g}}$  is an arbitrarily chosen direction, e.g. gravity. The relative amplitude of the transitions  $\Delta m_J = 0$  is proportional to the projection of the polarization vector on the magnetic field axis  $\zeta_0 = (\hat{\varepsilon} \cdot \hat{\mathbf{e}}_3)^2$  for  $\pi$ -polarized light. To estimate the amplitude of the transitions  $\Delta m_J = \pm 1$ , we must project onto the coordinates,

$$\hat{\mathbf{e}}_{\pm} = \frac{1}{\sqrt{2}}(\hat{\mathbf{e}}_1 \mp i\hat{\mathbf{e}}_2), \quad (14.194)$$

and we obtain  $\zeta_{\pm 1} = (\hat{\varepsilon} \cdot \hat{\mathbf{e}}_{\pm})^2$  for  $\sigma^{\pm}$ -polarized light. Hence,

$$H_{kl} = \zeta_{\Delta m_J} = \zeta_{m_l - m_k}. \quad (14.195)$$

With this generalization the Bloch equations can e.g. be employed to calculate Hanle resonances quantum mechanically. The Hanle effect occurs when a magnetic and an optical field compete for the quantization axis.

#### 14.5.4.4 Hyperfine and Zeeman splitting

The nuclear spin of the  ${}^6\text{Li}$  atom is  $I = 1$ , its electron spin is  $S = \frac{1}{2}$ . The excitation states are characterized by quantum numbers  $J_k, F_k, m_k$ . The electron angular orbital momentum is  $L_k = \delta_{k \geq 7}$ , and the electron angular orbital momentum is  $J_k = \frac{1}{2}\delta_{k \leq 6} + \frac{3}{2}\delta_{k \geq 7}$ . The hyperfine structure of the excited state  ${}^2P_{3/2}$  can be written as  $\nu_{hf1} = -2.8$  MHz,  $\nu_{hf2} = 0$  MHz, and  $\nu_{hf3} = 1.7$  MHz. Hence, the hyperfine splitting is inferior to the natural decay rate  $\Gamma = (2\pi) 6$  MHz,

$$Z_{kl} = \frac{\mu_B |\vec{\mathcal{B}}|}{2\pi\hbar} (g_{F_k} m_k - g_{F_l} m_l) \quad (14.196)$$

$$+ \nu_{hf1} \delta_{7 \leq l \leq 8} + \nu_{hf2} \delta_{8 \leq l \leq 13} + \nu_{hf3} \delta_{13 \leq l \leq 16},$$

where  $g_{F_k}$  is the Landé factor of hyperfine level  $F_k$ .

### 14.5.5 Exercises

#### 14.5.5.1 Ex: Derivation of three-level Bloch equations

Derive from the general formula (14.162) the three-level Bloch equations for the system  $|1\rangle \xleftrightarrow{\Omega_{12}} |2\rangle \xleftrightarrow{\Omega_{23}} |3\rangle$ .

### 14.5.5.2 Ex: Bloch equations for three levels

An excited  $\Lambda$ -shaped atom consists of two ground states  $|1\rangle$  and  $|3\rangle$ , which are coupled by two lasers with Rabi frequencies and detunings  $\Omega_{12}$  and  $\Delta_{12}$  respectively  $\Omega_{23}$  and  $\Delta_{23}$  through an excited level  $|2\rangle$ . Derive the Bloch equations from this system from the general master equation.

### 14.5.5.3 Ex: Adiabatic elimination

Derive the effective two-level Bloch equations for a  $\Lambda$ -type three-level system adiabatically eliminating the excited state under the Raman condition. **Help:** Start from the Liouvillean (14.164), set  $\rho_{22} = 0$ , assume  $\Gamma_{13} \ll \Gamma_{12}, \Gamma_{23} \ll |\Delta_{12}|, |\Delta_{23}|$ , and  $\Delta_{12} = -\Delta_{23}$ .

### 14.5.5.4 Ex: EIT & dark resonances

In this exercise we study so-called *dark resonances*, which are responsible for the phenomenon of *electromagnetically induced transparency* (EIT). Such resonances are observed in three-level systems  $|1\rangle$ - $|2\rangle$ - $|3\rangle$  in  $\Lambda$ -configuration, as shown in Fig. 14.6(a), when the laser detunings are chosen so as to satisfy  $\Delta_{12} = \Delta_{23}$ .

a. From the Bloch equations (14.164) show analytically that, in a stationary situation, the population of the excited state is  $\rho_{22}(\infty) = 0$  in the center of the dark resonance. Dark resonances can be observed experimentally. To reproduce the experiment by numerical simulations of the Bloch equations (14.164), write down the Liouville matrix  $\mathcal{M}_{red}$  reduced by the trace condition (14.168) and calculate the stationary Bloch vector from equation (14.169) varying the detunings of the two lasers  $\Delta_{12}$  and  $\Delta_{23}$ . Choosing the parameters such that  $\Gamma_{23} = \Gamma_{12}$ ,  $\Gamma_{13} = 0.01\Gamma_{12}$ ,  $\Omega_{12} = 2\Gamma_{12}$ , and  $\Omega_{23} = 0.2\Gamma_{12}$ , prepare a 3D curve [similar to Fig. 14.2(a)] of the population  $\rho_{22}(\infty)$ . Interpret the results.

### 14.5.5.5 Ex: STIRAP

In experiments with cold atoms it is often necessary to transfer populations between ground states, for example, between specific levels of a hyperfine structure. One possible procedure is the method of optical pumping, from the initial ground state to an excited state, which subsequently decays to the final state by spontaneous emission. The problem with this incoherent procedure is, that one can control into which ground state level the atom will decay, and that it heats atoms due to the photonic recoil associated with the scattering of light. In this exercise we studied an alternative method, called *Stimulated Raman Adiabatic Passage* (STIRAP), which allows the coherent transfer of population between two states by counter-intuitive pulse sequences:

a. Consider a three-level system in  $\Lambda$ -configuration, as shown in Fig. 14.6(a), initially being in the state  $|1\rangle$ . Write the system's Hamiltonian in the interaction picture. Now, choose  $\Delta_{12} = 0 = \Delta_{23}$ , and a temporal variation of the Rabi frequencies described by  $\Omega_{12}(t) = \Gamma_{12}(\frac{1}{2} + \frac{1}{\pi} \arctan \Gamma_{12}t)$  and  $\Omega_{23}(t) = \Gamma_{12}(\frac{1}{2} - \frac{1}{\pi} \arctan \Gamma_{12}t)$ . With this, solve the Schrödinger equation (14.172) iteratively within the time interval  $t \in [-40/\Gamma_{12}, 40/\Gamma_{12}]$ , while continuously adjusting the Rabi frequencies.

b. The dynamics can also be calculated via a numerical simulations of the Bloch



equations (14.164). Write down the Liouville matrix and prepare a simulation using the same parameters as in (b) and additionally  $\Gamma_{23} = \Gamma_{12}/2$ ,  $\Gamma_{13} = \Gamma_{12}/500$ .  
 c. Interpret the results.

#### 14.5.5.6 Ex: Adiabatic sweeps

In experiments with cold atoms it is often necessary to transfer populations between ground states, for example, between specific levels of a Zeeman structure. One possible procedure is the method of optical pumping, from the initial ground state to an excited state, which subsequently decays to the final state by spontaneous emission. The problem with this incoherent procedure is, that one can control into which ground state level the atom will decay, and that it heats atoms due to the photonic recoil associated with the scattering of light. In this exercise we study an alternative method, called *adiabatic sweep*, which allows the coherent transfer of population between the two outer states of a degenerate multiplet, as shown in Fig. 14.8, via an adiabatic ramp of the frequency of the incident radiation:

- Write down the Hamiltonian of the system in the interaction picture. Now, choose  $\Omega/2\pi = 8$  kHz and apply a linear ramp of the radiation detuning between  $-50$  kHz  $< \Delta(t)/2\pi < 50$  kHz during a time interval of 2 ms. With this, solve the Schrödinger equation (14.164) iteratively varying the detuning.
- Write down the Liouville matrix of the system and do a numerical simulation of the Bloch equations (14.164) using the same parameters as in (a). Interpret the results. What you observe when you introduce a decay rate between adjacent levels of  $\Gamma/2\pi = 200$  Hz?

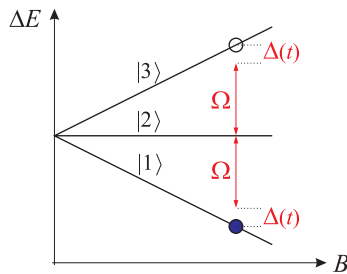


Figure 14.8: Energy levels of an atom in the ground state with Zeeman structure (for example,  $|J = 1, m_J = -1, 0, +1\rangle$ ) as a function of the applied magnetic field.

#### 14.5.5.7 Ex: Dispersive interaction between an atom and light

Radiation which is tuned far from a resonance can change the phase of an atomic dipole moment without changing the populations<sup>10</sup>. We study this effect in a three-level system in cascade configuration excited by two radiation fields, as illustrated in Fig. 14.6(c), simulating the Schrödinger equation and the Bloch equations.

- Write down the Hamiltonian  $\hat{H}$  for this system letting  $\Delta_{12} = 0$ .
- Now, consider the subsystem  $|2\rangle$ - $|3\rangle$ , write down its Hamiltonian  $\hat{H}_{23}$ , determine

<sup>10</sup>This type of interaction is used in the implementation of quantum gates in quantum computing.

the eigenvalues, and assume that this transition be excited very far-off resonance. That is, for  $\Delta_{23} \gg \Omega_{23}, \Gamma_{23}$  expand the eigenvalues of  $\hat{H}_{23}$  up to second order in  $\Omega_{23}$ . Finally, replace the submatrix  $\hat{H}_{23}$  in the complete Hamiltonian  $\hat{H}$  by the matrix of the expanded eigenvalues. This procedure corresponds to treating the transition  $|2\rangle\text{-}|3\rangle$  as a perturbation of the transition  $|1\rangle\text{-}|2\rangle$  until second order.

c. Assume that the atom is initially in the ground state and compute the time evolution of the state via the Schrödinger equation (14.172) using (a) the perturbed Hamiltonian and (b) the exact Hamiltonian for the following *sequence of pulses*:

(i) a  $\pi/2$ -pulse on the transition  $|1\rangle\text{-}|2\rangle$ ,

(ii) a pulse with a variable duration between 0 and  $\Delta t = \Omega_{23}^2/4\pi\Delta_{23}$  applied to the transition  $|2\rangle\text{-}|3\rangle$ ,

(iii) a  $\pi/2$ -pulse on the transition  $|1\rangle\text{-}|2\rangle$ . What you observe?

d. Establish the Liouville matrix  $\mathcal{L}$  for the same system and calculate the time evolution of the Bloch vector during the sequence by the Bloch equations (14.172) choosing the same parameters as in (c) and additionally  $\Gamma_{23} = 1$ ,  $\Gamma_{13} = \Gamma_{23}$ ,  $\Gamma_{12} = 0.01\Gamma_{23}$ , and  $\Omega_{12} \gg \Delta_{23}, \Gamma_{23}$ . Prepare a 3D curve [similar to Fig. 14.2(b)] of the population  $\rho_{22}(t)$ . Interpret the results.

#### 14.5.5.8 Ex: Fano profile of in dark resonance

The dark resonance studied in Exc. 14.5.5.4 may in some circumstances adopt an asymmetric profile. Calculate, for a three-level system in  $\Lambda$ -configuration, as shown in Fig. 14.6(a), starting from the Bloch equations (14.164) with the Liouville matrix  $\mathcal{M}_{red}$  reduced by the trace condition (14.168), the spectrum  $\rho_{22}(\Delta_2)$  for the following set of parameters:  $\Gamma_{12} = 2$ ,  $\Gamma_{23} = \Gamma_{12}/2$ ,  $\Gamma_{23} = 0.1\Gamma_{12}$ ,  $\Omega_{12} = 10\Gamma_{12}$ ,  $\Omega_{23} = 5\Gamma_{23}$ ,  $\Delta_{12} = -5\Gamma_{12}$  and  $\Delta_{23} = [-1 : .01 : 1]\Gamma_{23}$ . Interpret the spectrum in terms of a Fano resonance.

#### 14.5.5.9 Ex: Gas with negative permittivity

Study EIT on the strontium cascade system consisting of the transitions 689 nm and 497 nm and draw a spectrum of the permittivity. Compare with the permittivity of the 689 nm two-level system. What densities are necessary to get a negative permittivity?

#### 14.5.5.10 Ex: Gas with negative permeability

Theoretically, under certain conditions, gases may exhibit *negative* permittivity and permeability, and therefore refraction [630]<sub>DOI</sub>, [628]<sub>DOI</sub>, [629]<sub>DOI</sub>, [526]<sub>DOI</sub>, [420]. To study this phenomenon we consider a three-level system in  $\Lambda$ -configuration with an electric dipole transition and another magnetic dipole transition. The objective is to balance the electrical dipole moment excited by a probe laser and the magnetic dipole moment excited via a Raman transition by both, the probe laser and a control laser. The Raman transition simulates an effective magnetic field. Since the magnetic moment is smaller by a factor of  $\alpha^2$ , the electric moment must be reduced by detuning the probe laser, as shown in Fig. 14.9.

a. Consider a three-level system in  $\Lambda$ -configuration. The transitions  $|1\rangle\text{-}|2\rangle$  and  $|2\rangle\text{-}|3\rangle$  are assumed to be electric dipoles and  $|1\rangle\text{-}|3\rangle$  a magnetic dipole, such that,  $\Gamma_{12}, \Gamma_{23} \gg \Gamma_{13}$ . Extract from the Bloch equation (14.164) the equations for the coherences  $\rho_{12}$ ,

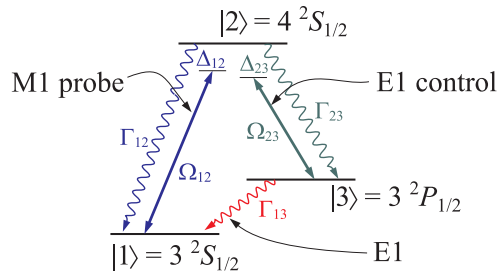


Figure 14.9:

$\rho_{13}$ , and  $\rho_{23}$ .

b. Suppose, that the excitation on the probe transition be so weak,  $\Omega_{12} \ll \Gamma_{12}$ , that it does not succeed to empty the ground state. In this approximation eliminate the dynamics of  $\rho_{23}$  and deduce the stationary solution for  $\rho_{12}$  and  $\rho_{13}$ .

c. Calculate the magnetic susceptibility  $\chi_m$  [629] with the following parameters  $\Gamma_{12} = 7 \cdot 10^7 \text{ s}^{-1}$ ,  $\Gamma_{23} = 3 \cdot 10^7 \text{ s}^{-1}$ ,  $\Gamma_{13} = 2 \cdot 10^7 \text{ s}^{-1}$ ,  $\Omega_{12} = 0.1\Gamma_{12}$ ,  $\Omega_{23} = 2 \cdot 10^8 \text{ s}^{-1}$ ,  $\Delta_{23} = 0$  in the regime  $\Delta_{12} = [-15\Gamma_{23}, 15\Gamma_{23}]$ .

d. Simulate the Bloch equations (14.164) and compare with the numerical solution.

#### 14.5.5.11 Ex: Magnetic dipole transitions in strontium

Magnetic dipole transitions are characterized by the selection rules  $\Delta J = 0, \pm 1$ ,  $\Delta S = 0$ ,  $\Delta L = 0$ , and  $\Delta n = 0$ . There are several transitions starting from the  $5s5p \ ^3P_J$  metastable states going to the  $5p^2 \ ^3P_J$  states with strong linewidths:

- $5s5p \ ^3P_1^o \leftrightarrow 5p^2 \ ^3P_2$  at 472.2278nm with  $\Gamma = (2\pi) \ 5.7 \text{ MHz}$
- $5s5p \ ^3P_1^o \leftrightarrow 5p^2 \ ^3P_1$  at 478.4320nm with  $\Gamma = (2\pi) \ 4.8 \text{ MHz}$

Check whether it is possible to reach negative permeability in a cold strontium gas.

#### 14.5.5.12 Ex: Cascade EIT scheme in strontium

Consider the Bloch equations for the  $^{88}\text{Sr}$  7-level system consisting of the following levels:  $|1\rangle \equiv (5s^2) \ ^1S_0$ ,  $|2-4\rangle \equiv (5s5p) \ ^3P_1$ , and  $|5-7\rangle \equiv (5s5d) \ ^3D_1$ , and check under which circumstances it is possible to observed dark resonances. The Sr level scheme can be consulted under (Sr level scheme). The Liouvillean can be consulted at (Sr Liouvillean).

## 14.6 Further reading

J. Weiner and P-T. Ho, Springer-Verlag, Berlin (2003), *Light-Matter Interaction: Fundamentals and Applications* [ISBN]

R. Loudon, Oxford Science Publications, Oxford (1982), *The quantum theory of light* [ISBN]

- M.O. Scully, *From lasers and masers to phaseonium and phasers* [DOI]
- I.I. Sobelman, Springer Verlag, Berlin (1972), *Introduction to the Theory of Atomic Spectra* [ISBN]
- M. Weissbluth, (Academic Press, Boston, 1989), *Photon-Atom Interactions* [ISBN]
- A. Corney, Clarendon Press, Oxford (1977), *Atomic and Laser Spectroscopy* [ISBN]
- C.M. Tokarsky Dieguez et al., *Os fundamentos quânticos da Ressonância Magnética Nuclear* [DOI]
- Y. Stalgies et al., *Light shift and Fano resonances in a single cold ion* [DOI]
- M. Fleischhauer et al., *Electromagnetically induced transparency, Optics in coherent media* [DOI]
- L.V. Hau et al., *Light Speed Reduction to 17 Metres per Second in an Ultracold Atomic Gas* [DOI]

### 14.6.1 on negative refraction

- A. Poddubny et al., *Hyperbolic metamaterials* [DOI]
- Jian-Qi Shen et al., *How to realize a negative refractive index material at the atomic level in an optical frequency range* [DOI]
- Jian-Qi Shen et al., *Negatively refracting atomic vapour* [DOI]
- Jian-Qi Shen et al., *Negative permeability in a  $\Lambda$ -type three-level atomic vapor* [DOI]
- F. Bello, *Negative index of refraction in a four-level system with magnetoelectric cross coupling and local field corrections* [DOI]
- Yi S. Ding et al., *Possible realization of negative refraction in Bose-Einstein condensates* [DOI]
- A. Alù et al., *Pairing an Epsilon-Negative Slab With a Mu-Negative Slab Resonance, Tunneling and Transparency* [DOI]
- M.Ö. Oktel et al., *Electromagnetically induced left-handedness in a dense gas of three-level atoms* [DOI]
- P.P. Orth et al., *Negative refraction with tunable absorption in an active dense gas of atoms* [DOI]
- D.E. Sikes et al., *Negative refraction using Raman transitions and chirality* [DOI]
- P. Shekhar et al., *Strong Coupling in Hyperbolic Metamaterials* [DOI]



## Chapter 15

# Atoms in quantized radiation fields

So far we have treated the optical field only as a stationary or propagating classical wave, while our two-level atom has been regarded as an entity obedient to the laws of quantum mechanics and subject to an induced perturbation by an oscillatory electromagnetic field. This procedure naturally leads to oscillations of the atomic states' populations and the coherences between them. However, in strong fields, when atomic energy spectrum is significantly modified, a non-perturbative, time-independent approach can be fruitful. Time-independent solutions for the Schrödinger equation for atoms coupled to fields is called *dressed states*. They were used for the first time to interpret the *splitting* of rotational molecular spectra in the presence of intense classical radiofrequency fields. While the semiclassical treatment is suitable for a wide variety of phenomena and has the virtue of mathematical simplicity and familiarity, it is sometimes worth considering the field as a quantum entity as well. In the dressed states picture, the atom-field interaction corresponds to an exchange of energy quanta between the field (photons) and the atom. This approach allows us to express photonic *number states*, also called *Fock states*, on equal footings with the discrete states of atom excitation and to write the state functions of the coupled atom-field system in a basis of photonic and atomic product states. Diagonalization of the dipole coupling terms in the system's Hamiltonian generates time-independent solutions of dressed states in a completely quantum Schrödinger equation.

We begin this chapter with the quantization of the light field and then express the atom-field interaction in a fully quantized form. We will examine some examples illustrating how the dressed states picture can provide useful information on the light-matter interactions.

### 15.1 Quantization of the electromagnetic field

We have already seen that the energy of a monochromatic light field with frequency  $\omega$  is quantized in small equal portions, such that the total energy is  $N\hbar\omega$ , where  $N$  is an integer number. The energy spectrum is the same as the one of the harmonic oscillator. Therefore, we can identify a light mode with an oscillator and adopt the entire formalism developed for the harmonic oscillator. The formalism will be assumed as known in the following. We will, for simplicity use the term *photon* (respectively *phonon*) for excitations of a harmonic oscillator mode. It is however important to be

aware that a photon is not a particle, as it simply *disappears when performing the transition from quantum to classical mechanics* [421].

### 15.1.1 Field operators

The basic idea behind field quantization is the replacement of the classical harmonic oscillators discussed in Sec. 3.5 by quantum oscillators. The simplest approach to perform this quantization is to introduce the scalar potential  $\Phi$  and the potential vector  $\mathbf{A}$  as done in electrodynamic theory <sup>1</sup>. In free space, without charges nor currents, and within the *Coulomb gauge* we have the solution of the wave equation (13.5) generalized to a distribution of wavevectors  $\mathbf{k}$  <sup>2</sup>,

$$\mathbf{A}(\mathbf{r}, t) = \sum_{\mathbf{k}} \vec{\epsilon}_{\mathbf{k}} [A_{0\mathbf{k}}^+ e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} + A_{0\mathbf{k}}^- e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)}], \quad (15.1)$$

where we already isolated the vectorial character due to the polarization  $\vec{\epsilon}_{\mathbf{k}}$  of the light mode  $\mathbf{k}$ . Obviously,  $A_{0\mathbf{k}}^- = (A_{0\mathbf{k}}^+)^*$ . As each amplitude and polarization of the wave given by the vector potential  $\mathbf{A}_{\mathbf{k}}$  and  $\mathbf{A}_{\mathbf{k}}^*$  must satisfy the wave equation separately, we arrive at the dispersion relation,

$$\omega_{\mathbf{k}} = ck. \quad (15.2)$$

With the results (13.7) and (13.8) we know that the energy in each radiative mode containing  $n_{\mathbf{k}}$  photons is,

$$E_{\mathbf{k}} = \hbar\omega_{\mathbf{k}}N_{\mathbf{k}} = u_{\mathbf{k}}V = 2\varepsilon_0V\omega_{\mathbf{k}}^2\overline{\mathbf{A}_{0\mathbf{k}}^2} = 2\varepsilon_0V\omega_{\mathbf{k}}^2(A_{0\mathbf{k}}^-A_{0\mathbf{k}}^+ + A_{0\mathbf{k}}^+A_{0\mathbf{k}}^-), \quad (15.3)$$

where the bar denotes cycle-averaging. The second quantization now consists in interpreting the mode as a *quantum harmonic oscillator*, that is, we understand the observables as *operators* satisfying commutation rules, such as  $[\hat{A}_{0\mathbf{k}}, \hat{A}_{0\mathbf{k}'}^+] \propto \delta_{\mathbf{k},\mathbf{k}'}$ , and hence being affected by quantum fluctuations:

$$\hat{H}_{\mathbf{k}} = \hbar\omega_{\mathbf{k}}(\hat{n}_{\mathbf{k}} + \frac{1}{2}) = 2\varepsilon_0V\omega_{\mathbf{k}}^2(\hat{A}_{0\mathbf{k}}^- \hat{A}_{0\mathbf{k}}^+ + \hat{A}_{0\mathbf{k}}^+ \hat{A}_{0\mathbf{k}}^-). \quad (15.4)$$

We introduce normalized field operators following the commutation rule (3.74) via,

$$\hat{a}_{\mathbf{k}}\sqrt{\frac{\hbar}{4\varepsilon_0V\omega_{\mathbf{k}}}} \equiv \hat{A}_{0\mathbf{k}}^+ \quad \text{and} \quad \hat{a}_{\mathbf{k}}^\dagger\sqrt{\frac{\hbar}{4\varepsilon_0V\omega_{\mathbf{k}}}} \equiv \hat{A}_{0\mathbf{k}}^-, \quad (15.5)$$

such that,

$$\hat{H}_{\mathbf{k}} = \hbar\omega_{\mathbf{k}}(\hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}} + \frac{1}{2}). \quad (15.6)$$

The analogy allows us to interpret them as *creation operator* and *annihilation operator* of photons. Finally, we can rewrite (15.1) as,

$$\boxed{\hat{\mathbf{A}}_{\mathbf{k}}(\mathbf{r}, t) = \sqrt{\frac{\hbar}{4\varepsilon_0V\omega_{\mathbf{k}}}} \vec{\epsilon}_{\mathbf{k}} \left[ \hat{a}_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} + \hat{a}_{\mathbf{k}}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} \right]}. \quad (15.7)$$

<sup>1</sup>See the script *Electrodynamics* by the same author [Scripts/EleetroMagnetismScript](#).

<sup>2</sup>The atom-light interaction may depend on the polarization of the light with respect to the quantization axis of the atom, as defined e.g. by a magnetic field. In these cases we need to extend the index  $\mathbf{k}$  to include the polarization state  $(\mathbf{k}, \lambda)$ .

We already know such combinations of operators and their complex conjugates from the quantum harmonic oscillator (3.83).

In the Coulomb gauge, the electric and magnetic field operators for the cavity modes can be constructed from,

$$\begin{aligned} \hat{\mathcal{E}}_{\mathbf{k}} &= -\frac{\partial \hat{\mathbf{A}}_{\mathbf{k}}}{\partial t} = \imath \sqrt{\frac{\hbar \omega_{\mathbf{k}}}{2\varepsilon_0 V}} \left( \hat{a}_{\mathbf{k}} e^{\imath(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} - \hat{a}_{\mathbf{k}}^\dagger e^{-\imath(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} \right) \vec{\epsilon}_k \\ \hat{\mathcal{B}}_{\mathbf{k}} &= \nabla \times \hat{\mathbf{A}}_{\mathbf{k}} = \imath \sqrt{\frac{\hbar \omega_{\mathbf{k}}}{2\varepsilon_0 V}} \left( \hat{a}_{\mathbf{k}} e^{\imath(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} - \hat{a}_{\mathbf{k}}^\dagger e^{-\imath(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} \right) \mathbf{k} \times \vec{\epsilon}_k \end{aligned} \quad (15.8)$$

We can calculate the cycle-averaged energy of the  $\mathbf{k}$ -th cavity mode from a quantum version of Eq. (15.3),

$$\bar{E}_{\mathbf{k}} = \frac{\varepsilon_0}{2} \int \langle n_{\mathbf{k}} | \hat{\mathcal{E}}_{\mathbf{k}} \cdot \hat{\mathcal{E}}_{\mathbf{k}} | n_{\mathbf{k}} \rangle dV . \quad (15.9)$$

The result (15.6) is exactly Planck's quantum hypothesis (although strictly speaking, he rather suggested a quantization of oscillators in the conducting walls of the cavity, not of the field) on the distribution of the spectral intensity radiated by a black body. We now can see that it follows naturally from the quantization of the cavity field modes. Solve Excs. 15.1.4.1, Exc. 15.1.4.2, and 15.1.4.3.

### 15.1.2 Interaction of quantized fields with atoms

With the results of the previous section the complete field Hamiltonian reads,

$$\hat{H}_{field} = \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \left( \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \frac{1}{2} \right) . \quad (15.10)$$

Now, that we have a clear picture of the quantized field with the energies in the modes given by Eq. (15.9) and the photon number states given by the eigenstates  $|n\rangle$  of the quantized harmonic oscillator, we are in a position to consider our two-level atom interacting with this quantized radiation field. If for the moment, we exclude spontaneous emission and stimulated processes, the Hamiltonian of the combined atom-field system is,

$$\hat{H} = \hat{H}_{atom} + \hat{H}_{field} + \hat{H}_{atom:field} . \quad (15.11)$$

We describe the atom by a two-level system,

$$\hat{H}_{atom} = \hbar \omega_g |g\rangle \langle g| + \hbar \omega_e |e\rangle \langle e| = \hbar \omega_g |g\rangle \langle g| + \hbar(\omega_g + \omega_0) |e\rangle \langle e| , \quad (15.12)$$

where  $\hat{H}_{field}$  is the Hamiltonian of the quantized field, expressed by Eq. (15.6), and  $\hat{H}_{atom:field}$  the atom-field interaction. For the Hamiltonian without interaction,  $\hat{H} = \hat{H}_{atom} + \hat{H}_{field}$ , the eigenstates are simply product states of the atomic states and the photon number states,

$$|g, n\rangle = |g\rangle |n\rangle \quad \text{and} \quad |e, n\rangle = |e\rangle |n\rangle . \quad (15.13)$$

The left side of Fig. 15.1 shows, how the eigenenergies of the product states consist of two ladders, being displaced by the energy difference  $\hbar\Delta$ , which corresponds to the



detuning. We write the Hamiltonian of the atom Eq. (15.12) as the sum of projectors on unperturbed eigenstates using the completeness relation and the orthogonality of eigenstates. With the same idea we can rewrite the dipole operator defined in Eq. (13.30),

$$\hat{\mathbf{d}} = \sum_i |\psi_i\rangle\langle\psi_i| \hat{\mathbf{d}} \sum_j |\psi_j\rangle\langle\psi_j| = \sum_{i,j} |i\rangle\langle i| e^{i(\omega_i - \omega_j)t} \hat{\mathbf{d}} |j\rangle\langle j| = \sum_{i,j} e^{i(\omega_i - \omega_j)t} \mathbf{d}_{ij} |i\rangle\langle j|. \quad (15.14)$$

using  $|\psi_n(t)\rangle = e^{-i\omega_n t} |n\rangle$ . Note that  $\hat{\mathbf{d}}$  only has non-diagonal elements.

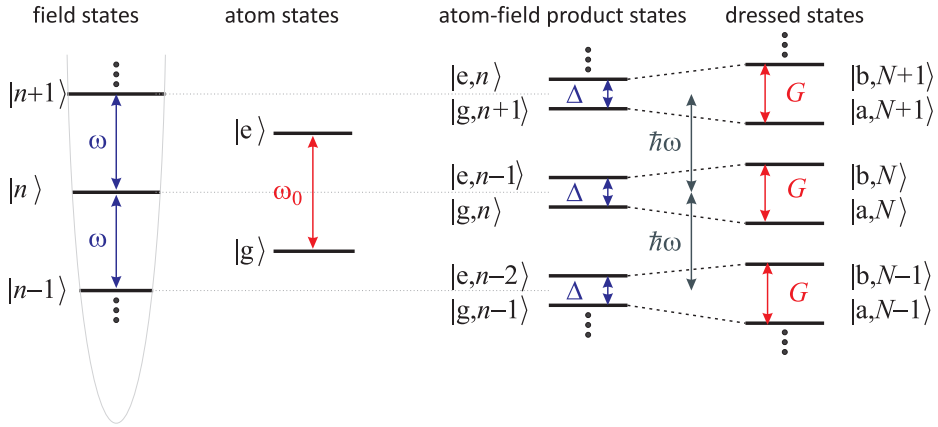


Figure 15.1: (Left) Photons number states and the two stationary states of the two-levels atom. (Center) Double ladder showing the basis of products states of photon number and atomic states. (Right) Dressed states constructed by diagonalization of the full Hamiltonian in the basis of the product states.

Now, let us use the electric field of Eqs. (15.8) to describe the atom-field interaction through the Hamiltonian  $\hat{H}_{atom:field} = -\hat{\mathbf{d}} \cdot \hat{\mathcal{E}}$ ,

$$\hat{H}_{atom:field} = i \sum_{\mathbf{k}} \sum_{i,j} \sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2\epsilon_0 V}} \mathbf{d}_{ij} e^{i(\omega_i - \omega_j)t} |i\rangle\langle j| \cdot \vec{\epsilon}_{\mathbf{k}} \left[ \hat{a}_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} - \hat{a}_{\mathbf{k}}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} \right]. \quad (15.15)$$

For our two-level atom interacting with a single mode radiation field, we only have,

$$\hat{H}_{atom:field} = i\sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2\epsilon_0 V}} \mathbf{d}_{ge} \left[ e^{i(\omega_e - \omega_g)t} |g\rangle\langle e| + e^{i(\omega_g - \omega_e)t} |e\rangle\langle g| \right] \cdot \vec{\epsilon}_{\mathbf{k}} \left[ \hat{a}_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} - \hat{a}_{\mathbf{k}}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} \right]. \quad (15.16)$$

### 15.1.2.1 Rotating wave approximation for dressed states

We can simplify the notation by identifying  $\hat{\sigma}^+ = |e\rangle\langle g|$  and  $\hat{\sigma}^- = |g\rangle\langle e|$  of the Eqs. (14.72) and introducing as an abbreviation the *Rabi frequency*,

$$\frac{1}{2} \hbar\Omega(\mathbf{r}) \equiv \sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2\epsilon_0 V}} \mathbf{d}_{ge} \cdot \vec{\epsilon}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (15.17)$$

The interaction Hamiltonian then becomes,

$$\hat{H}_{atom:field} = \frac{i}{2}\hbar\Omega(\mathbf{r})e^{-i(\omega_{\mathbf{k}}-\omega_0)t}\hat{\sigma}^+\hat{a}_{\mathbf{k}} + \frac{i}{2}\hbar\Omega(\mathbf{r})e^{-i(\omega_{\mathbf{k}}+\omega_0)t}\hat{\sigma}^-\hat{a}_{\mathbf{k}} - \frac{i}{2}\hbar\Omega^*(\mathbf{r})e^{i(\omega_{\mathbf{k}}+\omega_0)t}\hat{\sigma}^+\hat{a}_{\mathbf{k}}^\dagger - \frac{i}{2}\hbar\Omega^*(\mathbf{r})e^{i(\omega_{\mathbf{k}}-\omega_0)t}\hat{\sigma}^-\hat{a}_{\mathbf{k}}^\dagger. \quad (15.18)$$

This Hamiltonian contains four terms describing the following processes <sup>3</sup>,

- $|g, n\rangle \longrightarrow |e, n-1\rangle$  the atom is excited by the absorption of a photon;
- $|e, n\rangle \longrightarrow |g, n-1\rangle$  the atom is deexcited by the absorption of a photon;
- $|g, n\rangle \longrightarrow |e, n+1\rangle$  the atom is excited by the emission of a photon;
- $|e, n\rangle \longrightarrow |g, n+1\rangle$  the atom is deexcited by the emission of a photon.

Obviously, only the first and fourth terms respect energy conservation (in first-order processes) and can serve as initial and final states in real physical processes. Fig. 15.3 shows schemes of these four terms. We see, that neglecting the second and third process (i.e., terms  $\propto \hat{\sigma}^\pm \hat{a}^\pm$  of the Hamiltonian) is equivalent to making the rotating wave approximation (RWA), where we despise the terms rotating with the frequency  $\pm(\omega_{\mathbf{k}} + \omega_0)$ , and that we really only need to consider the coupling between the two dressed states  $|g, n\rangle$  and  $|e, n-1\rangle$ .

Finally, within the RWA the Hamiltonian reads,

$$\hat{H}_{atom:field} = \frac{i}{2}\hbar\Omega(\mathbf{r})e^{-i\Delta_{\mathbf{k}}t}\hat{\sigma}^+\hat{a}_{\mathbf{k}} - \frac{i}{2}\hbar\Omega^*(\mathbf{r})e^{i\Delta_{\mathbf{k}}t}\hat{\sigma}^-\hat{a}_{\mathbf{k}}^\dagger, \quad (15.19)$$

where we introduced the detuning  $\Delta_{\mathbf{k}} \equiv \omega_{\mathbf{k}} - \omega_0$  as short hand notation.

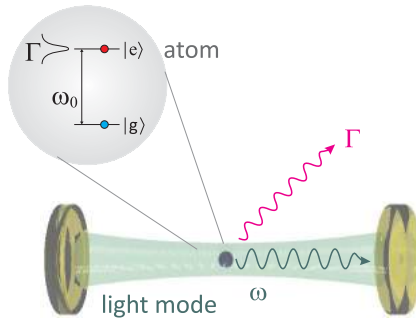


Figure 15.2: Two-level atom interacting with a cavity mode.

It is important to note that the first and fourth term can be important in higher order processes, such as multiphotonic absorption or Raman scattering processes, where the excited state would be a virtual level. In fact, when the Rabi frequency is very large,  $\Omega \simeq \omega$ , the excitation and deexcitation processes follow each other so rapidly, that energy conservation can be violated for short times. The energy shift caused by terms neglected in the RWA are called *Bloch-Siegert shift* <sup>4</sup>.

<sup>3</sup>Remember that the four processes contained in the Hamiltonian are all coherent (absorption and stimulated emission), and that spontaneous emission must be treated separately see next Sec. 15.4.

<sup>4</sup>The shift is not observed, when the non-rotating terms  $\sigma^\pm a^\pm$  are forbidden by other conservation or selection rules. For example, when a resonance is excited by  $\sigma^\pm$  light, the RWA is accurate.

### 15.1.3 Dressed states

Within the new dressed states basis, the atom-light coupling problem is reduced to diagonalizing the Hamiltonian of a quasi-degenerate two-level atom ( $|\Delta| \ll \omega_0$ ), in which the non-diagonal elements are given by  $\frac{1}{2}\hbar\Omega$ . The eigenenergies of the complete Hamiltonian  $\hat{H}$  are,

$$E_{\pm} = \frac{\hbar}{2}(\omega_{g,n} + \omega_{e,n-1}) \pm \frac{\hbar}{2}G . \quad (15.20)$$

where  $\hbar\omega_{g,n}$  and  $\hbar\omega_{e,n-1}$  are the energies of the product states  $\hbar\omega_g + n\hbar\omega_{\mathbf{k}}$  and  $\hbar\omega_e + (n-1)\hbar\omega_{\mathbf{k}}$ . The separation between constituents of the same dressed state is  $G = \sqrt{\Omega^2 + \Delta^2}$ .

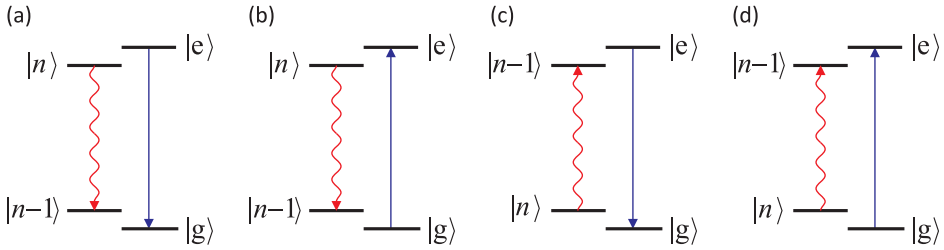


Figure 15.3: Illustration of the four processes in the atom-field interaction. Terms (b) and (c) conserve energy in first-order processes, while (a) and (d) do not conserve.

The atom-field product states offer a natural basis for the Hamiltonian of Eq. (15.11). The states resulting from the diagonalization of the Hamiltonian on this basis are called *dressed states*. As indicated in Fig. 15.1, the neighboring doublets the double ladder 'repel' each other under the influence of the interaction  $\hat{H}_{atom:field}$  in Eq. (15.11). The mixed coefficients form the familiar problem of two levels, now called  $|a\rangle$  and  $|b\rangle$ . From Fig. 15.1 we see,

$$\begin{pmatrix} |a, N\rangle \\ |b, N\rangle \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} |g, n\rangle \\ |e, n-1\rangle \end{pmatrix} . \quad (15.21)$$

with

$$\tan 2\theta = \frac{\Omega}{\Delta} . \quad (15.22)$$

The numbers  $n$  denote the amount of photons in the laser beam, the numbers  $N$  denote the amount of energy packets within the system, that is, the photons *plus* the possible excitation of the atom.

## 15.1.4 Exercises

### 15.1.4.1 Ex: Photon statistics

An optical resonator contains on average 10 photons in the mode  $TEM_{00q}$ . What is the probability of finding, at any time, 1 photon resp. 10 photons, when the light is (a) thermal, (b) coherent? For case (a), what is the temperature of the light for  $\lambda = 633 \text{ nm}$ ?

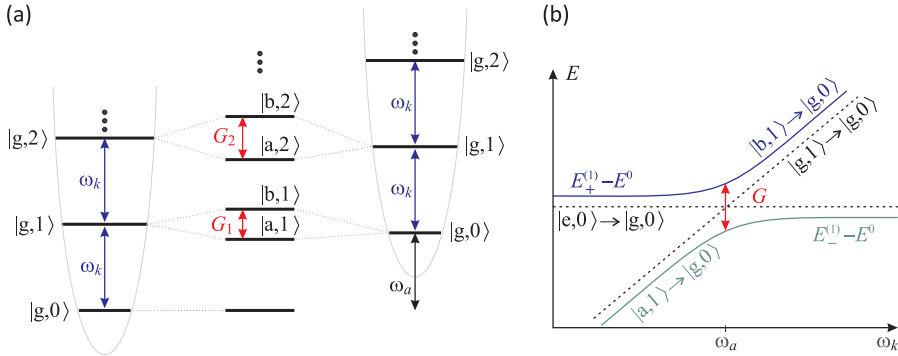


Figure 15.4: (a) Rabi splitting of the lowest dressed states. (b) Avoided crossing of dressed states.

### 15.1.4.2 Ex: Thermal mixture

We consider a thermal non-interacting atomic gas in one dimension. Instead of describing the state of the atomic ensemble, we can consider a single atom with a distributed probability of having a given velocity  $v$ . The density operator of the continuous degree of freedom can be written,

$$\hat{\rho} = \int dv \sqrt{\frac{m}{2\pi k_B T}} e^{-mv^2/2k_B T} |v\rangle\langle v| ,$$

and the trace of an arbitrary observable  $\hat{A}$ ,

$$\langle \hat{A} \rangle = \text{Tr } \hat{\rho} \hat{A} = \int du \langle u | \hat{\rho} \hat{A} | u \rangle .$$

Now imagine a device capable of measuring the speed of a single atom randomly chosen within the cloud.

- Express the probability of measuring a specific velocity  $v'$  for this atom using the density operator.
- Express the expectation value of the average velocity by the density operator.

### 15.1.4.3 Ex: Converting a pure state into a mixture by incomplete measurement

Consider a dressed two-level atom with the atomic states  $|1\rangle$  and  $|2\rangle$  and the photon number state  $|n\rangle$ .

- Write down the general normalized dressed state and the density operator.
- Now, perform a measurement of the atomic state tracing over the atomic degree of freedom and verify whether the resulting density operator represents a pure state.
- Now, perform a measurement of the photon number and verify whether the resulting density operator represents a pure state.



Note that we can simplify the above Hamiltonian  $\hat{H}_n$  applying the unitary transform,

$$U \equiv \begin{pmatrix} e^{-i(n-1/2)\omega t} & 0 \\ 0 & e^{-i(n-1/2)\omega t} \end{pmatrix}, \quad (15.27)$$

yielding,

$$\tilde{H}_n = U^\dagger \hat{H}_n U + i\dot{U}^\dagger U = \begin{pmatrix} \frac{\Delta}{2} & \frac{\Omega}{2}\sqrt{n} \\ \frac{\Omega}{2}\sqrt{n} & -\frac{\Delta}{2} \end{pmatrix}. \quad (15.28)$$

The eigenvalues can be easily calculated by <sup>5</sup>,

$$\det \sum_n \hat{H}_n = \sum_n \det \tilde{H}_n, \quad (15.29)$$

defining the detuning between radiation and the atomic transition,  $\Delta \equiv \omega - \omega_0$ , and the generalized  $n$ -photon Rabi frequency,  $\varpi_n \equiv \sqrt{\Delta^2 + n\Omega^2} = |\varpi_n|e^{i\mathbf{k}\cdot\mathbf{R}}$ , which contains the spatial mode function of the radiation field. This gives the diagonal matrix of eigenvalues,

$$\hat{E}_n = \begin{pmatrix} (n - \frac{1}{2})\omega + \frac{\varpi_n}{2} & 0 \\ 0 & (n - \frac{1}{2})\omega - \frac{\varpi_n}{2} \end{pmatrix}. \quad (15.30)$$

From the transformation  $\hat{H}_n U_n = U_n \hat{E}_n$ , under the condition that  $U_n$  is unitary and hermitian,  $U_n^\dagger U_n = 1$ , and using the abbreviation  $\tan 2\phi_n \equiv \sqrt{n}\Omega/\Delta$ , we obtain:

$$U_n = \begin{pmatrix} \cos \phi_n & \sin \phi_n \\ -\sin \phi_n & \cos \phi_n \end{pmatrix}. \quad (15.31)$$

The eigenvectors corresponding to the eigenvalues  $\hat{E}_n$  are obtained by  $\hat{H}_n|x\rangle = e_{nx}|x\rangle$ , that is,  $\hat{E}_n U_n^{-1}|x\rangle = e_{nx} U_n^{-1}|x\rangle$ . Knowing  $\hat{E}_n|y\rangle = e_{ny}|y\rangle$ , we obtain  $|x\rangle = U_n|y\rangle$ . The temporal evolution of the Jaynes-Cummings state,  $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle$ , is described by the transformation,

$$\begin{aligned} e^{-i\hat{H}_n t} &= U_n e^{-i\hat{E}_n t} U_n^\dagger = e^{-i(n-1/2)\omega t} \times \\ &\times \begin{pmatrix} \cos^2 \phi_n e^{-i\varpi_n t/2} + \sin^2 \phi_n e^{i\varpi_n t/2} & \cos \phi_n \sin \phi_n (e^{i\varpi_n t/2} - e^{-i\varpi_n t/2}) \\ \cos \phi_n \sin \phi_n (e^{i\varpi_n t/2} - e^{-i\varpi_n t/2}) & \sin^2 \phi_n e^{-i\varpi_n t/2} + \cos^2 \phi_n e^{i\varpi_n t/2} \end{pmatrix}, \end{aligned} \quad (15.32)$$

which is essentially the same, as the time evolution derived in Exc. 2.4.7.1. The transition probability between dressed states is,

$$|\langle 2, n-1 | e^{-i\hat{H}_n t} | 1, n \rangle|^2 = \frac{4n\Omega^2\Delta^2}{\varpi_n^2} \sin^2 \frac{\varpi_n t}{2}. \quad (15.33)$$

<sup>5</sup>The following rules apply to determinants,

$$\det(AB) = \det A \det B \quad \text{and} \quad (\det A)^{-1} = \det A^{-1}.$$

The temporal evolution follows with [370],

$$\hat{\rho}(t) = e^{-i\hat{H}_n t} \hat{\rho}(0) e^{i\hat{H}_n t} \equiv \mathcal{L}(t) \hat{\rho}(0). \quad (15.34)$$

Do the Exc. 15.2.4.1.

A genuine phenomenon observed in the Jaynes-Cummings model, the temporal disappearance of any signatures of quantum coherence in the light field known as *quantum collapse and revival* is studied in Exc. 15.2.4.2.

## 15.2.1 Classical and quantum limits

### 15.2.1.1 The limit of high laser intensities and resonant interaction

The classical limit is recovered for  $n \rightarrow \infty$ , where a single photon makes no difference, that is, we can treat the states  $|n\rangle$  and  $|n+1\rangle$  as equivalent. Then, we can approximate the Hamiltonian of the system (15.25) by the trace of this same Hamiltonian taken over the number of photons,

$$\hat{H}_{semi} = \lim_{n \rightarrow \infty} \text{Tr}_{field} \hat{\rho} \hat{H} = \sum_m \langle m | \hat{\rho} \hat{H} | m \rangle. \quad (15.35)$$

This situation, as illustrated in Fig. 15.5, describes well the state of a laser as a coherent state,  $|\alpha\rangle = \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle e^{-|\alpha|^2/2}$ . For  $n \rightarrow \infty$ , the uncertainty of the Poisson distribution is small,  $\Delta n/\bar{n} = 1/\sqrt{\bar{n}} \rightarrow 0$ , such that the light mode is characterized by the average number of photons, and fluctuations are negligible. This allows us to replace the Poisson distribution,  $P_n = |\langle n | \alpha \rangle|^2 = \delta_{n\bar{n}}$ ,

$$\begin{aligned} \hat{H}_{semi} &= \hat{H}_{field} + \hat{H}_{atom} + \hat{H}_{atom:field} = \sum_m \langle m | \alpha \rangle \langle \alpha | \hat{H} | m \rangle = \langle \alpha | \hat{H} | \alpha \rangle \simeq \langle \bar{n} | \hat{H} | \bar{n} \rangle \\ &= \hat{H}_{\bar{n}} = \begin{pmatrix} (\bar{n}-1)\omega & 0 \\ 0 & \bar{n}\omega \end{pmatrix} + \begin{pmatrix} \frac{\omega_0}{2} & 0 \\ 0 & -\frac{\omega_0}{2} \end{pmatrix} + \begin{pmatrix} 0 & \frac{\varpi_{\bar{n}}}{2} \\ \frac{\varpi_{\bar{n}}^*}{2} & 0 \end{pmatrix}. \end{aligned} \quad (15.36)$$

Now, in the case of a resonant interaction,  $\Delta = 0$ , the Jaynes-Cummings evolution is,

$$e^{-i\hat{H}_{\bar{n}} t} = \frac{1}{\sqrt{2}} e^{-i(\bar{n}-1/2)\omega t} \begin{pmatrix} \cos \frac{1}{2} \varpi_{\bar{n}} t & i \sin \frac{1}{2} \varpi_{\bar{n}} t \\ i \sin \frac{1}{2} \varpi_{\bar{n}} t & \cos \frac{1}{2} \varpi_{\bar{n}} t \end{pmatrix}, \quad (15.37)$$

which is a result already obtained in Exc. 2.4.7.1.

**Example 65 (Resonant  $\pi/2$ -pulse):** In this example, we consider resonant  $\pi/2$ -pulses, that is,  $\sqrt{\bar{n}}\Omega t = \frac{1}{2}\pi$ . The Jaynes-Cummings evolution now simplifies to,

$$e^{-i\hat{H}_{\bar{n}} t} = \frac{1}{2} e^{-i(\bar{n}-1/2)\omega t} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}. \quad (15.38)$$

For large  $\bar{n}$ , a resonant  $\pi/2$ -pulse does (ignoring irrelevant dynamical phases),

$$\begin{pmatrix} |2\rangle|\bar{n}-1\rangle \\ |1\rangle|\bar{n}\rangle \end{pmatrix} \xrightarrow{\pi/2} \begin{pmatrix} (|2\rangle|\bar{n}-1\rangle + i|1\rangle|\bar{n}\rangle) \\ (i|2\rangle|\bar{n}-1\rangle + |1\rangle|\bar{n}\rangle) \end{pmatrix}, \quad (15.39)$$

that is, for a coherent field,

$$\begin{pmatrix} |2\rangle|\alpha\rangle \\ |1\rangle|\alpha\rangle \end{pmatrix} \xrightarrow{\pi/2} \begin{pmatrix} (|2\rangle + i|1\rangle)|\alpha\rangle \\ (i|2\rangle + |1\rangle)|\alpha\rangle \end{pmatrix}. \quad (15.40)$$

Obviously, the structure of the field  $|\alpha\rangle$  is not affected, and we recover the dynamics of a two-level atom excited by a resonant classical *radiation* as described by the Bloch equations (14.62).

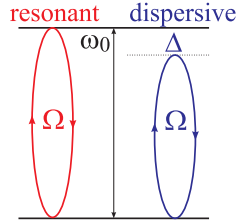


Figure 15.5: Atomic level scheme for the implementation of resonant interactions with classical radiation fields (on the lower transition) and dispersive interactions with quantum fields (on the upper transition).

### 15.2.1.2 Dispersive interaction, the limit of large detunings

The dispersive Jaynes-Cummings dynamics can be implemented by irradiating a light field, which is sufficiently detuned to avoid Rayleigh scattering processes, as shown in Fig. 15.5. This interaction results in a phase shift of the atomic levels. For  $|\Delta| \gg \sqrt{n}\Omega$  we consider the radiative coupling as a small perturbation,

$$\hat{H}_n = \hat{H}_n^{(0)} + \hat{H}_n^{(1)} = \begin{pmatrix} (n - \frac{1}{2})\omega + \frac{\Delta}{2} & 0 \\ 0 & (n - \frac{1}{2})\omega - \frac{\Delta}{2} \end{pmatrix} + \begin{pmatrix} 0 & \frac{\Omega}{2}\sqrt{n} \\ \frac{\Omega}{2}\sqrt{n} & 0 \end{pmatrix}. \quad (15.41)$$

In the unperturbed case we have,  $\hat{H}_n^{(0)}|\psi_{j,n}\rangle_0 = E_{j,n}|\psi_{j,n}\rangle_0$ , where the  $n$ -photon subspace is spanned by the basis  $|j\rangle = (1 \ 0)$  and  $(0 \ 1)$ . In second perturbation order,

$$\langle\psi_{j,n}|\hat{H}_n|\psi_{j,n}\rangle \simeq \langle j|\hat{H}_n^{(1)}|j\rangle + \sum_{j \neq i} \frac{\langle j|\hat{H}_n^{(1)}|i\rangle\langle i|\hat{H}_n^{(1)}|j\rangle}{E_{j,n}^{(0)} - E_{i,n}^{(0)}} = \mp \frac{n\Omega^2}{4\Delta}, \quad (15.42)$$

where the upper sign holds for  $|j\rangle = (1 \ 0)$ . This result was already obtained in the Excs. 6.1.3.4 and 14.3.5.14. In matrix notation,

$$\hat{H}_n^{(1)} \simeq \begin{pmatrix} n\Omega^2/4\Delta & 0 \\ 0 & -n\Omega^2/4\Delta \end{pmatrix}. \quad (15.43)$$

The temporal propagation operator (15.32) then simplifies to,

$$e^{-i\hat{H}_n^{(1)}t} = \begin{pmatrix} e^{in\Omega^2t/4\Delta} & 0 \\ 0 & e^{-in\Omega^2t/4\Delta} \end{pmatrix}. \quad (15.44)$$

The fact that the ground and excited atomic states evolve with different phase factors is important, as we will show in the following example.



**Example 66 (Dispersive  $\pi$ -pulse):** As in the previous case, we consider a two-level atom subject to a coherent field, but now tuned out of resonance. Introducing the abbreviation  $\varphi \equiv \Omega^2 t / 4\Delta$ , the Jaynes-Cummings evolution is,

$$e^{-i\hat{H}_n^{(1)}t} = \begin{pmatrix} e^{in\varphi} & 0 \\ 0 & e^{-in\varphi} \end{pmatrix}. \quad (15.45)$$

The fact that the phase shift  $n\varphi$  depends on the number of photons, and that it goes in opposite directions for the ground and excited states, is crucial. We have already studied in Exc. 14.5.5.7, that the dispersive interaction of the atom with a radiation field can phase-shift the Bloch vector. Now, we observe that in addition, it causes a phase shift of the probability amplitude of having  $n$  photons in the radiation field by a value proportional to  $n$ , i.e. (ignoring irrelevant dynamical phases),

$$\begin{pmatrix} |2\rangle|n-1\rangle \\ |1\rangle|n\rangle \end{pmatrix} \underset{n\varphi}{\curvearrowright} \begin{pmatrix} e^{in\varphi}|2\rangle|n-1\rangle \\ e^{-in\varphi}|1\rangle|n\rangle \end{pmatrix}. \quad (15.46)$$

Applying this result to Glauber states,

$$\begin{pmatrix} |2\rangle|\alpha\rangle \\ |1\rangle|\alpha\rangle \end{pmatrix} \underset{n\varphi}{\curvearrowright} \begin{pmatrix} |2\rangle \sum_n \frac{\alpha^n}{\sqrt{n!}} e^{in\varphi} |n\rangle \\ |1\rangle \sum_n \frac{\alpha^n}{\sqrt{n!}} e^{-in\varphi} |n\rangle \end{pmatrix} = \begin{pmatrix} |2\rangle|\alpha e^{i\varphi}\rangle \\ |1\rangle|\alpha e^{-i\varphi}\rangle \end{pmatrix}. \quad (15.47)$$

Apparently, the phase of the radiation field is shifted by a value  $\varphi$ , which depends on the state of the atom.

We note here, that the dynamics studied in the last example provides a method of *transferring coherence from an atomic superposition to a quantum correlation of a radiation field*. All we have to do, is to bring the atom into a superposition of states  $|1\rangle + |2\rangle$ , and the field will automatically evolve toward a Schrödinger cat state  $|\alpha e^{i\varphi}\rangle + |\alpha e^{-i\varphi}\rangle$ . The transfer of quantum correlations between coupled degrees of freedom is one of the characteristics of the Jaynes-Cummings model. As examples we will study the phenomena of *quantum collapse and revival* in Exc. 15.2.4.3 and of *vacuum Rabi splitting* in 15.2.4.4.

## 15.2.2 Observables and correlations of the Jaynes-Cummings dynamics

In the limit of low laser intensities we must consider photonic distributions that are not necessarily coherent. The stationary solution of the Schrödinger equation consists of the dressed states  $|1, n\rangle$  and  $|2, n-1\rangle$ . If we now expand a general Jaynes-Cummings state in amplitudes  $c_{jn}(t)$ ,

$$|\psi\rangle = \sum_n (c_{1,n}|1, n\rangle + c_{2,n-1}|2, n-1\rangle), \quad (15.48)$$

they will follow the Schrödinger equation,

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_{2,n-1} \\ c_{1,n} \end{pmatrix} = \hat{H}_n \begin{pmatrix} c_{2,n-1} \\ c_{1,n} \end{pmatrix}. \quad (15.49)$$

The evolution of the coefficients  $c_{jn}$  completely describes the Jaynes-Cummings dynamics of the system through the formula (15.32). Obviously, the Jaynes-Cummings state is normalized because,

$$\langle \psi | \psi \rangle = \text{Tr} |\psi\rangle\langle\psi| = \sum_n (|c_{1,n}|^2 + |c_{2,n}|^2) = 1. \quad (15.50)$$

As dissipation processes are neglected, we get a pure state described by,

$$\hat{\rho} = |\psi\rangle\langle\psi|. \quad (15.51)$$

The Jaynes-Cummings dynamics involves two coupled degrees of freedom characterized by with their respective observables. If we are interested in them, we can do two things: (a) We ignore the degrees of freedom NOT under study by NOT DOING a measurement of the other degrees. That is, we simply remove the non-interesting degrees of freedom from the state. For example, if our focus is on the optical mode, we ignore the atomic state,

$$|\gamma\rangle \equiv \sum_{j=1,2} \langle j | \psi \rangle = \sum_n c_{1,n} |n\rangle + c_{2,n-1} |n-1\rangle. \quad (15.52)$$

Our new density operator remains pure, that is,

$$\hat{\rho}_{field}^{(pure)} = \sum_{i,j=1,2} \langle j | \hat{\rho} | i \rangle = \sum_{i,j=1,2} \langle j | \psi \rangle \langle \psi | i \rangle = |\gamma\rangle\langle\gamma|. \quad (15.53)$$

On the other hand, ignoring the optical mode via,

$$|j\rangle = \sum_n \langle n | \psi \rangle = \sum_n c_{1,n} |1\rangle + c_{2,n-1} |2\rangle. \quad (15.54)$$

Again, our new density operator remains pure, that is,

$$\hat{\rho}_{atom}^{(pure)} = \sum_{m,n} \langle m | \hat{\rho} | n \rangle = |j\rangle\langle j|. \quad (15.55)$$

(b) We trace over the degrees of freedom NOT under study by DOING a measurement. For example, if again our focus is on the optical mode, we trace over the atomic states,

$$\begin{aligned} \hat{\rho}_{field}^{(mix)} &= \text{Tr}_{atom} \hat{\rho} = \sum_{j=1,2} \langle j | \hat{\rho} | j \rangle = \sum_{j=1,2} \langle j | \psi \rangle \langle \psi | j \rangle \\ &= \sum_{n,m} c_{1,m}^* c_{1,n} |n\rangle \langle m| + c_{2,m-1}^* c_{2,n-1} |n-1\rangle \langle m-1| \neq \hat{\rho}_{field}^{(pure)}. \end{aligned} \quad (15.56)$$

It is clear, that this incomplete measurement converts the reduced density operator into a statistical mixture, which is free of inneratomic correlations of the type  $c_{2,m}^* c_{1,n}$ , but this means that we also loose possible field correlations. On the other hand, tracing over the field mode,

$$\begin{aligned} \hat{\rho}_{atom}^{(mix)} &= \text{Tr}_{field} \hat{\rho} = \sum_{n=0}^{\infty} \langle n | \hat{\rho} | n \rangle = \sum_{n=0}^{\infty} \langle n | \psi \rangle \langle \psi | n \rangle \\ &= \sum_n (c_{1,n} |1\rangle + c_{2,n} |2\rangle) (c_{1,n}^* \langle 1| + c_{2,n}^* \langle 2|) \neq \hat{\rho}_{atom}^{(pure)}. \end{aligned} \quad (15.57)$$

After these preliminary remarks let us have a look a some interesting observables.

### 15.2.2.1 Temporal evolution of the Bloch vector

The expectation value for field observables  $\hat{A}|n\rangle = A_n|n\rangle$  is,

$$\langle\psi|\hat{A}|\psi\rangle = \text{Tr} \hat{\rho}\hat{A} \sum_{i,n} \langle i|\langle n|\psi\rangle\langle\psi|\hat{A}|n\rangle|i\rangle = \sum_n A_n(|c_{1,n}|^2 + |c_{2,n}|^2). \quad (15.58)$$

And for the annihilation operator  $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$  we have,

$$\langle\psi|\hat{a}|\psi\rangle = \sum_n \sqrt{n}(c_{1,n-1}^*c_{1,n} + c_{2,n-1}^*c_{2,n}). \quad (15.59)$$

To determine the internal state of the atom, we must trace over the light field. The populations and coherences are, therefore,

$$\rho_{ij} = \langle i|\text{Tr}_{field} \hat{\rho}|j\rangle = \langle i|\sum_n \langle n|\psi\rangle\langle\psi|n\rangle|j\rangle = \sum_n c_{i,n}c_{j,n}^*. \quad (15.60)$$

The projection onto the atomic state is done by,

$$\frac{|j\rangle\langle j|\psi\rangle}{\langle\psi|j\rangle\langle j|\psi\rangle} = \frac{\sum_m c_{j,n}|j,n\rangle}{\sum_m |c_{j,m}|^2}. \quad (15.61)$$

With this, we can calculate the atomic Bloch vector (??), whose norm is interestingly NOT preserved, since,

$$\begin{aligned} |\vec{\rho}| &= \left\| \begin{pmatrix} 2\text{Re} \rho_{12} \\ 2\text{Im} \rho_{12} \\ \rho_{22} - \rho_{11} \end{pmatrix} \right\| = 2|\rho_{12}|^2 - 2\rho_{11}\rho_{22} = -2 \det \hat{\rho} \\ &= 2 \sum_n c_{1,n}c_{2,n}^* \sum_n c_{1,n}^*c_{2,n} - 2 \sum_n |c_{2,n}|^2 \sum_n |c_{1,n}|^2 \neq 1. \end{aligned} \quad (15.62)$$

### 15.2.2.2 The photon number distribution

To determine the state of the light field, we must trace over the atomic state. For example, the probability amplitude of encountering the state  $|\psi\rangle$  in  $|n\rangle$  is,

$$\langle n|\psi\rangle = c_{1,n}|1\rangle + c_{2,n}|2\rangle, \quad (15.63)$$

such that,

$$p_n = \langle n|\text{Tr}_{atom} \hat{\rho}|n\rangle = \langle n|\sum_{i=1,2} \langle i|\psi\rangle\langle\psi|i\rangle|n\rangle = |\langle n|\psi\rangle|^2 = |c_{1,n}|^2 + |c_{2,n}|^2. \quad (15.64)$$

### 15.2.2.3 The Glauber-Sudarshan Q-function

To characterize the optical field separately from the atomic state, we can try, by a calculation similar to (15.58), to project the Jaynes-Cummings state onto a basis of

coherent states. Thus, the probability amplitude of encountering the state  $|\psi\rangle$  in  $|\alpha\rangle$  is,

$$\begin{aligned} \langle\alpha|\psi\rangle &= e^{-|\alpha|^2/2} \sum_n \frac{\alpha^{*n}}{\sqrt{n!}} (c_{1,n}|1\rangle + c_{2,n}|2\rangle) \\ |\langle\alpha|\psi\rangle|^2 &= e^{-|\alpha|^2} \sum_n \frac{\alpha^{*n}\alpha^m}{\sqrt{n!}\sqrt{m!}} (c_{1,m}^*c_{1,n} + c_{2,m}^*c_{2,n}), \end{aligned} \quad (15.65)$$

such that,

$$\pi Q(\alpha) \equiv \langle\alpha|\text{Tr}_{atom} \hat{\rho}|\alpha\rangle = e^{-|\alpha|^2} \left( \left| \sum_n c_{1,n} \frac{\alpha^n}{\sqrt{n!}} \right|^2 + \left| \sum_n c_{2,n} \frac{\alpha^n}{\sqrt{n!}} \right|^2 \right). \quad (15.66)$$

We will derive this result in Exc. 15.2.4.5. This quantity, called *Q-function*, allows the illustration of the state in a coordinate system spanned by  $\text{Re } \alpha$  and  $\text{Im } \alpha$  [83]. It is generally easy to calculate, but does not exhibit much information, e.g., on interference phenomena caused by quantum correlations. In the following section, we will calculate the Wigner function, which can also be evaluated from the Jaynes-Cummings coefficients [224].

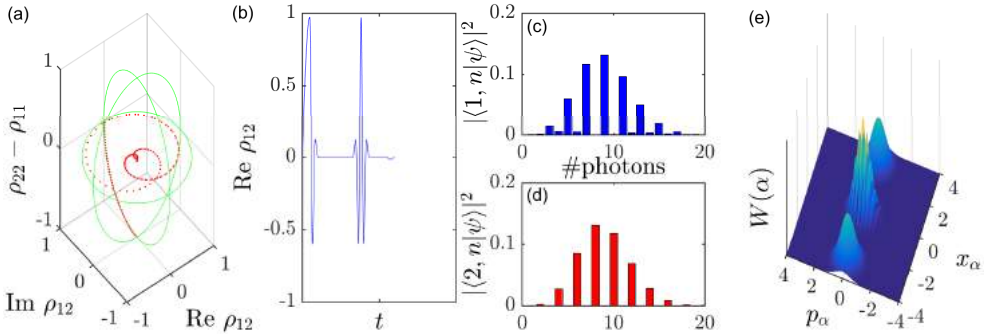


Figure 15.6: (code) Evolution of the state during a Jaynes-Cummings type interaction: (a) Bloch vector, (b,c) photon distribution after projection on the ground and excited atomic state, (d) time evolution of the coherence  $\rho_{12}$  showing the phenomenon of collapse and revival, and (e)  $W(\alpha)$  function.

The Jaynes-Cummings dynamics illustrated in Fig. 15.6 demonstrates the transfer of coherence between an atom and a light field. In Exc. 15.2.4.6 we study how to create, via a sequence of Ramsey pulses, a Schrödinger cat state in a light field.

#### 15.2.2.4 The Wigner function in the Glauber picture

We found in (15.44) that a dispersive phase shift of the atomic state  $|2\rangle$  leads to a time-dependent phase shift of the Glauber field,

$$|\psi\rangle = \sum_N (c_{1,n}|1, n\rangle + c_{2,n-1}|2, n-1\rangle) = |1, \beta\rangle + e^{i\varphi(t)}|2, \beta\rangle \quad \text{or} \quad \hat{\rho} = |\psi\rangle\langle\psi|, \quad (15.67)$$

with

$$c_{1,n} = e^{-|\beta|^2/2} \frac{\beta^n}{\sqrt{n!}} \quad \text{and} \quad c_{2,n} = e^{-|\beta|^2/2} \frac{(e^{i\varphi} \beta)^n}{\sqrt{n!}}. \quad (15.68)$$

We will now concentrate on the field state by explicitly IGNORING the atomic states  $|j\rangle$ ,

$$|\gamma\rangle = \sum_{j=1,2} \langle j|\psi\rangle = |\beta\rangle + |e^{i\varphi}\beta\rangle \quad \text{or} \quad \hat{\rho}_{field}^{(pure)} = \sum_{i,j=1,2} \langle j|\psi\rangle \langle \psi|i\rangle = |\gamma\rangle \langle \gamma|. \quad (15.69)$$

From the optical cat pure state wavefunction (15.69), we can easily calculate the Wigner function in the Glauber picture, as done in (3.204) and Exc. 3.7.5.4,

$$W(\alpha) = \frac{2}{C^2\pi} \left( e^{-2|\alpha-\beta|^2} + e^{-2|\alpha-\beta e^{i\varphi}|^2} \pm 2e^{-|\beta|^2} \text{Re} e^{-2(\beta e^{i\varphi} - \alpha)(\beta^* - \alpha^*) + |\beta|^2 e^{i\varphi}} \right). \quad (15.70)$$

Now, what happens if we MEASURE the atomic state before we analyze the field state? The incomplete measurement corresponds to tracing over the atomic degrees of freedom, which transforms our initially pure state (15.67) into a statistical mixture. With  $|\psi\rangle$  given by (15.67),

$$\hat{\rho}_{field}^{(mix)} = \text{Tr}_{atom} \hat{\rho} = \sum_{j=1,2} \langle j|\psi\rangle \langle \psi|j\rangle = |\beta\rangle \langle \beta| + |e^{i\varphi}\beta\rangle \langle e^{i\varphi}\beta| \neq |\gamma\rangle \langle \gamma|. \quad (15.71)$$

Calculating the Wigner function from this density operator consequently must yield a different result, because any correlations are lost. A movie of the dynamics can be watched here ([watch movie](#)) [121, 177, 8, 692].

### 15.2.2.5 The Wigner function in the Fock picture

Let us now calculate the Wigner function in the Fock state picture. This will allow us to consider more general states later on. We start from the expansion,

$$|\psi\rangle = \sum_n c_{1,n} |1, n\rangle + c_{2,n-1} |2, n-1\rangle. \quad (15.72)$$

As before, we can now choose to DO or NOT DO a measurement of the atomic state. If we do a measurement tracing over the atomic states, we calculate the normally ordered characteristic function using the density operator (15.56),

$$\begin{aligned} \chi_N(\lambda) &= \text{Tr} \hat{\rho}_{field}^{(mix)} e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} = \sum_{n'} \langle n' | \hat{\rho}_{field}^{(mix)} e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} | n' \rangle \\ &= \sum_{n,m} c_{1,m}^* c_{1,n} \langle m | e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} | n \rangle + c_{2,m-1}^* c_{2,n-1} \langle m-1 | e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} | n-1 \rangle. \end{aligned} \quad (15.73)$$

Obviously, this formula does not contain inneratomic correlations and, since non-classical field correlation would be entangled with atomic superposition states, we expect no interesting field correlations, neither.



and the dynamical evolution by  $c'_{jn} \equiv e^{-\kappa n t/2} c_{jn}$ . Note, that the dissipation due to cavity losses can also be taken into account by a *master equation*. Do the Exc. 16.2.6.1.

## 15.2.4 Exercises

### 15.2.4.1 Ex: Time-evolution in the Jaynes-Cummings model

Derive the equations of motion for  $\hat{\sigma}^-$ ,  $\hat{\sigma}_z$ , and  $\hat{a}$  in the Jaynes-Cummings model. Show that the number of photons is not a constant of motion, but the total number of excitations.

### 15.2.4.2 Ex: The Jaynes-Cummings model

Consider the Jaynes-Cummings Hamiltonian.

a. Determine from the Schrödinger equation the system of differential equations for the temporal evolution of the coefficients  $c_{2,n}(t)$  and  $c_{1,n+1}(t)$  in the interaction picture within the rotating wave approximation (RWA).

b. Calculate the time evolution for the start condition  $c_{2,n}(0) = 1$  and  $c_{1,n+1}(0) = 0$  for the particular case  $\omega = \omega_0$ .

c. Generalize the result of item (a) for a multimode field, for which initially (i) all modes of field  $\mathbf{k}$  are empty  $|0\rangle$  and (ii) the atom is in the excited state  $|a\rangle$ . Use the ansatz,

$$|\psi(t)\rangle = c_2(t)e^{-iE_2t/\hbar}|2, 0\rangle + \sum_{\mathbf{k}} c_{1,\mathbf{k}}(t)e^{-i[E_1/\hbar + \omega_{\mathbf{k}}]t}|1, \mathbf{k}\rangle,$$

and determine the equations of motion for the amplitudes  $c_2$  and  $c_{1,\mathbf{k}}$ .

### 15.2.4.3 Ex: Quantum collapse and revival in the Jaynes-Cummings model

Consider the Jaynes-Cummings Hamiltonian and show that the quantum coherence between the two atomic levels can disappear altogether for long periods and reappear later. Explain how this is possible.

### 15.2.4.4 Ex: Vacuum Rabi splitting

Calculate the Autler-Townes splitting for an excited atom interacting with an empty cavity.

### 15.2.4.5 Ex: The $Q$ -function in a Jaynes-Cummings state

Calculate the  $Q$ -function for a Jaynes-Cummings state from its definition (15.66).

### 15.2.4.6 Ex: Creation of quantum correlations in an optical mode

We will show in this exercise how, via coherent operations in a three-level system, we can create Schrödinger-type quantum-type correlations in an optical mode. In the system shown in Fig. 15.7 we imagine the lower transition excited by  $\pi/2$ -pulses of a classical resonant microwave radiation (as described by the operation (15.37)). The upper transition is excited by quantum laser pulses tuned very far out of resonance,

thus creating a dispersive dynamics (as described by the operation (15.37)). At time  $t = 0$  the atom is in state  $|1\rangle$ . Now, we apply the following pulse sequence: (i) a microwave pulse with  $\sqrt{n}\Omega_{12}t = \pi/2$ , (ii) an optical pulse with  $\Omega_{23}^2 t/4\Delta_{23} = \pi$ , (iii) another microwave  $\pi/2$ -pulse, and finally (iv) an optical pulse of light which is resonant with the transition  $|2\rangle$ - $|3\rangle$  and projects the population of the atom into one of the states of the microwave transition. Describe the evolution of the state of the system during the sequence and determine the final state of the optical mode.

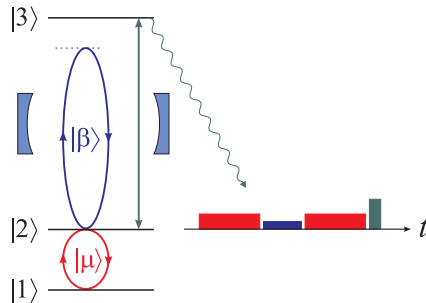


Figure 15.7: (a) Level scheme and (b) pulse sequence.

#### 15.2.4.7 Ex: Master equation derived from JC model Hamiltonian for two-level systems

Write down the Liouvillean for a JC system in matrix form for a density operator defined like,

$$(\dots \rho_{11}^{n-1} \quad \rho_{22}^n \quad \rho_{12}^n \quad \rho_{21}^n \quad \rho_{11}^n \quad \rho_{22}^{n+1} \quad \dots)$$

#### 15.2.4.8 Ex: Laguerre polynomials

Calculate the Wigner function for the field generated by a Jaynes-Cummings dynamics in the photon picture.

## 15.3 Correlation functions

In the preceding sections and in Sec. 3.7 we have learned, how to characterize quantum fields by (quasi-)probability distribution functions, and how to represent correlations in the Fock or the Glauber basis. But we did not propose experimental schemes allowing to detect them. Experimental devices, such as interferometers or photon correlators, necessarily involve space or time coordinates. Hence, we need to devise quantities for the characterization of correlations, that are compatible with experimental devices. The *correlation functions* are such quantities, and in the next section we will focus our attention them.

In order to be able to distinguish classical from genuinely quantum correlations, we will first a classical description, before introducing a quantum description of the light field [440].



### 15.3.1 Classical first and second order coherence

The coherence properties of a light field (or a matter wave) are measured by  $n^{\text{th}}$  space time order correlation functions. In quantum mechanics, these are defined by,

$$g^{(n)}(\mathbf{r}_1, t_1, \dots, \mathbf{r}_{2n}, t_{2n}) \equiv \frac{\langle \hat{\mathcal{E}}^-(\mathbf{r}_1, t_1) \dots \hat{\mathcal{E}}^-(\mathbf{r}_n, t_n) \hat{\mathcal{E}}^+(\mathbf{r}_{n+1}, t_{n+1}) \dots \hat{\mathcal{E}}^+(\mathbf{r}_{2n}, t_{2n}) \rangle}{\sqrt{\langle \hat{\mathcal{E}}^-(\mathbf{r}_1, t_1) \hat{\mathcal{E}}^+(\mathbf{r}_1, t_1) \rangle \dots \langle \hat{\mathcal{E}}^-(\mathbf{r}_{2n}, t_{2n}) \hat{\mathcal{E}}^+(\mathbf{r}_{2n}, t_{2n}) \rangle}}. \quad (15.78)$$

In the following, we will only consider temporal coherences, e.g. one or more collinear light beams,  $\mathbf{k}_m \parallel \mathbf{k}_n$ , impinging on a photodetector,  $(t_m - \frac{z_m}{c}) - (t_n - \frac{z_n}{c}) = \tau$ , since  $\hat{\mathcal{E}}(\mathbf{r}, t) = \hat{\mathcal{E}}(\omega t - \mathbf{k} \cdot \mathbf{r})$ , we can define the the 1<sup>st</sup> and 2<sup>nd</sup> order correlation functions  $g^{(1)}$  and  $g^{(2)}$ , which are particularly important,

$$\boxed{g^{(1)}(\tau) \equiv \frac{\langle \hat{\mathcal{E}}^-(t) \hat{\mathcal{E}}^+(t + \tau) \rangle}{\langle \hat{\mathcal{E}}^-(t) \hat{\mathcal{E}}^+(t) \rangle} \quad \text{and} \quad g^{(2)}(\tau) \equiv \frac{\langle \hat{\mathcal{E}}^-(t) \hat{\mathcal{E}}^-(t + \tau) \hat{\mathcal{E}}^+(t + \tau) \hat{\mathcal{E}}^+(t) \rangle}{\langle \hat{\mathcal{E}}^-(t) \hat{\mathcal{E}}^+(t) \rangle^2}}. \quad (15.79)$$

Ignoring the quantized nature of light, we may substitute the field operators by complex numbers,  $\hat{\mathcal{E}}^+ \rightarrow \mathcal{E}$  and  $\hat{\mathcal{E}}^- \rightarrow \mathcal{E}^*$  and interpret the brackets as pure time averages,

$$\langle \dots \rangle_t = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \dots dt. \quad (15.80)$$

Defining the intensity as  $I = 2\varepsilon_0 c \mathcal{E}^* \mathcal{E}$ , the coherences become,

$$g^{(1)}(\tau) \equiv \frac{2\varepsilon_0 c}{I} \langle \mathcal{E}^*(t) \mathcal{E}(t + \tau) \rangle \quad \text{and} \quad g^{(2)}(\tau) \equiv \left( \frac{2\varepsilon_0 c}{I} \right)^2 \langle I(t) I(t + \tau) \rangle. \quad (15.81)$$

The correlation functions must be calculated from the field operators simultaneously respecting *time order* and *normal order*. These functions are useful quantities to describe phenomena such as photon *bunching* or to understand the fluorescence spectra or the scattering of light from correlated atoms.  $g^{(1)}$  measures the *coherence* of a light field (how much it resembles a sine wave).  $g^{(2)}$  measures, for a given degree of coherence, the deviation of the light field from the quantum state that most closely approximates a classical light (how much it resembles a laser).

The correlation functions  $g^{(1)}$  and  $g^{(2)}$  are experimentally measured in *Young's experiment* and in the *Hanbury-Brown-Twiss experiment*. The experimental schemes are explained in Figs. 15.8.

Coherence and chaos are contrary properties of light. They leave their imprint in the spectrum of the light or in the autocorrelation functions. The emission spectrum of a light source generally emerges as a combination of various physical effects: The active medium gives rise resonances and broadenings, a resonator containing the active medium imprints a modal structure, and the coupling to a thermal bath gives rise to a thermal distribution of the radiation energy according to  $P_n = e^{-\hbar\omega(n+1/2)/k_B T} / \sum_n e^{-\hbar\omega(n+1/2)/k_B T}$ .

### 15.3.2 The Wiener-Khintchine theorem

When the time dependence of a wave is given by  $\mathcal{E}(t)$ , we call

$$R_{\mathcal{E}}(\tau) = \langle \mathcal{E}^*(t) \mathcal{E}(t + \tau) \rangle_t \quad (15.82)$$

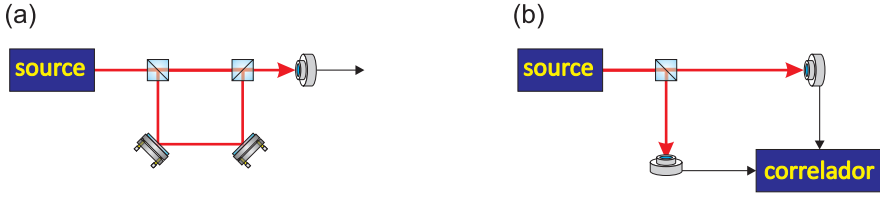


Figure 15.8: (a) Scheme of Young's experiment. (b) Scheme of the experiment of Hanbury, Brown, and Twiss. Young's experiment reveals the coherence of a field, that is, its ability to interfere. In contrast, the Hanbury-Brown-Twist experiment reveals correlations between the (quasi-)particles constituting the field, that is, effects due to quantum statistics or interactions.

the autocorrelation function and the power density

$$S_{\mathcal{E}}(\omega) = (\mathcal{F}R_{\mathcal{E}})(\omega) = |(\mathcal{F}\mathcal{E})(\omega)|^2 \quad (15.83)$$

the *spectrum*. This relation is called the *Wiener-Khinchine theorem*. We may also consider the normalized quantities, dividing (15.82) and (15.83) by  $R_{\mathcal{E}}(0) = \langle \hat{\mathcal{E}}^*(t)\hat{\mathcal{E}}(t) \rangle_t = \int_{-\infty}^{\infty} |(\mathcal{F}\mathcal{E})(\omega)|^2 d\omega = \int_{-\infty}^{\infty} S_{\mathcal{E}}(\omega) d\omega$ . We obtain,

$$g^{(1)}(\tau) = \frac{R_{\mathcal{E}}(\tau)}{R_{\mathcal{E}}(0)}, \quad (15.84)$$

and,

$$F_{\mathcal{E}}(\omega) \equiv (\mathcal{F}g^{(1)})(\omega) = \frac{S_{\mathcal{E}}(\omega)}{R_{\mathcal{E}}(0)} = \frac{1}{2\pi} \int_{-\infty}^{\infty} g^{(1)}(\tau) e^{i\omega\tau} d\tau. \quad (15.85)$$

The quantity  $F_{\mathcal{E}}(\omega)$  is called line profile or *spectrum*. Note that, since,

$$g^{(1)}(-\tau) = g^{(1)}(\tau)^*, \quad (15.86)$$

we may also write,

$$F_{\mathcal{E}}(\omega) = \text{Re} \frac{1}{\pi} \int_0^{\infty} g^{(1)}(\tau) e^{i\omega\tau} d\tau. \quad (15.87)$$

### 15.3.3 Coherent and chaotic light

The temporal and spectral properties of a light field are largely determined by the processes leading to its generation in the light source, that is, whether the light is generated by stimulated or spontaneous emission, by a laser or by blackbody radiation, by a single atom or by atomic gases subject to collisional and Doppler-broadening.

#### 15.3.3.1 Correlation functions for laser light

First-order coherent light satisfies  $|g^{(1)}(\tau)| = 1$ , incoherent light  $|g^{(1)}(\tau)| = 0$ , and for partially coherent light, we get intermediate values. Second-order coherent light satisfies  $g^{(2)}(-\tau) = g^{(2)}(\tau)$  and  $1 \leq g^{(2)}(0) \leq \infty$  and  $0 \leq g^{(2)}(\tau) \leq \infty$  and  $g^{(2)}(0) \geq$

$g^{(2)}(\tau) \xrightarrow{\tau \gg \tau_c} 1$ . Let us now look at some specific cases, for which the correlation functions and spectra can be calculated.

With the definitions (15.79) it is easy to calculate the autocorrelation functions and the spectrum of a *laser* light field,

**laser**

$$\begin{aligned}
 \mathcal{E}(t) &= e^{i\omega_0 t} \\
 \Rightarrow g^{(1)}(\tau) &= \frac{t^{-1} \int e^{-i\omega_0 \tau} dt}{t^{-1} \int dt} = e^{-i\omega_0 \tau} \\
 \Rightarrow \mathcal{F}[g^{(1)}(\tau)] &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega - \omega_0)\tau} d\tau = \delta(\Delta) \\
 g^{(2)}(\tau) &= 1
 \end{aligned} \tag{15.88}$$

We see that the absolute values of the first and second-order coherences are constant, and that the spectrum is narrow like a  $\delta$ -function.

### 15.3.3.2 Correlation functions for laser light subject to white noise

For a laser subject to *white phase noise* ( $\zeta$  be a normally distributed random number) we have ,

**noisy laser**

$$\begin{aligned}
 \mathcal{E}(t) &= e^{i[\omega_0 t + \zeta(t)]} \\
 \Rightarrow g^{(1)}(\tau) &= \frac{\int e^{-i[\omega_0 \tau + \zeta(t+\tau) - \zeta(t)]} dt}{\int dt} = e^{i\omega_0 \tau - i\gamma|\tau|} \\
 \Rightarrow \mathcal{F}[g^{(1)}(\tau)] &= \frac{\gamma/\pi}{\Delta^2 + \gamma^2} \\
 g^{(2)}(\tau) &= 1
 \end{aligned} \tag{15.89}$$

We see, that the first-order coherence decays exponentially,  $|g^{(1)}(\tau)| = e^{-\gamma|\tau|}$ <sup>6</sup>, such that the spectrum has a *Lorentzian profile*. This result has already been derived in Sec. 13.3.1 for the natural linewidth of a transition subject to spontaneous emission. We understand the connection by interpreting spontaneous emission as being induced by *vacuum fluctuations, which do have a white noise spectrum*, indeed.

**Example 67 (Laser broadening due to spontaneous emission):** Laser light is generated by stimulated emission on a transition between two quantized levels. The alternance of absorption and stimulated emission induces coherent Rabi oscillations ensuring the coherence of the emitted light. But we have seen earlier that spontaneous emission leads to randomly occurring interruptions of the coherent Rabi oscillations. The probability of finding a coherent interval decreases exponentially with the evolution time,

$$p(\tau)d\tau = \gamma e^{-\gamma\tau} d\tau ,$$

<sup>6</sup>Note that, in order to satisfy (15.86), we must take the absolute value of the delay  $|\tau|$ .

where  $\gamma$  is the spontaneous decay rate of the dipole moment. From  $\mathcal{E}(t) = e^{i\omega_0 t + i\zeta(t)}$  we calculate,

$$\begin{aligned} R_{\mathcal{E}}(\tau) &= \langle e^{i\omega_0 t + i\zeta(t)} e^{-i\omega_0(t+\tau) - i\zeta(t+\tau)} \rangle = e^{-i\omega_0 \tau} \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t e^{i[\zeta(t) - \zeta(t+\tau)]} dt \\ &= e^{-i\omega_0 \tau} \int_{\tau}^{\infty} p(\tau') d\tau' = e^{-i\omega_0 \tau} e^{-\gamma|\tau|}, \end{aligned}$$

and,

$$F_{\mathcal{E}}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{R_{\mathcal{E}}(\tau)}{R_{\mathcal{E}}(0)} e^{i\omega \tau} d\tau = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega_0 \tau} e^{-\gamma|\tau|} e^{i(\omega - \omega_0)\tau} d\tau = \frac{\gamma/\pi}{\Delta^2 + \gamma^2}.$$

An alternative derivation from Bloch or rate equations is shown in Excs. 15.4.4.3 and 15.4.4.4.

### 15.3.3.3 Correlation functions with pressure broadening

In Sec. 14.4.2 we have already seen, that collision or *pressure broadening* can be treated by assuming that the light is emitted as a superposition of coherent waves all having the same frequency, but being randomly interrupted by phase jumps,

$$\mathcal{E}(t) = \sum_n E_n(t) \quad \text{with} \quad \mathcal{E}_n(t) = e^{i\omega_0 t + i\phi_n(t)}. \quad (15.90)$$

The autocorrelation function is then,

$$\begin{aligned} \langle \mathcal{E}^*(t) \mathcal{E}(t + \tau) \rangle &= \frac{1}{t} \int \sum_n e^{-i\omega_0 t - i\phi_n(t)} \sum_m e^{i\omega_0 t + i\omega_0 \tau + i\phi_m(t + \tau)} dt \\ &= e^{i\omega_0 \tau} \sum_{n,m} \frac{1}{t} \int e^{i\phi_m(t + \tau) - i\phi_n(t)} dt = N \langle \mathcal{E}_n^*(t) \mathcal{E}_m(t + \tau) \rangle \delta_{nm}. \end{aligned} \quad (15.91)$$

The crossed terms  $n \neq m$  of this expressions vanish. The pressure broadening is homogeneous, but the fact that the wavepackets are scattered by different atoms results in a modified first-order coherence,

$$\langle \mathcal{E}_n^*(t) \mathcal{E}_n(t + \tau) \rangle = e^{i\omega_0 \tau} \sum_n \int e^{i\phi_n(t + \tau) - i\phi_n(t)} dt = e^{i\omega_0 \tau} \int_{\tau}^{\infty} p(\tau) d\tau. \quad (15.92)$$

The probability density of finding a coherent interval of duration  $\tau$  is  $p(\tau) d\tau = \gamma_c e^{-\gamma_c \tau} d\tau$ , which finally gives,

$$\langle \mathcal{E}^*(t) \mathcal{E}(t + \tau) \rangle = N e^{i\omega_0 \tau - \gamma_c |\tau|}. \quad (15.93)$$

The calculation for the  $2^{nd}$  order correlation function (15.81) is analogous,

$$\begin{aligned} \langle \mathcal{E}^*(t) \mathcal{E}^*(t + \tau) \mathcal{E}(t + \tau) \mathcal{E}(t) \rangle &= \sum_{n,m,n',m'} \langle \mathcal{E}_m^*(t) \mathcal{E}_n(t) \mathcal{E}_{m'}^*(t + \tau) \mathcal{E}_{n'}(t + \tau) \rangle \\ &= \sum_n \langle \mathcal{E}_n^*(t) \mathcal{E}_n(t) \mathcal{E}_n^*(t + \tau) \mathcal{E}_n(t + \tau) \rangle \\ &+ \left( \sum_{n \neq m} \langle \mathcal{E}_n^*(t) \mathcal{E}_n(t) \mathcal{E}_m^*(t + \tau) \mathcal{E}_m(t + \tau) \rangle + \langle \mathcal{E}_m^*(t) \mathcal{E}_n(t) \mathcal{E}_n^*(t + \tau) \mathcal{E}_m(t + \tau) \rangle \right), \end{aligned} \quad (15.94)$$

neglecting all terms which do not satisfy either  $E_n^*(t)E_n(t)$  or  $E_n^*(t)E_n(t + \tau)$ . Now, assuming a large amount of identical atoms,

$$\begin{aligned} & \langle \mathcal{E}^*(t)\mathcal{E}^*(t + \tau)\mathcal{E}(t + \tau)\mathcal{E}(t) \rangle \\ &= N \langle \mathcal{E}_n^*(t)\mathcal{E}_n(t)\mathcal{E}_n^*(t + \tau)\mathcal{E}_n(t + \tau) \rangle + N(N - 1) (\langle \mathcal{E}_n^*(t)\mathcal{E}_n(t) \rangle^2 + |\langle \mathcal{E}_n(t)\mathcal{E}_n^*(t + \tau) \rangle|^2) \\ &\simeq N^2 (\langle \mathcal{E}_n^*(t)\mathcal{E}_n(t) \rangle^2 + |\langle \mathcal{E}_n(t)\mathcal{E}_n^*(t + \tau) \rangle|^2) . \end{aligned} \quad (15.95)$$

Finally, exploiting the result (15.91) and the definitions of the 1<sup>st</sup> and 2<sup>nd</sup> order correlations functions,

$$g^{(2)}(\tau) = \frac{\langle \mathcal{E}_n^*(t)\mathcal{E}_n(t) \rangle^2 + |\langle \mathcal{E}_n(t)\mathcal{E}_n^*(t + \tau) \rangle|^2}{\langle \mathcal{E}_n^*(t)\mathcal{E}_n(t) \rangle^2} = 1 + |g^{(1)}(\tau)|^2 . \quad (15.96)$$

In summary,

#### pressure broadening

$$\begin{aligned} \mathcal{E}(t) &= \sum_n e^{i\omega_0 t + i\phi_n(t)} \\ \Rightarrow g^{(1)}(\tau) &= e^{i\omega_0 \tau - \gamma_c |\tau|} \\ \Rightarrow \mathcal{F}[g^{(1)}(\tau)] &= \frac{\gamma/\pi}{\Delta^2 + \gamma_c^2} \\ g^{(2)}(\tau) &= 1 + e^{-\gamma_c |\tau|} \end{aligned} . \quad (15.97)$$

The spectrum is a Lorentzian with the full linewidth  $\gamma' = \gamma + \gamma_c$ .

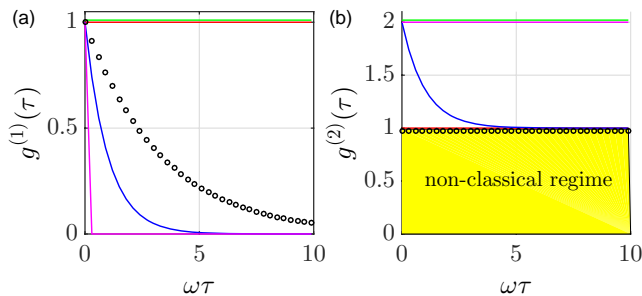


Figure 15.9: (code) First and second-order correlation functions for (red) a laser, (cyan) a laser subject to phase noise, (blue) a laser subject to collision broadening, (magenta) chaotic light, and (green) spectrally filtered thermal light.

### 15.3.3.4 Correlation functions with thermal broadening

For light emitted by an ensemble of non-colliding atoms in thermal motion, we must allow for different frequencies,  $E_n(t) = e^{i\omega_n t + i\phi_n}$ , but time-independent phases,

$$\begin{aligned} \langle \mathcal{E}^*(t)\mathcal{E}(t+\tau) \rangle &= \int \sum_n e^{-i\omega_n t - i\phi_n} \sum_m e^{i\omega_m t + i\omega_m \tau + i\phi_m} dt \\ &= \sum_{n,m} \int e^{-i\omega_n t - i\phi_n + i\omega_m t + i\omega_m \tau + i\phi_m} dt = \sum_n e^{i\omega_n \tau} . \end{aligned} \quad (15.98)$$

The crossed terms  $n \neq m$  of this expressions vanish. *Doppler broadening* is inhomogeneous. Hence, the probability density for frequencies emitted by thermal atoms is a Gaussian,  $p(\omega)d\omega = (2\pi\delta)^{-1/2} e^{-(\omega_n - \omega_0)^2 / 2\delta^2} d\omega$ , such that,

**thermal ensemble**

$$\begin{aligned} \langle \mathcal{E}^*(t)\mathcal{E}(t+\tau) \rangle &= N(2\pi\delta)^{-1/2} \int e^{i\omega_n \tau} e^{-(\omega_n - \omega_0)^2 / 2\delta^2} d\omega_n \\ \Rightarrow g^{(1)}(\tau) &= e^{i\omega_0 \tau - \delta^2 \tau^2 / 2} \\ \Rightarrow \mathcal{F}[g^{(1)}(\tau)] &= \sqrt{\frac{\ln 2}{\pi \delta^2}} e^{-\ln 2 \cdot \omega^2 / \delta^2} \\ g^{(2)}(\tau) &= 1 + e^{-\delta^2 \tau^2 / 2} \end{aligned} \quad (15.99)$$

For a totally emission *chaotic light*,

**chaotic line**

$$\begin{aligned} g^{(1)}(\tau) &= \delta(0) \\ \mathcal{F}[g^{(1)}(\tau)] &= 1 \\ g^{(2)}(\tau) &= 1 + |g^{(1)}(\tau)| \end{aligned} \quad (15.100)$$

The last expression is known as *Bloch-Siegert relation*. Mono-mode chaotic light can be seen as incoherent multi-mode light, where all modes except a single mode are filtered by a Fabry-Pérot etalon. This light is characterized by  $|g^{(1)}(\tau)| = 1$  and  $g^{(2)}(\tau) = 2$ , despite the coherence length being  $\tau \rightarrow \infty$ . Do the Excs. 15.3.5.1 to 15.3.5.3.

## 15.3.4 Photon counting statistics

### 15.3.5 Exercises

#### 15.3.5.1 Ex: Correlation functions for two light modes

- Calculate  $|g^{(1)}(\tau)|$ ,  $F_{\mathcal{E}}(\omega)$ , and  $|g^{(2)}(\tau)|$  for two interfering and non-interfering modes neglecting fluctuations.
- What changes when one mode is broadened by random noise, e.g. induced by spontaneous emission?

### 15.3.5.2 Ex: Correlation functions and spectra of phase- and amplitude-modulated light

- Calculate  $g^{(1)}(\tau)$ ,  $S_{\mathcal{E}}(\omega)$ , and  $g^{(2)}(\tau)$  for amplitude-modulated light:  $\mathcal{E}_{am}(t) = e^{i\omega_0 t}(1 + M \cos \Omega t)$ .
- Calculate  $g^{(1)}(\tau)$ ,  $S_{\mathcal{E}}(\omega)$ , and  $g^{(2)}(\tau)$  for phase-modulated light:  $\mathcal{E}_{pm}(t) = e^{i\omega_0 t + iM \cos \Omega t}$ .
- Repeat the calculation (a) for exponentially decaying amplitude-modulated light:  $\mathcal{E}_{dam}(t) = e^{-\gamma t} e^{i\omega_0 t}(1 + M \cos \Omega t)$ .

### 15.3.5.3 Ex: Phase modulation

- Show that it is not possible to construct a periodic phase modulation function such that the signal has only two sidebands.
- From  $1 = |e^{iM \sin \Omega t}|^2$  derive a sum rule for the Bessel functions.
- Discuss the difference of the spectra  $\sum_{k=-\infty}^{\infty} J_k(M) e^{ik\Omega t}$  and  $\sum_{k=-\infty}^{\infty} |J_k(M)| e^{ik\Omega t}$ .

## 15.4 Spontaneous emission and light scattering

### 15.4.1 Interaction of atoms with vacuum modes

The Jaynes-Cummings Hamiltonian (15.11), discussed in Sec. 15.2, describes the purely coherent dynamics of a single immobile two-level atom interacting with a single cavity mode. The model is simple enough to allow for analytical solutions. However, it does not include processes of spontaneous emission, which can be understood as the interaction of the atom with the light modes of the vacuum. That is, we must extend the Hamiltonian,

$$\hat{H} = \hat{H}_{atom} + \hat{H}_{field} + \hat{H}_{atom:field} + \hat{H}_{vacuum} + \hat{H}_{atom:vacuum} . \quad (15.101)$$

The evolution of the system represented by the Hamiltonian (15.101) is described by a total density operator,  $\hat{\rho}_{total}(t)$ , obeying the *von Neumann equation*,

$$\boxed{\frac{d\hat{\rho}_{total}}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}_{total}]}, \quad (15.102)$$

which has the solution,

$$\hat{\rho}_{total}(t) = e^{-i\hat{H}t/\hbar} \hat{\rho}_{total}(0) e^{i\hat{H}t/\hbar} \equiv e^{-i\mathcal{L}t} \hat{\rho}_{total}(0) . \quad (15.103)$$

Often, we are only interested in *either* the evolution of the light field, *or* the internal state of the atom. In these cases, we calculate the trace over all those degrees of freedom, which are we are NOT interested in,

$$\hat{\rho}_{atom} = \text{Tr}_{light} \hat{\rho}_{total} \quad \text{and} \quad \hat{\rho}_{light} = \text{Tr}_{atom} \hat{\rho}_{total} . \quad (15.104)$$

The procedure is the following. We begin choosing the initial state of the electromagnetic vacuum as the photonic vacuum  $\hat{\rho}_{field} = |\{0\}\rangle\langle\{0\}|$  and defining a projection operator onto this state,  $\hat{P} \dots \equiv \hat{\rho}_{field}(0) \text{Tr}_{field} \dots = \hat{P}^2 \dots$ . Then we apply to the von Neumann equation the rotating wave, the Markov and the Born approximations.

Finally, tracing over the vacuum field variables, we obtain after some calculations the *Bloch-Lindblad equation* or *master equation* [566] for the atom interacting with the driving field. For a discussion of the validity of the Born-Markov approximation [509]. For the relation between the Markov approximation and the Fermi's Golden Rule [9].

We emphasize that the Hamiltonian (15.101) describes the interaction of light with a *single immobile atom* at the most fundamental level. However, it excludes many-body effects introduced by quantum statistics or interatomic interactions (to be discussed in Chp. 26.9), as well as the center-of-mass motion of the atom and the impact of photonic recoil (to be discussed in Chp. 18.4).

In the following section we give a simplified derivation concentrating us on the situation of a single motionless atom, excited by a laser and emitting photons into the electromagnetic vacuum.

### 15.4.1.1 Spontaneous emission

Spontaneous emission can be understood as an energy diffusion process from a system with a restricted number of degrees of freedom into a large thermal bath. For example, although a two-dimensional Hilbert space is sufficient to describe a laser-driven two-level atom, this atom couples to a huge phase-space by spontaneously emitting photons into arbitrary directions. We account for this fact by including in the Hamiltonian not only the interaction of the atom with the incident laser (wavevector  $\mathbf{k}_0$ , frequency  $\omega_{\mathbf{k}_0}$ , coupling force  $g_{\mathbf{k}_0}$ ), but also with the modes of the electromagnetic vacuum (wavevector  $\mathbf{k}$ , frequency  $\omega_{\mathbf{k}}$ , coupling force  $g_{\mathbf{k}}$ ). We will see, that with this Hamiltonian, we can derive, in a calculation known as *Weisskopf-Wigner theory*, the Schrödinger equation for the amplitudes of the atomic levels (14.95) including spontaneous emission.

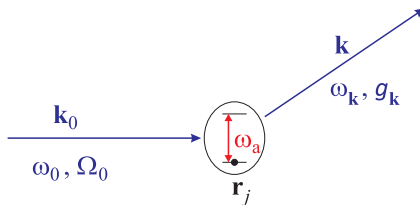


Figure 15.10: Scattering of a laser beam by an atom.

Denoting the frequency of the atomic resonance by  $\omega_a$ , the interaction part of the Hamiltonian is,

$$\hat{H} = \hbar g_{\mathbf{k}_0} (\hat{\sigma}^- e^{-i\omega_a t} + \hat{\sigma}^+ e^{i\omega_a t}) \left( \hat{a}_{\mathbf{k}_0}^\dagger e^{i\omega_0 t - i\mathbf{k}_0 \cdot \mathbf{r}} + \hat{a}_{\mathbf{k}_0} e^{-i\omega_0 t + i\mathbf{k}_0 \cdot \mathbf{r}} \right) + \sum_{\mathbf{k}} \hbar g_{\mathbf{k}} (\hat{\sigma}^- e^{-i\omega_a t} + \hat{\sigma}^+ e^{i\omega_a t}) \left( \hat{a}_{\mathbf{k}}^\dagger e^{i\omega_{\mathbf{k}} t - i\mathbf{k} \cdot \mathbf{r}} + \hat{a}_{\mathbf{k}} e^{-i\omega_{\mathbf{k}} t + i\mathbf{k} \cdot \mathbf{r}} \right). \quad (15.105)$$

$\Omega_0$  is the Rabi frequency of the interaction between the atom and the pump mode (which, here, is treated as classical field),  $\hat{\sigma}^-$  is the atomic deexcitation operator,  $\hat{a}_{\mathbf{k}}$  is the annihilation operator of a photon, and  $g_{\mathbf{k}} = d\sqrt{\omega/(\hbar\epsilon_0 V)}$  describes the coupling



between the atom and a vacuum mode whose volume is  $V$ . The atom has two states, the ground state  $|g\rangle$  and excited state  $|e\rangle$ . Since we are considering only one atom fixed in space <sup>7</sup>, we can as well locate it at the origin  $\mathbf{r} = 0$ . In addition, considering a high power incident laser,

$$\hat{a}_{\mathbf{k}_0}|n_0\rangle_{\mathbf{k}_0} = \sqrt{n_0}|n_0 - 1\rangle_{\mathbf{k}_0} \simeq \sqrt{n_0}|n_0\rangle_{\mathbf{k}_0} , \quad (15.106)$$

$\hat{a}_{\mathbf{k}_0}$  is approximately an observable proportional to the root of the intensity. As  $[\hat{a}_{\mathbf{k}_0}, \hat{a}_{\mathbf{k}_0}^\dagger] \simeq 0$ , we can disregard the quantum nature of the incident field and replace,  $\Omega_0 \equiv 2\sqrt{n_0}g_{\mathbf{k}_0}$ . Within the rotating wave approximation (RWA), the Hamiltonian becomes,

$$\hat{H} = \frac{\hbar}{2}\Omega_0 [\hat{\sigma}^- e^{i\Delta_0 t} + h.c.] + \hbar \sum_{\mathbf{k}} \left[ g_{\mathbf{k}} \hat{\sigma} \hat{a}_{\mathbf{k}}^\dagger e^{i\Delta_{\mathbf{k}} t} + h.c. \right] , \quad (15.107)$$

where we introduced the abbreviations,

$$\Delta_0 \equiv \omega_0 - \omega_a \quad \text{and} \quad \Delta_{\mathbf{k}} \equiv \omega_{\mathbf{k}} - \omega_a . \quad (15.108)$$

The general state of the system is given by,

$$|\Psi(t)\rangle = \alpha(t)|0\rangle_a|0\rangle_{\mathbf{k}} + \beta(t)|1\rangle_a|0\rangle_{\mathbf{k}} + \sum_{\mathbf{k}} \gamma_{\mathbf{k}}(t)|0\rangle_a|1\rangle_{\mathbf{k}} , \quad (15.109)$$

where  $|j\rangle_a$  denotes the atomic state and  $|n\rangle_{\mathbf{k}}$  the number of photons in the scattering mode.

The temporal evolution of the amplitudes is obtained by inserting the Hamiltonian (15.107) and the ansatz (15.109) into the Schrödinger equation,

$$\frac{\partial}{\partial t}|\Psi(t)\rangle = -\frac{i}{\hbar}\hat{H}|\Psi(t)\rangle . \quad (15.110)$$

As verified in Exc. 15.4.4.1, we obtain,

$$\begin{aligned} \dot{\alpha}(t) &= -i\frac{\Omega_0}{2}e^{i\Delta_0 t}\beta(t) \\ \dot{\beta}(t) &= -i\frac{\Omega_0}{2}\alpha(t)e^{-i\Delta_0 t} - \sum_{\mathbf{k}} ig_{\mathbf{k}}\gamma_{\mathbf{k}}(t)e^{-i\Delta_{\mathbf{k}} t} \\ \dot{\gamma}_{\mathbf{k}}(t) &= -ig_{\mathbf{k}}e^{i\Delta_{\mathbf{k}} t}\beta(t) . \end{aligned} \quad (15.111)$$

Now, we chose the initial conditions,

$$\alpha(0) = 1 \quad \text{and} \quad \beta(0) = 0 \quad \text{and} \quad \gamma_{\mathbf{k}}(0) = 0 , \quad (15.112)$$

we integrate the third equation,

$$\gamma_{\mathbf{k}}(t) = -ig_{\mathbf{k}} \int_0^t e^{i\Delta_{\mathbf{k}} t'} \beta(t') dt' , \quad (15.113)$$

and we substitute it in the second equation,

$$\dot{\beta}(t) = -i\frac{\Omega_0}{2}\alpha(t)e^{-i\Delta_0 t} - \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \int_0^t e^{i\Delta_{\mathbf{k}}(t'-t)} \beta(t') dt' . \quad (15.114)$$

<sup>7</sup>We do not let the atom be accelerated by photonic recoil.

### 15.4.1.2 The Markov approximation

For small systems (which certainly is the case of a single atom), we can apply the *Markov approximation*<sup>8</sup> claiming that the temporal variation of the amplitudes  $\beta(t')$  is slower than the evolution of the system given by  $e^{i(\omega_{\mathbf{k}} - \omega_a)t}$  in the integro-differential equation, which is equivalent to an arbitrarily high-order equation. Hence, substituting  $\beta(t') \rightarrow \beta(t)$  into the integro-differential equation, we reduce it to a simple first-order differential equation.

In practice, we redefine the integration variable,  $t'' \equiv t - t'$ , to obtain,

$$\begin{aligned} \frac{d}{dt}\beta(t) &= -i\frac{\Omega_0}{2}\alpha(t) - \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \int_0^t e^{i(\omega_{\mathbf{k}} - \omega_a)(t-t')} \beta(t') dt' \\ &= -i\frac{\Omega_0}{2}\alpha(t) - \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \int_0^t e^{-i(\omega_{\mathbf{k}} - \omega_a)t''} \beta(t-t'') dt'' , \end{aligned} \quad (15.115)$$

and implement the Markov approximation by setting  $\beta(t-t'') \simeq \beta(t)$ , and with  $\lim_{t \rightarrow \infty} \int_0^t e^{-i(\omega_{\mathbf{k}} - \omega_a)t''} dt'' = \pi\delta(\omega_{\mathbf{k}} - \omega_a)$ , and replacing  $\sum_{\mathbf{k}} \rightarrow \frac{V}{(2\pi)^3} \int d^3\mathbf{k}$ , we arrive at,

$$\begin{aligned} \frac{d}{dt}\beta(t) &\simeq -i\frac{\Omega_0}{2}\alpha(t) - \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \beta(t) \pi\delta(\omega_{\mathbf{k}} - \omega_a) \\ &= -i\frac{\Omega_0}{2}\alpha(t) - \frac{V}{(2\pi)^3} \beta(t) \int g_{\mathbf{k}}^2 \pi\delta(\omega_{\mathbf{k}} - \omega_a) d^3\mathbf{k} \\ &= -i\frac{\Omega_0}{2}\alpha(t) - \frac{V}{(2\pi)^3} \beta(t) 4\pi g_{\mathbf{k}_a}^2 \pi k_a^2 \frac{1}{c} = -i\frac{\Omega_0}{2}\alpha(t) - \frac{\Gamma}{2}\beta(t) . \end{aligned} \quad (15.116)$$

In the last step we introduced, as an abbreviation, the spontaneous emission rate,

$$\Gamma \equiv \sum_{\mathbf{k}} 2g_{\mathbf{k}}^2 \pi\delta(\omega_{\mathbf{k}} - \omega_a) = \frac{V}{\pi c} k_a^2 g_{\mathbf{k}_a}^2 , \quad (15.117)$$

Finally,

$$\boxed{\frac{d}{dt}\alpha(t) = -i\frac{\Omega_0}{2}\beta(t) \quad \text{and} \quad \frac{d}{dt}\beta(t) = -i\frac{\Omega_0}{2}\alpha(t) - \frac{\Gamma}{2}\beta(t)} . \quad (15.118)$$

These are exactly the equations for the probability amplitudes (14.95) derived from the Schrödinger equation, only that now, the spontaneous emission term has been derived explicitly. Solve the Exc. 15.4.4.2.

**Example 68 (Emission stimulated by vacuum fluctuations):** Spontaneous emission can be regarded as an emission stimulated by vacuum fluctuations. To see this, we write down the resonant optical cross section of a driven two-level atom without degeneracies,  $\sigma_0 = \lambda^2/2\pi$ , and the intensity of an incident laser field,  $\bar{I} = cN\hbar\omega_0/V$ , generating the Rabi frequency,

$$\Omega_a^2 = \sigma_0 \frac{\bar{I}}{\hbar\omega_a} \Gamma = \frac{2\pi c}{k_a^2} \frac{N}{V} \Gamma . \quad (15.119)$$

<sup>8</sup>The approximation does not necessarily hold for large clouds of atoms.

Now, we assume that the field is, in fact, a vacuum mode containing only half a photon,  $N = 1/2$ , which corresponds to vacuum fluctuations in the mode  $k_a$ . Then,

$$\Omega_{1/2}^2 = \frac{\pi c}{k_a^2 V} \Gamma = g^2. \quad (15.120)$$

## 15.4.2 Resonance fluorescence and (in-)coherent light scattering

The typical situation for a spectroscopy experiment is illustrated in Fig. 15.11: When a beam of light, understood as a plane wave, strikes an atom (or a cloud of many atoms), a part of the light is absorbed and reemitted into a direction indicated by a solid angle  $d\Omega$ . Light scattering is, of course, a second order process involving two atomic transitions, one absorption and one emission.

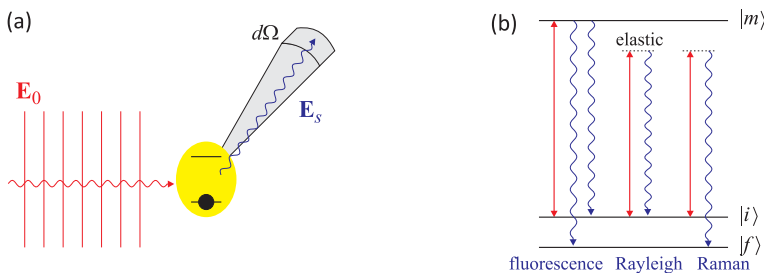


Figure 15.11: (a) Geometry of a scattering experiment. (b) Spectral contributions of light scattered elastically and inelastically by a three-level atom.

Radiation can be absorbed or scattered by an atom in different ways, depending on whether the interaction is an *elastic scattering* or an *inelastic scattering* process, a coherent or incoherent, a spontaneous or (bosonically) stimulated process. These properties characterize many processes, in particular, resonance fluorescence (i.e. absorption and reemission), *Rayleigh scattering*, or *Raman scattering*. In the following, we will clarify this classification.

Every scattering process is either spontaneous or stimulated<sup>9</sup>. Rayleigh scattering is elastic, that is, the kinetic energy of the scattering atom is the same, before and after the scattering process. In contrast, Raman scattering is inelastic. Spontaneous emission is due to the decay of population from an excited state, and spontaneous Rayleigh scattering is due to the decay of an induced dipole moment. Both spontaneous processes can be regarded as being stimulated by vacuum fluctuations.

<sup>9</sup>Classical theories of light scattering through the excitation of an electronic motion based on the models of Lorentz or Drude can be found in the script [Electrodynamics](#). Although being classical, these model are useful for a deeper understanding of many aspects of *Compton scattering*, *Thomson scattering*, and *Rayleigh scattering*.

### 15.4.2.1 Deriving the source field expression

We will now calculate the electric field due to spontaneous emission by an atom from the interaction Hamiltonian for atom-vacuum coupling (15.105) in the RWA,

$$\hat{H} = \sum_{\mathbf{k}} \hbar g_{\mathbf{k}} \hat{\sigma}^- \hat{a}_{\mathbf{k}}^\dagger e^{i\omega_{\mathbf{k}}t - i\omega_a t - i\mathbf{k}\cdot\mathbf{R}} + h.c. . \quad (15.121)$$

Now, we assume isotropic coupling,  $g_{\mathbf{k}} = g_k$ , and  $\omega_{\mathbf{k}} = \omega_k$ , and for simplicity we position the atom in the origin,  $\mathbf{R} = 0$ . We use the Heisenberg equation with the commutation rule  $[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}, \mathbf{k}'}$  to derive the temporal evolution of the field operators,

$$\frac{d\hat{a}_{\mathbf{k}}}{dt} = \frac{1}{i\hbar} [\hat{a}_{\mathbf{k}}, \hat{H}] = -i\hat{\sigma}^- g_k e^{i(\omega_k - \omega_a)t} . \quad (15.122)$$

Neglecting for simplicity polarization, the electric field is given by,

$$\hat{\mathcal{E}}_{sct}^+(\mathbf{r}, t) = \sum_{\mathbf{k}} \mathcal{E}_1 \hat{a}_{\mathbf{k}}(t) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)} , \quad (15.123)$$

where  $\mathbf{r}$  is now the observation point of the electric field. We restrict to the far-field and substitute the annihilation operator with the integral of Eq. (15.122) using the initial condition  $\hat{a}_{\mathbf{k}}(0) = 0$ ,

$$\hat{\mathcal{E}}_{sct}^+(\mathbf{r}, t) = \sum_{\mathbf{k}} \mathcal{E}_1 g_k \int_0^t \hat{\sigma}^-(t') e^{i(\omega_k - \omega_a)t'} dt' e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)} . \quad (15.124)$$

Now, we substitute the sum over  $\mathbf{k}$  by an integral, as done in (15.116),

$$\hat{\mathcal{E}}_{sct}^+(\mathbf{r}, t) = -i \frac{V}{(2\pi)^3} \int_{\mathbb{R}^3} \mathcal{E}_1 g_k \int_0^t \hat{\sigma}^-(t') e^{i(\omega_k - \omega_a)t'} dt' e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)} d^3k . \quad (15.125)$$

Using the relationships,

$$g_k = \frac{d_{12}\mathcal{E}_1}{\hbar} \quad \text{and} \quad \mathcal{E}_1 = \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}} , \quad (15.126)$$

the final result of the integration yields [440],

$$\hat{\mathcal{E}}_{sct}^+(\mathbf{r}, t) \simeq -i \frac{d_{12}k_a^2}{4\pi\varepsilon_0 r} \hat{\sigma}^-(t - \frac{r}{c}) . \quad (15.127)$$

### 15.4.2.2 Resonance fluorescence

When we introduced the second quantization (15.8) we learned that the field of light emitted by a radiator in the radiation zone ( $\lambda \ll r$ ) is, taking into account retardation<sup>10</sup>, given by,

$$\langle \hat{\mathcal{E}}_s^+(\mathbf{r}, t) \rangle \propto \langle \hat{\sigma}^- \rangle \propto \tilde{\rho}_{21} \quad \text{and} \quad \langle \hat{\mathcal{E}}_s^-(\mathbf{r}, t) \hat{\mathcal{E}}_s^+(\mathbf{r}, t) \rangle \propto \langle \hat{\sigma}^+ \hat{\sigma}^- \rangle \propto \rho_{22} . \quad (15.128)$$

<sup>10</sup>The classical version of this formula is can be found in the script [Electrodynamics](#), Sec. 9.1.3, Eq. (8.41).

Therefore, the electric field emitted by an atom and the intensity of scattered light are given by,

$$\left. \begin{aligned} \langle \hat{\mathcal{E}}_s^+(\mathbf{r}, t) \rangle &= -\frac{e\omega_a^2 \hat{\epsilon} \cdot \mathbf{r}_{12}}{4\pi\epsilon_0 c^2 r} \tilde{\rho}_{21}(t - \frac{r}{c}) e^{-i\omega(t-r/c)} \\ \bar{I}_s = c\epsilon_0 \langle \hat{\mathcal{E}}_s^-(\mathbf{r}, t) \hat{\mathcal{E}}_s^+(\mathbf{r}, t) \rangle &= \frac{\alpha \hbar \omega_a^4 |\hat{\epsilon} \cdot \mathbf{r}_{12}|^2}{4\pi c^2 r^2} \rho_{22}(t - \frac{r}{c}) \end{aligned} \right\}, \quad (15.129)$$

with the definition of the Sommerfeld constant  $\alpha = e^2/4\pi\epsilon_0 \hbar c$ . We calculate the total flux of emitted photons,

$$\begin{aligned} W_{fi}^{(sp)} &= \int \frac{\bar{I}_s r^2}{\hbar \omega_a} d\Omega = \frac{1}{\hbar \omega_a} \int \frac{\alpha \hbar \omega_a^4 |\mathbf{r}_{12}|^2 \cos^2 \theta}{4\pi c^2} \rho_{22}(t - \frac{r}{c}) \sin \theta d\theta d\phi \\ &= \frac{8\pi}{3\hbar \omega_a} \frac{\alpha \hbar \omega_a^4 |\mathbf{r}_{12}|^2}{4\pi c^2} \rho_{22}(t - \frac{r}{c}) = \frac{2\alpha}{3c^2} \omega_a^3 |\mathbf{r}_{12}|^2 \rho_{22}(t - \frac{r}{c}). \end{aligned} \quad (15.130)$$

The result coincides with the spontaneous emission rate  $\Gamma$  calculated in (13.37).

A *differential scattering cross section* can be defined by,

$$\frac{d\sigma}{d\Omega} \equiv \frac{\omega \bar{I}_s r^2}{\omega_s \bar{I}_0}. \quad (15.131)$$

### 15.4.2.3 Coherently scattered light and saturation

The total intensity of the scattered light being  $\bar{I}_s$ , the fraction of the coherently scattered light is,

$$\frac{\bar{I}_s^{\text{coh}}}{\bar{I}_s} = \frac{\langle \hat{\mathcal{E}}_s^-(\mathbf{r}, t) \rangle \langle \hat{\mathcal{E}}_s^+(\mathbf{r}, t) \rangle}{\langle \hat{\mathcal{E}}_s^-(\mathbf{r}, t) \hat{\mathcal{E}}_s^+(\mathbf{r}, t) \rangle}. \quad (15.132)$$

Inserting the expressions (15.129) and the stationary solution of the Bloch equations (14.99),

$$\frac{\bar{I}_s^{\text{coh}}}{\bar{I}_s} = \frac{|\tilde{\rho}_{21}(\infty)|^2}{\rho_{22}(\infty)} = \frac{1}{1+s} = 1 - \frac{\bar{I}_s^{\text{incoh}}}{\bar{I}_s}. \quad (15.133)$$

That is, since the resonance fluorescence is proportional to the excited state population,  $S_{tot} \equiv \rho_{22}(\infty)$ , the coherent and incoherent parts of the fluorescence are,

$$\boxed{S_{coh} = |\rho_{21}(\infty)|^2 = \frac{s/2}{(1+s)^2} \quad \text{and} \quad S_{incoh} = \rho_{22}(\infty) - |\rho_{21}(\infty)|^2 = \frac{s^2/2}{(1+s)^2}}. \quad (15.134)$$

Hence,  $S_{incoh} = s S_{coh}$ .

We note, that the integral of the fluorescence spectrum is,

$$\int_{-\infty}^{\infty} \frac{\Omega^2}{4\Delta^2 + 2\Omega^2 + \Gamma^2} d\Delta = \frac{\pi}{2} \frac{\Omega^2}{\sqrt{2\Omega^2 + \Gamma^2}} \xrightarrow{\Omega \ll \Gamma} \frac{\pi\Omega^2}{2\Gamma}. \quad (15.135)$$

### 15.4.3 The spectrum of resonance fluorescence

The *correlation functions* defined in (15.79) represent an interesting concept for describing resonance fluorescence and for phenomena such as *antibunching* observed in resonance fluorescence.

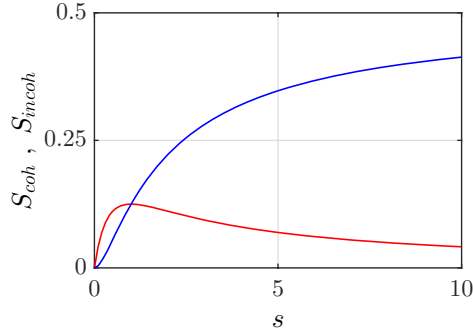


Figure 15.12: (code) Elastic (red) versus inelastic scattering (blue).

### 15.4.3.1 The quantum regression theorem

From (15.85) we see that, to compute the spectra of *resonance fluorescence*, we only need to compute the correlation function  $g^{(1)}$ , i.e. the amplitudes of the field  $\hat{\mathcal{E}}(t)$ , which in turn are related to the field operators (15.8). The field operators follow the solutions of the Bloch equation, which, being linear, have the following generic form,

$$\rho_{ij}(t + \tau) = \sum_{k,l} \alpha_{ijkl}(\tau) \rho_{ij}(t) + \beta_{ij}(\tau). \quad (15.136)$$

The trace condition is satisfied, when  $(i, j), (k, l) \neq (1, 1)$ .

To be able to explore this relationship (15.85), needed to calculate the correlation functions, we have to invoke the so-called *quantum regression theorem*,

$$\langle \hat{A}(t + \tau) \rangle = \sum_i \xi_i(\tau) \langle \hat{A}_i(t) \rangle \implies \langle \hat{B}(t) \hat{A}(t + \tau) \hat{C}(t) \rangle = \sum_i \xi_i(\tau) \langle \hat{B}(t) \hat{A}_i(t) \hat{C}(t) \rangle. \quad (15.137)$$

**Example 69 (Quantum regression applied to the Langevin equation):** We have,

$$\begin{aligned} \dot{A}_\mu &= D_\mu(t) + F_\mu(t) \\ \langle F_\mu(t) F_\nu(t') \rangle &= 2 \langle D_{\mu\nu} \rangle \delta(t - t'). \end{aligned} \quad (15.138)$$

We know,

$$\langle A_\mu(t) F_\nu(t) \rangle = \langle D_{\mu\nu} \rangle \quad \text{and} \quad \langle F_\mu(t) A_\nu(t) \rangle = \langle D_{\mu\nu} \rangle \quad (15.139)$$

and the quantum regression theorem gives,

$$\frac{d}{dt} \langle A_\mu(t) A_\nu(t') \rangle = \langle D_\mu(t) A_\nu(t') \rangle, \quad (15.140)$$

because if  $t' < t$ , the term  $\langle F_\mu(t) A_\nu(t') \rangle$  vanishes for a *Markovian process*.

### 15.4.3.2 Bloch equation for a two-level system

The Fourier transform of the first-order coherence,  $g^{(1)}(\tau) = e^{-i\omega\tau}G(\tau)$ , gives,

$$F(\nu) = (\mathcal{F}g^{(1)})(\nu) = \mathcal{F}[e^{-i\omega\tau}] \star \mathcal{F}[G(\tau)] = \delta(\nu - \omega) \star \mathcal{F}[G(\tau)] = (\mathcal{F}G)(\nu - \omega). \quad (15.141)$$

Therefore, we can look at the unshifted spectrum,  $(\mathcal{F}G)(\nu)$ . Since the fluorescence spectrum is determined by the first-order coherence, which depends on the field operators, which in turn depend on the atomic populations and coherences, we have to solve the Bloch equation.

For a two-level atom the Bloch equations, having been reduced by the normalization condition (14.169) are,

$$\dot{\vec{\rho}}_{red} = \mathcal{M}\vec{\rho}_{red} + \mathbf{b} = \begin{pmatrix} -\Gamma & -\frac{i}{2}\Omega & \frac{i}{2}\Omega \\ -i\Omega & -\frac{1}{2}\Gamma - i\Delta & 0 \\ i\Omega & 0 & -\frac{1}{2}\Gamma + i\Delta \end{pmatrix} \begin{pmatrix} \rho_{22} \\ \rho_{12} \\ \rho_{21} \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{i}{2}\Omega \\ -\frac{i}{2}\Omega \end{pmatrix} \quad (15.142)$$

with the solution (14.171), that is,  $\vec{\rho}(t + \tau) = e^{\mathcal{M}\tau}\vec{\rho}(t) + (1 - e^{\mathcal{M}\tau})\vec{\rho}(\infty)$  with  $\rho(\infty) = -\mathcal{M}^{-1}\mathbf{b}$ . This solution can be cast in the following form,

$$\rho_{kl}(t + \tau) = \sum_{(mn)} \alpha_{(kl)(mn)}(\tau)\rho_{mn}(t) + \beta_{(kl)}(\tau), \quad (15.143)$$

where  $(mn), (kl) = (22), (12), (21)$  identifying,

$$\alpha_{(kl)(mn)}(\tau) = \begin{pmatrix} \alpha_{22,22} & \alpha_{12,22} & \alpha_{21,22} \\ \alpha_{22,12} & \alpha_{12,12} & \alpha_{21,12} \\ \alpha_{22,21} & \alpha_{12,21} & \alpha_{21,21} \end{pmatrix} \equiv \begin{pmatrix} (e^{\mathcal{L}\tau})_{11} & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} = e^{\mathcal{M}\tau} \quad (15.144)$$

$$\beta_{(kl)}(\tau) = \begin{pmatrix} \beta_{22} \\ \beta_{12} \\ \beta_{21} \end{pmatrix} \equiv \begin{pmatrix} -[(1 - e^{\mathcal{M}\tau})\mathcal{M}^{-1}\mathbf{b}]_1 \\ \cdot \\ \cdot \end{pmatrix} = -(1 - e^{\mathcal{M}\tau})\mathcal{M}^{-1}\mathbf{b}.$$

Using quantum operators in the interaction image,  $|k\rangle\langle l| = \hat{\sigma}_{kl}$ , we have,

$$\langle \hat{\sigma}_{12}(t) \rangle = \langle \hat{\sigma}_{21}^\dagger(t) \rangle = \rho_{12}(t)e^{i\omega_0 t} \quad \text{and} \quad \langle \hat{\sigma}_{22}(t) \rangle = \langle \hat{\sigma}_{12}(t)\hat{\sigma}_{21}(t) \rangle = \rho_{22}(t). \quad (15.145)$$

yielding,

$$\langle e^{(k-l)i\omega_0(t+\tau)}\hat{\sigma}_{kl}(t + \tau) \rangle = \sum_{(mn)} \alpha_{(kl)(mn)}(\tau)\langle e^{(m-n)i\omega_0 t}\hat{\sigma}_{mn}(t) \rangle + \beta_{(mn)}(\tau)\langle 1 \rangle, \quad (15.146)$$

or,

$$\begin{aligned} & \langle \hat{\sigma}_{kl}(t + \tau) \rangle & (15.147) \\ & = \sum_{(mn)} e^{(l-k)i\omega_0\tau} \alpha_{(kl)(mn)}(\tau)\langle e^{(l-k+m-n)i\omega_0 t}\hat{\sigma}_{mn}(t) \rangle + e^{(l-k)i\omega_0\tau} \beta_{(mn)}(\tau)\langle e^{(l-k)i\omega_0 t} \rangle. \end{aligned}$$

Applying the quantum regression theorem to the Bloch equations, we get for an arbitrary time-dependent function  $f(t)$ ,

$$\boxed{\langle f(t)\hat{\sigma}_{kl}(t+\tau) \rangle = \sum_{(mn)} e^{(l-k)\omega_0\tau} \alpha_{(kl)(mn)}(\tau) \langle e^{(l-k+m-n)\omega_0 t} f(t)\hat{\sigma}_{mn}(t) \rangle + e^{(l-k)\omega_0\tau} \beta_{(mn)}(\tau) \langle e^{(l-k)\omega_0 t} f(t) \rangle} \quad (15.148)$$

### 15.4.3.3 Correlation functions

We now look at the radiation field, which is related to the dipole moment operator via,

$$\hat{\mathcal{E}}^- = \gamma \hat{\sigma}_{21}, \quad (15.149)$$

where  $\gamma$  is simply a constant. Substituting this relation in the correlation functions (15.79) we obtain,

$$\begin{aligned} g^{(1)}(\tau) &= \frac{\langle \hat{\sigma}_{21}(t)\hat{\sigma}_{12}(t+\tau) \rangle}{\langle \hat{\sigma}_{21}(t)\hat{\sigma}_{12}(t) \rangle} = \frac{\langle \hat{\sigma}_{21}(t)\hat{\sigma}_{12}(t+\tau) \rangle}{\langle \hat{\sigma}_{22}(t) \rangle} \quad (15.150) \\ g^{(2)}(\tau) &= \frac{\langle \hat{\sigma}_{21}(t)\hat{\sigma}_{21}(t+\tau)\hat{\sigma}_{12}(t+\tau)\hat{\sigma}_{12}(t) \rangle}{\langle \hat{\sigma}_{21}(t)\hat{\sigma}_{12}(t) \rangle^2} = \frac{\langle \hat{\sigma}_{22}(t)\hat{\sigma}_{22}(t+\tau) \rangle}{\langle \hat{\sigma}_{22}(t) \rangle^2}. \end{aligned}$$

Now we can calculate, letting  $\xi_i(\tau) \equiv \alpha_{(12)(mn)}$ ,  $\hat{C}(t) \equiv 1$ , and  $\hat{B}(t) \equiv \hat{\sigma}_{21}(t)$ ,

$$g^{(1)}(\tau) = \frac{\sum_{(mn)} e^{i\omega_0(t+\tau)} e^{(m-n)\omega_0 t} \alpha_{(12)(mn)}(\tau) \langle \hat{\sigma}_{21}(t)\hat{\sigma}_{mn}(t) \rangle + e^{i\omega_0(t+\tau)} \beta_{(12)}(\tau) \langle \hat{\sigma}_{21}(t) \rangle}{\langle \hat{\sigma}_{22}(t) \rangle} \quad (15.151)$$

$$g^{(2)}(\tau) = \frac{\sum_{(mn)} e^{(m-n)\omega_0 t} \alpha_{(22)(mn)}(\tau) \langle \hat{\sigma}_{22}(t)\hat{\sigma}_{mn}(t) \rangle + \beta_{(22)}(\tau) \langle \hat{\sigma}_{22}(t) \rangle}{\langle \hat{\sigma}_{22}(t) \rangle^2}.$$

Using  $\hat{\sigma}_{21}\hat{\sigma}_{mn} = \hat{\sigma}_{2n}\delta_{m1}$ ,

$$g^{(1)}(\tau) = e^{i\omega_0\tau} \frac{\alpha_{(12)(12)}(\tau) \langle \hat{\sigma}_{21}(t)\hat{\sigma}_{12}(t) \rangle + \beta_{(12)}(\tau) \langle e^{i\omega_0 t} \hat{\sigma}_{21}(t) \rangle}{\langle \hat{\sigma}_{22}(t) \rangle} \quad (15.152)$$

$$g^{(2)}(\tau) = \frac{\alpha_{(22)(21)}(\tau) \langle e^{i\omega_0 t} \hat{\sigma}_{22}(t)\hat{\sigma}_{21}(t) \rangle + \alpha_{(22)(22)}(\tau) \langle \hat{\sigma}_{22}(t)\hat{\sigma}_{22}(t) \rangle + \beta_{(22)}(\tau) \langle \hat{\sigma}_{22}(t) \rangle}{\langle \hat{\sigma}_{22}(t) \rangle^2}.$$

Returning to the density operator and letting  $t \rightarrow \infty$ ,

$$g^{(1)}(\tau) = e^{i\omega_0\tau} \left[ \alpha_{(12)(12)}(\tau) + \beta_{(12)}(\tau) \frac{\rho_{21}(\infty)}{\rho_{22}(\infty)} \right] \quad \text{and} \quad g^{(2)}(\tau) = e^{i\omega_0\tau} \frac{\beta_{(22)}(\tau)}{\rho_{22}(\infty)}, \quad (15.153)$$

that is,

$$\boxed{\begin{aligned} g^{(1)}(\tau) &= e^{i\omega_0\tau} \left[ [e^{\mathcal{M}\tau}]_{(12)(12)} - [(\mathbb{I} - e^{\mathcal{M}\tau})\mathcal{M}^{-1}\mathbf{b}]_{(12)} \frac{[\mathcal{M}^{-1}\mathbf{b}]_{(21)}}{[\mathcal{M}^{-1}\mathbf{b}]_{(22)}} \right] \\ g^{(2)}(\tau) &= e^{i\omega_0\tau} \frac{[(\mathbb{I} - e^{\mathcal{M}\tau})\mathcal{M}^{-1}\mathbf{b}]_{(22)}}{[\mathcal{M}^{-1}\mathbf{b}]_{(22)}} \end{aligned}} \quad (15.154)$$



These correlation functions can easily be calculated via a numerical resolution of the Bloch equations (15.142). Fig. 15.13 shows the correlation functions and the fluorescence spectrum derived by Fourier transform of the first-order correlation function (15.84). Assuming resonant excitation,  $\Delta = 0$ , analytic formulas can be derived, as will be exercised in Excs. 15.4.4.3 and Exc. 15.4.4.4.

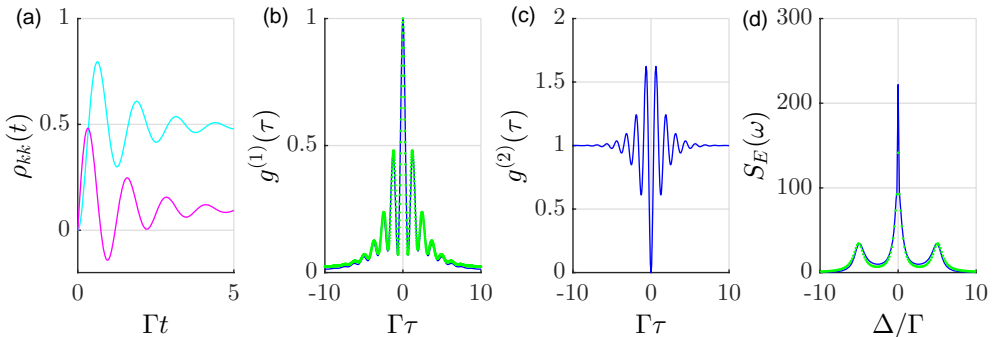


Figure 15.13: (code) (a) Temporal evolution of the excited state population  $\rho_{22}(t)$  (cyan) and coherence  $\rho_{12}(t)$  (magenta) of a laser-driven two-level atom with  $\Omega = 5\Gamma$ . (b) Correlation function  $g^{(1)}(\tau)$  and (c)  $g^{(2)}(\tau)$ . The blue curves in (b-c) are obtained by numerical simulations of the Bloch equations and subsequent application of the quantum regression theorem (15.154). The green dots are obtained from an analytic solution derived in Exc. 15.4.4.3. (d) Mollow spectrum obtained by numerical FFT of  $g^{(1)}(\tau)$ .

The spectrum 15.13(d) exhibits three lines known as the *Mollow triplet*. Note that the spontaneous emission triplet is only observed in the presence of a driving laser, because it is the laser excitation which causes the splitting. Indeed, the splitting and the position of the lines are easily understood in the dressed states picture visualized in Fig. 15.1: The coupling of the two-level atom to a light field splits up the levels  $|n\rangle$  and  $|n+1\rangle$  by an amount corresponding to the Rabi frequency  $\Omega$ . Now, the transition from the two excited state  $|n+1\rangle$  levels to the ground state  $|n\rangle$  levels can occur on three different frequencies. In Exc. 15.4.4.5 we calculate the Mollow spectrum for a transition between one ground and three excited Zeeman states. Fig. 15.14 illustrates the various methods to analyze scattered light, but not all of them yield information on the Mollow triplet.

#### 15.4.3.4 Mollow spectrum from effective Hamiltonian

The Mollow triplet is easily understood in the dressed states picture. On the other hand, we know that (for classical light) the semi-classical picture is totally equivalent (its just a unitary transform of the dressed states picture). Developing a physical picture the Mollow triplet in the semi-classical framework may give us a deeper insight. Generally, the Mollow spectrum is anyhow calculated using the semi-classical Bloch equations, via the correlation function  $g^{(1)}(\tau)$  and the Wiener-Khintchine theorem, but the on the way the physical intuition is lost.

For example, looking at the stationary solution of the Bloch equations (14.99), we see that  $\vec{\rho}(\infty)$  is time-independent, so that we might be *surprised to see correlations*

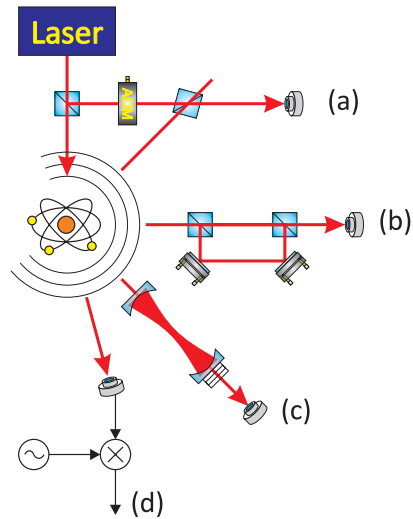


Figure 15.14: Schemes for analyzing resonance fluorescence: (a) Heterodyning [529], (b) temporal correlation, (c) spectrum [650], (d) demodulation. Only the schemes (b) and (c) yield information on the Mollow triplet.

*in time domain* (and consequently a structured spectrum) at all. This surprise results from a common misconception that may arise considering the damping of  $\bar{\rho}(t)$  predicted by the Bloch model, as illustrated e.g. in Fig. 14.2: It seems that the atoms eventually cease oscillating between the ground and excited states. In most experiments, measurement are made on a large number of atoms and indeed the oscillations are damped.

In fact, however, every individual atom undergoes a complicated unpredictable trajectory alternating times of coherent evolution with spontaneous emission events (called quantum jumps). The damped behavior only results as an average over many such quantum trajectories. In this light, the reason for  $g^{(1)}$ -type correlations is a subtle interplay between coherently and incoherently scattered light: *The spontaneous emission probability is amplitude-modulated with the Rabi frequency.*

An alternative way to calculate the Mollow spectrum consists in solving the Schrödinger equation with the effective Hamiltonian, as done in Exc. 15.4.4.2 and 15.4.4.6. The results are shown in Fig. 15.15. While providing an intuitive picture of the origin of the Mollow triplet a quantitatively correct treatment requires a Monte-Carlo wavefunction simulation [496] (see Sec. 16.1.2).

#### 15.4.3.5 Weak excitation and the role of collisions

For the case of a weakly excited two-level atom,  $|\Omega| \ll \Gamma$ , we have analytic solutions (14.105) of the Bloch equation. We can then take the coefficients  $\alpha_{ijkl}$  and  $\beta_{ij}$  and

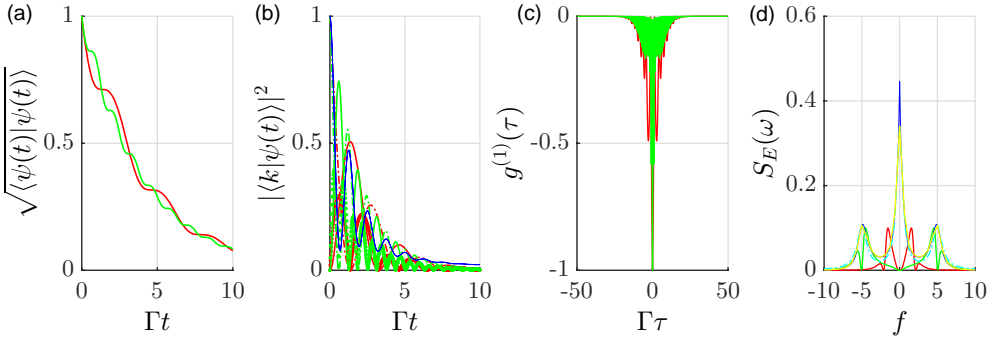


Figure 15.15: (code) (a) Time evolution of the norm of a decaying driven two-level atom. (b) Time evolution of the ground and excited state amplitudes. (c) First-order auto-correlation function, and (d) spectrum.

insert them into the correlation functions,

$$\begin{aligned}
 g^{(1)}(\tau) &= e^{-i\omega\tau} , \\
 g^{(2)}(\tau) &= 1 + e^{-2\gamma\tau} - 2 \cos \Delta\tau , \\
 F(\omega_s) &= (\mathcal{F}g^{(1)})(\omega_s) = \delta(\omega_s - \omega) .
 \end{aligned}
 \tag{15.155}$$

These functions show that the spectrum is essentially composed of *Rayleigh scattering* at the frequency of the incident light. The  $\delta$ -shaped fluorescence spectrum shows, that the contribution of elastically scattered light dominates below saturation, which confirms the results (15.134) illustrated in Fig. 15.12. The light is 'antibunched' and, at higher  $\tau$  exhibits a damped oscillation around the value 1.

If pressure broadening is taken into account, the two-level Bloch equations are given by (14.99), where  $\gamma' = \gamma + \gamma_{coll}$  is the width of the collision-broadened line. Within this model and in the limit  $\Omega \ll \Gamma$ , the resonance fluorescence spectrum is given by [440],

$$F(\omega_s) = \frac{\gamma' - \Gamma}{\gamma'} \frac{\gamma'/\pi}{(\omega_0 - \omega_s)^2 + \gamma'^2} + \frac{\Gamma}{\gamma'} \delta(\omega_s - \omega) .
 \tag{15.156}$$

So, we find that, even at low intensities, a continuous spectrum due to *inelastic scattering* appears around the resonance frequency  $\omega_0$  additionally to the elastic Rayleigh peak.

## 15.4.4 Exercises

### 15.4.4.1 Ex: Derivation of the rate equations for two-level atoms

Inserting the ansatz (15.109) into the Schrödinger equation, derive the equations of motion (15.111) for the wavefunction amplitudes.

**15.4.4.2 Ex: Non-Hermitian time evolution**

Study the time evolution  $|\psi(t)\rangle = e^{-i\hat{H}_{eff}t/\hbar}|\psi(0)\rangle$  with the effective Hamiltonian,

$$\hat{H}_{eff} = \begin{pmatrix} 0 & \frac{\hbar}{2}\Omega \\ \frac{\hbar}{2}\Omega & -\frac{i\hbar}{2}\Gamma \end{pmatrix}$$

starting from the initial condition  $\langle 2|\psi(0)\rangle = 1$ . Calculate the evolution of  $|\psi(t)\rangle$  and the norm  $\langle\psi(t)|\psi(t)\rangle$ . Plot the time evolution of the norm for various ratios  $\Omega/\Gamma$  and interpret the curves.

**15.4.4.3 Ex: Resonance fluorescence and antibunching via Bloch equations**

- Derive the analytic solution of the Bloch equations for a resonantly driven two-level atom.
- Calculate the 1<sup>st</sup>-order correlation function  $g^{(1)}(\tau)$  from the formula (15.154).
- Derive the spectrum of resonance fluorescence [495].
- Derive the 2<sup>nd</sup>-order correlation function  $g^{(2)}(\tau)$  from the formula (15.154).

**15.4.4.4 Ex: Resonance fluorescence via rate equations**

Repeat Exc. 15.4.4.3 neglecting coherences, i.e. replacing the Bloch equations by rate equations,

$$\dot{\vec{\rho}} = \begin{pmatrix} -R & R + \Gamma & 0 & 0 \\ R & -R - \Gamma & 0 & 0 \\ 0 & 0 & -\gamma & 0 \\ 0 & 0 & 0 & -\gamma \end{pmatrix} \vec{\rho},$$

where  $R = \Omega^2/2\gamma$  is the pump rate.

**15.4.4.5 Ex: Fluorescence spectrum of a four-level system**

A more realistic transition, allowing for a vectorial nature of the radiation field, involves one ground and three excited Zeeman states (e.g. the strontium  $^1S_0$ - $^1P_1$  transition). In this case, the emitted light is,

$$\hat{\mathcal{E}}^-(t) = \hat{\mathcal{E}}_{\sigma^-}^-(t) + \hat{\mathcal{E}}_{\pi}^-(t) + \hat{\mathcal{E}}_{\sigma^+}^-(t).$$

Calculate the first-order correlation function and the fluorescence spectrum of this transition.

**15.4.4.6 Ex: Semi-classical picture of the Mollow triplet**

Calculate the first-order correlation function from the solution of the Schrödinger equation with the effective Hamiltonian derived in Exc. 15.4.4.2.

**15.4.4.7 Ex: Monte-Carlo simulation of the Mollow triplet**

Implement a Monte-Carlo simulation of the Mollow triplet for a driven two-level atom according to [167, 496].

## 15.5 Light scattering from multi-level atoms

### 15.5.1 Quantum beats

The phenomenon of *quantum beats* is another simple example of effects beyond semi-classical theory, requiring a full second-quantized calculation. In semi-classical theory (SCT), there is an interference or beat note term for both V-type and  $\Lambda$ -type atoms, while in quantum electrodynamics (QED) only V-type atoms exhibits a beat term.

In the semi-classical picture, the state vector of electrons is [626],

$$\psi(t) = c_1 e^{-i\omega_1 t} |1\rangle + c_2 e^{-i\omega_2 t} |2\rangle + c_3 e^{-i\omega_3 t} |3\rangle. \quad (15.157)$$

Writing the non-vanishing dipole matrix elements as  $d_{12} = e\langle 1|r|2\rangle$ ,  $d_{23} = e\langle 2|r|3\rangle$  a three-level atom has two microscopic oscillating dipoles,

$$P(t) = d_{12}(c_1^* c_2) e^{i\omega_{12} t} + d_{23}(c_2^* c_3) e^{i\omega_{23} t} + c.c. . \quad (15.158)$$

In the semi-classical picture, the radiated field will be a sum of these two terms,

$$\mathcal{E}^+ = \mathcal{E}_1 e^{-i\omega_{12} t} + \mathcal{E}_2 e^{-i\omega_{23} t}. \quad (15.159)$$

This leads to an interference or beat note term in a square-law detector,

$$|\mathcal{E}^+|^2 = |\mathcal{E}_{12}|^2 + |\mathcal{E}_{23}|^2 + \mathcal{E}_{12}^* \mathcal{E}_{23} e^{i(\omega_{12} - \omega_{23})t} + c.c. , \quad (15.160)$$

regardless of whether state  $|2\rangle$  decays simultaneously to  $|1\rangle$  and  $|3\rangle$  or vice versa.

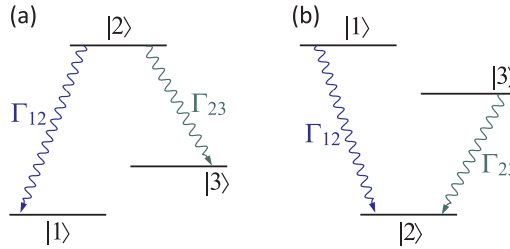


Figure 15.16: Level configuration of a  $\Lambda$ -system (left) and a V-system (right).

#### 15.5.1.1 Quantum electrodynamics calculation

For the quantum electrodynamical calculation, we use the creation and annihilation operators from second quantization of quantum mechanics. Let  $\hat{\mathcal{E}}_n^+ = \hat{a}_n e^{-i\omega_n t}$  be the annihilation operator and  $\hat{\mathcal{E}}_n^- = \hat{a}_n^\dagger e^{i\omega_n t}$  be the creation operator with  $n = (12)$  or  $n = (23)$ . Then the beat note becomes,

$$\langle \psi_V(t) | \hat{\mathcal{E}}_{12}^-(t) \hat{\mathcal{E}}_{23}^+(t) | \psi_V(t) \rangle \quad \text{and} \quad \langle \psi_\Lambda(t) | \hat{\mathcal{E}}_{12}^-(t) \hat{\mathcal{E}}_{23}^+(t) | \psi_\Lambda(t) \rangle \quad (15.161)$$

for the  $\Lambda$  and the V-system, respectively. The state vector for each type of system is,

$$|\psi_V(t)\rangle = \sum_{i=1,2,3} c_i |i, 0\rangle + c_1 |c, 1_{12}\rangle + c_2 |c, 1_{23}\rangle \quad (15.162)$$

and,

$$|\psi_\Lambda(t)\rangle = \sum_{i=1,2,3} c'_i |i, 0\rangle + c'_1 |b, 1_{12}\rangle + c'_2 |c, 1_{23}\rangle . \quad (15.163)$$

The beat note term becomes,

$$\begin{aligned} \langle \psi_V(t) | \hat{\mathcal{E}}_1^-(t) \hat{\mathcal{E}}_2^+(t) | \psi_V(t) \rangle &= \kappa \langle 1_{12} 0_{23} | a_1^\dagger a_2 | 0_{12} 1_{23} \rangle e^{i(\omega_{12} - \omega_{23})t} \langle 3|3 \rangle \\ &= \kappa e^{i(\omega_{12} - \omega_{23})t} \langle 3|3 \rangle \end{aligned} \quad (15.164)$$

for the  $V$ -system and

$$\begin{aligned} \langle \psi_\Lambda(t) | \hat{\mathcal{E}}_1^-(t) \hat{\mathcal{E}}_2^+(t) | \psi_\Lambda(t) \rangle &= \kappa' \langle 1_{12} 0_{23} | a_1^\dagger a_2 | 0_{12} 1_{23} \rangle e^{i(\omega_{12} - \omega_{23})t} \langle 2|3 \rangle \\ &= \kappa' e^{i(\omega_{12} - \omega_{23})t} \langle 2|3 \rangle \end{aligned} \quad (15.165)$$

for the  $\Lambda$ -system. However, orthogonality of the eigenstates requires  $\langle 3|3 \rangle = 1$  and  $\langle 2|3 \rangle = 0$ . Therefore, there is a quantum beat note term for  $V$ -type atoms, but not for  $\Lambda$ -type atoms.

This difference originates in quantum mechanical uncertainty. A  $V$ -type atom decays to state  $|3\rangle$  via the emission with  $\omega_{12}$  and  $\omega_{23}$ . Since both transitions decayed to the same state, one cannot determine along which path each decayed, similar to Young's double-slit experiment. However,  $\Lambda$ -type atoms decay to two different states. Therefore, in this case we can identify the path by the end product.

Quantum beat spectroscopy is a technique which allows for Doppler-free resolution provided the separation of the adjacent levels is less than the Doppler width. It consists in generating a coherently distributed population of two upper states, e.g. via a short laser pulse, and detecting the beat frequency.

## 15.5.2 Two-photon transitions

We will now apply the *Kramers-Heisenberg formula* (6.112) to photon scattering processes  $\omega \rightarrow \omega_s$ . The states are then product states of atomic excitations and photonic modes  $|m, n, n_s\rangle$ . In particular, the final state must take into account the mode into which light is scattered,

$$\begin{aligned} \frac{1}{\tau} &= \frac{2\pi}{\hbar^2} \sum_f \sum_{\mathbf{k}_s} \left| \langle f, n-1, 1 | \hat{H}^{(2)} | i, n, 0 \rangle \right. \\ &\quad \left. + \frac{1}{\hbar} \sum_m \frac{\langle f, n-1, 1 | \hat{H}^{(1)} | m \rangle \langle m | \hat{H}^{(1)} | i, n, 0 \rangle}{\omega_i - \omega_m} \right|^2 \delta(\omega_f - \omega_i) . \end{aligned} \quad (15.166)$$

The initial energy is  $\omega_i \rightarrow n\omega$ , the final energy  $\omega_f \rightarrow (n-1)\omega + \omega_s + \omega_f$ , two intermediate states are possible,  $|m\rangle \rightarrow |m, n-1, 0\rangle$  and  $|m\rangle \rightarrow |m, n, 1\rangle$  over which we must sum, that is  $\omega_m \rightarrow \omega_m + (n-1)\omega$  and  $\omega_m \rightarrow \omega_m + n\omega + \omega_s$ . They are illustrated by the Feynman diagrams in Fig. xx. Hence, and neglecting the non-linear

contribution  $\hat{H}^{(2)}$ ,

$$\frac{1}{\tau} = \frac{2\pi}{\hbar^3} \sum_f \sum_{\mathbf{k}_s} \left| \sum_m \frac{\langle f, n-1, 1 | \hat{H}^{(1)} | m, n, 0 \rangle \langle m, n, 0 | \hat{H}^{(1)} | i, n, 0 \rangle}{\omega - \omega_m} \right. \quad (15.167)$$

$$\left. + \frac{\langle f, n-1, 1 | \hat{H}^{(1)} | m, n-1, 1 \rangle \langle m, n-1, 1 | \hat{H}^{(1)} | i, n, 0 \rangle}{-\omega_m - \omega_s} \right|^2 \delta(\omega_f - \omega + \omega_s) .$$

Evaluated far from resonance,  $\omega \gg \omega_m$ , this result leads to Thomson and Compton scattering. Close to resonance the second term of the sum may be neglected.

The matrix elements can be evaluated by the electric dipole Hamiltonian in second quantization,

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \sum_{\mathbf{k}_s} \left| \sum_m \frac{\Omega_{fm} \Omega_{mi}}{\omega - \omega_m} \right|^2 \delta(\omega_f - \omega + \omega_s) . \quad (15.168)$$

We convert the transition rate into a cross section via,

$$\sum_{\mathbf{k}_s} \rightarrow \frac{V}{(2\pi)^3} \int \int k_s^2 dk_s d\Omega = \frac{V}{(2\pi c)^3} \int \int \omega_s^2 d\omega_s d\Omega . \quad (15.169)$$

### 15.5.2.1 Transition rates for $n$ -photon processes

It is adequate to move to a continuum of final states of the field. The sum over the final states includes a sum over the modes  $\mathbf{k}$  and the polarizations  $\lambda$ ,

$$\sum_f = \sum_{\mathbf{k}} \sum_{\lambda} \rightarrow \frac{1}{h^3} \int_{\mathbb{R}^6} d^3 p d^3 r \sum_{\lambda} = \frac{V}{(2\pi c)^3} \int_{\Omega} d\Omega d\omega \omega^2 \sum_{\lambda} . \quad (15.170)$$

We now insert for the matrix element (first term in ()) the cartesian multipole expansion () and obtain,

$$\frac{1}{\tau} = \frac{2\pi}{\hbar^2} \sum_f \left| \langle f | -ie \sqrt{\frac{\hbar\omega}{2\varepsilon_0 V}} [\hat{\varepsilon} \cdot \mathbf{d}_E + \dots] | i \rangle \right|^2 \delta(\omega - \omega_f) \sum_{\lambda} \quad (15.171)$$

$$\rightarrow \frac{2\pi}{\hbar^2} \frac{V}{(2\pi c)^3} \frac{e^2 \hbar \omega}{2\varepsilon_0 V} \omega^2 \sum_{\lambda} \int |\hat{\varepsilon} \cdot \langle g | \mathbf{d}_E | e \rangle + i \hat{\varepsilon} \cdot \langle g | \mathbf{q}_E | e \rangle \cdot \mathbf{k} \dots - \dots|^2 d\Omega .$$

Finally, letting  $\sum_{\lambda} = 2$ ,

$$\frac{1}{\tau} = \frac{\alpha \omega^3}{\pi c^2} \int |\hat{\varepsilon} \cdot \langle g | \text{multipole-tensor} | e \rangle \text{wavenumber-tensor}|^2 d\Omega . \quad (15.172)$$

For example, for dipole radiation, letting  $\hat{\varepsilon} = \hat{\mathbf{e}}_z$ ,

$$\frac{1}{\tau} = \frac{\alpha \omega^3}{\pi c^2} \int |\hat{\varepsilon} \cdot \langle g | \mathbf{d}_E | e \rangle|^2 d \cos \theta d\phi \quad (15.173)$$

$$= \frac{\alpha \omega^3}{\pi c^2} |\langle g | \mathbf{d}_E | e \rangle|^2 \int |\cos \theta|^2 d \cos \theta d\phi = \frac{4\alpha \omega^3}{3c^2} |\langle g | \mathbf{d}_E | e \rangle|^2 .$$

15.5.2.2 Absorption

In first order perturbation theory we have Fermi's Golden rule,

$$\frac{1}{\tau} = \frac{2\pi}{\hbar^2} \sum_f |\langle f | \hat{H}_{int} | i \rangle|^2 \delta(\omega_f - \omega_i) . \tag{15.174}$$

In the dipolar approximation,  $\hat{H}_{int} = -\mathbf{d} \cdot \vec{\mathcal{E}}$ , and separating the field and atomic degrees of freedom,  $|f\rangle = |N_f\rangle |A_f\rangle$ , we get for absorption processes,

$$\frac{1}{\tau} = \frac{2\pi e^2}{\hbar^2} \sum_{N_f} \left| \langle N_f | \hat{\mathcal{E}}^- | N_i \rangle \cdot \langle A_f | \hat{\mathcal{E}} \cdot \hat{\mathbf{d}} | A_i \rangle \right|^2 \delta(\omega_f - \omega_i) . \tag{15.175}$$

Generalizing to a statistical mixture of Fock states via  $\sum_{N_f, N_i} \langle N_i | \hat{E}^+ | N_f \rangle p_i \langle N_f | \hat{E}^- | N_i \rangle = \text{Tr}(\hat{\rho} \hat{\mathcal{E}}^+ \hat{\mathcal{E}}^-)$ , we may also write,

$$\frac{1}{\tau} = \frac{2\pi e^2}{\hbar^2} |M_{abs}|^2 \delta(\omega_f - \omega_i) \text{Tr}(\hat{\rho} \hat{\mathcal{E}}^+ \hat{\mathcal{E}}^-) , \tag{15.176}$$

where

$$|M_{abs}|^2 \equiv \langle A_f | \hat{\mathcal{E}} \cdot \hat{\mathbf{d}} | A_i \rangle . \tag{15.177}$$

For an incoming photon  $\omega$ , we get  $\omega_f = E_f$  and  $\omega_i = E_i + \omega$ . See Fig. 15.17(a).

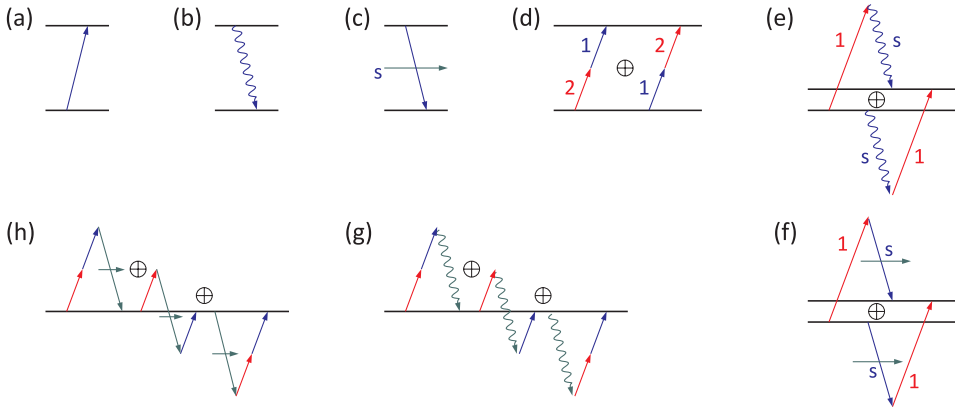


Figure 15.17: Feynman graphs for (a) absorption, (b) spontaneous emission, (c) stimulated emission, (d) two-photon absorption, (e) spontaneous Raman, (f) stimulated Raman, (g) spontaneous second harmonic generation, (h) and stimulated second harmonic generation.

15.5.2.3 Spontaneous and stimulated emission

In complete analogy to the absorption process, but now using the scattered field,  $\hat{H}_{int} = -\mathbf{d} \cdot \vec{\mathcal{E}}_s$ , we get for emission processes,

$$\frac{1}{\tau} = \frac{2\pi e^2}{\hbar^2} |M_{em}|^2 \delta(\omega_f - \omega_i) \text{Tr}(\hat{\rho} \hat{\mathcal{E}}_s^+ \hat{\mathcal{E}}_s^-) , \tag{15.178}$$



where

$$|M_{em}|^2 \equiv \langle A_f | \hat{\varepsilon}_s \cdot \hat{\mathbf{d}} | A_i \rangle . \quad (15.179)$$

For an outgoing photon  $\omega_s$ , we get  $\omega_f = E_f + \omega_s$  and  $\omega_i = E_i$ .

#### 15.5.2.4 Two-photon absorption

In second order perturbation theory we have the Kramers-Heisenberg rule,

$$\frac{1}{\tau} = \frac{2\pi}{\hbar^2} \sum_f \left| \sum_m \frac{\langle f | \hat{H}_{int} | m \rangle \langle m | \hat{H}_{int} | i \rangle}{\omega - \omega_m} \right|^2 \delta(\omega_f - \omega_i) . \quad (15.180)$$

In the dipolar approximation,  $\hat{H}_{int} = -\mathbf{d} \cdot \hat{\mathcal{E}}_1 - \mathbf{d} \cdot \hat{\mathcal{E}}_2$ , and separating the field and atomic degrees of freedom,  $|f\rangle = |N_f\rangle |A_f\rangle$ , we get for two-photon absorption processes,

$$\begin{aligned} \frac{1}{\tau} = & \frac{2\pi e^4}{\hbar^4} \sum_{N_f} \left| \sum_{N_m, A_m} \frac{\langle N_f | \mathcal{E}_2^- | N_m \rangle \langle N_m | \mathcal{E}_1^- | N_i \rangle \langle A_f | \hat{\varepsilon}_2 \cdot \hat{\mathbf{d}} | A_m \rangle \langle A_m | \hat{\varepsilon}_1 \cdot \hat{\mathbf{d}} | A_i \rangle}{\omega_1 - \omega_m} \right. \\ & \left. + \frac{\langle N_f | \mathcal{E}_1^- | N_m \rangle \langle N_m | \mathcal{E}_2^- | N_i \rangle \langle A_f | \hat{\varepsilon}_1 \cdot \hat{\mathbf{d}} | A_m \rangle \langle A_m | \hat{\varepsilon}_2 \cdot \hat{\mathbf{d}} | A_i \rangle}{\omega_2 - \omega_m} \right|^2 \delta(\omega_f - \omega_1 - \omega_2) . \end{aligned} \quad (15.181)$$

Generalizing to a statistical mixture of Fock states via  $\sum_{N_f, N_i} p_i \langle N_f | \hat{\mathcal{E}}_2^- \hat{\mathcal{E}}_1^- | N_i \rangle = \text{Tr}(\hat{\rho} \hat{\mathcal{E}}_1^+ \hat{\mathcal{E}}_2^+ \hat{\mathcal{E}}_2^- \hat{\mathcal{E}}_1^-)$ , we may also write,

$$\frac{1}{\tau} = \frac{2\pi e^4}{\hbar^4} |M_{tpa}|^2 \delta(\omega_f - \omega_i) \text{Tr}(\hat{\rho} \hat{\mathcal{E}}_1^+ \hat{\mathcal{E}}_2^+ \hat{\mathcal{E}}_2^- \hat{\mathcal{E}}_1^-) , \quad (15.182)$$

where

$$M_{tpa} \equiv \langle A_f | \hat{\varepsilon}_2 \cdot \hat{\mathbf{d}} G(E_i + \omega_1) \hat{\varepsilon}_1 \cdot \hat{\mathbf{d}} | A_i \rangle + \langle A_f | \hat{\varepsilon}_1 \cdot \hat{\mathbf{d}} G(E_i + \omega_2) \hat{\varepsilon}_2 \cdot \hat{\mathbf{d}} | A_i \rangle . \quad (15.183)$$

For two incoming photons  $\omega$ , we get  $\omega_f = E_f$  and  $\omega_i = E_i + \omega_1 + \omega_2$ . Here,  $G$  denotes the *photon propagator*,

$$G(\omega) = \sum_m \frac{|A_m\rangle \langle A_m|}{\omega - E_m} . \quad (15.184)$$

#### 15.5.2.5 Spontaneous and stimulated Raman process

In complete analogy to the two-photon absorption process, but now using the incident and the scattered fields,  $\hat{H}_{int} = -\mathbf{d} \cdot \hat{\mathcal{E}}_1 - \mathbf{d} \cdot \hat{\mathcal{E}}_s$ , we get for spontaneous and stimulated Raman processes,

$$\frac{1}{\tau} = \frac{2\pi e^4}{\hbar^4} |M_{ram}|^2 \delta(\omega_f - \omega_i) \text{Tr}(\hat{\rho} \hat{\mathcal{E}}_1^+ \hat{\mathcal{E}}_s^- \hat{\mathcal{E}}_s^+ \hat{\mathcal{E}}_1^-) , \quad (15.185)$$

where

$$M_{ram} \equiv \langle A_f | \hat{\varepsilon}_s \cdot \hat{\mathbf{d}} G(E_i + \omega_1) \hat{\varepsilon}_1 \cdot \hat{\mathbf{d}} | A_i \rangle + \langle A_f | \hat{\varepsilon}_1 \cdot \hat{\mathbf{d}} G(E_i - \omega_s) \hat{\varepsilon}_s \cdot \hat{\mathbf{d}} | A_i \rangle . \quad (15.186)$$

For an incoming photon  $\omega_1$  and a scattered photon  $\omega_s$ , we get  $\omega_f = E_f + \omega_s$  and  $\omega_i = E_i + \omega_1$ .

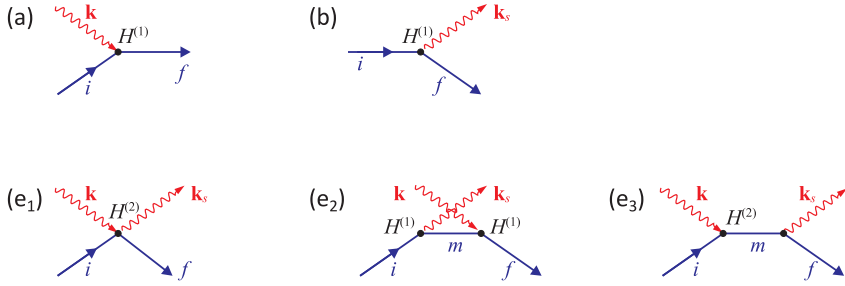


Figure 15.18: Feynman graphs for (a) absorption, (b) spontaneous emission, (c) stimulated emission, (e)(i-iii) spontaneous Raman.

### 15.5.2.6 General $n$ -photon processes

The transition probability in  $n$ -th order perturbation theory can be formulated in a general way as,

$$\frac{1}{\tau} = \frac{2\pi e^2}{\hbar^{2n}} |M_{fi}^{(n)}|^2 \delta(\omega_f - \omega_i) \text{Tr} (\hat{\rho} \hat{\mathcal{E}}_1^\pm \hat{\mathcal{E}}_2^\pm \dots \hat{\mathcal{E}}_2^\mp \hat{\mathcal{E}}_1^\mp), \quad (15.187)$$

where

$$\begin{aligned} M_{fi}(\omega_n, \dots, \omega_1) \equiv & \mathcal{S}_p \langle A_f | \hat{\varepsilon}_n \hat{\mathbf{d}} G(E_i \pm \omega_1 \pm \dots \pm \omega_{n-2} \pm \omega_{n-1}) \dots \\ & \dots \hat{\varepsilon}_{n-1} \hat{\mathbf{d}} G(E_i \pm \omega_1 \pm \dots \pm \omega_{n-2}) \dots \\ & \dots \hat{\varepsilon}_1 \cdot \hat{\mathbf{d}} G(E_i \pm \omega_1) | A_i \rangle. \end{aligned} \quad (15.188)$$

The upper signs hold for absorbed photons (up to  $n$ ), the lower for emitted photons,  $\omega_f = E_f + \omega_1 + \dots + \omega_n$  and  $\omega_i = E_i + \omega_1 + \dots + \omega_n$ .

For  $n$ -photon processes, there are theoretically up to  $n + 1$  different types, each one with  $n!$  possible temporal sequences, which can be illustrated in Feynman graphs. Additionally, for every emitted photon can be either spontaneous or stimulated. The number of possible time sequences is reduced, if some absorbed or emitted photons have the same frequency by  $m!$  (if  $m$  is the number of identical photons).

For example there are  $(3+1)$  different types of three-photon processes: 3 photons in, 2 photons in 1 out, 1 photon in 2 out, 3 photons out.

For example second harmonic generation:  $3!$  possible time sequences, 2 processes, 2 equivalent photons =  $\frac{3!2}{2!}$  possible Feynman graphs.

## 15.5.3 Exercises

### 15.5.3.1 Ex: Two-photon transitions in rubidium

Considering the following transitions of rubidium,  $5S_{1/2} - 5P_{1/2}$  at 795 nm with  $\Gamma_{795} = (2\pi) 6$  MHz linewidth  $5S_{1/2} - 5P_{3/2}$  at 780 nm with  $\Gamma_{780} = (2\pi) 6$  MHz, and  $5P_{3/2} - 5D_{5/2}$  at 776 nm with  $\Gamma_{776} = (2\pi) 700$  kHz linewidth. Calculate the rate for resonant two-photon transitions from the ground state to the  $5D_{5/2}$  level without bothering about hyperfine splitting induced by a laser intensity of  $I = 1$  mW/cm<sup>2</sup>.

### 15.5.3.2 Ex: Spin relaxation in a dipole trap

Consider a transition in a hypothetical atomic species without nuclear spin between two levels  ${}^2S_{1/2}$  and  ${}^2P_{1/2}$  driven far-off resonance. Calculate the spin relaxation rate as a function of the detuning.

### 15.5.3.3 Ex: Rayleigh scattering and spin relaxation

Derive the rates for Rayleigh scattering and spin relaxation for  ${}^{87}\text{Rb}$  driven far-off resonance. **Help:** Determine the hyperfine structure of the D1 and D2 lines and calculate the transition rates between sublevels from the Kramers-Heisenberg formula.

## 15.6 Beam splitting and quantum amplification

We have learned in Sec. 15.2 how a two-level quantum systems couples to a harmonic oscillator via terms in the Hamiltonian containing expressions such as  $\hat{\sigma}_+ \hat{a}$ . We will now see how two quantum harmonic oscillators couple together via terms such as  $\hat{a}^\dagger \hat{b}$ , where  $\hat{a}$  and  $\hat{b}$  are the field operators of two oscillator modes. A device providing such a coupling is called *beam splitter*. It *mixes two modes* according to the Hamiltonian,

$$\hat{H} = \frac{\hbar}{2} \Omega (\hat{a} \hat{b}^\dagger + \hat{a}^\dagger \hat{b}) . \quad (15.189)$$

The beam splitter can be described in the Schrödinger or the Heisenberg picture exploiting the formalism introduced in Sec. 3.5.

### 15.6.1 The beam splitter in various representations

#### 15.6.1.1 Schrödinger picture

In the Schrödinger picture, if  $|\psi_0\rangle = |\alpha_0\rangle|\beta_0\rangle$  is the state of the modes before the beam splitter, the Schrödinger equation,  $i\hbar\partial_t|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$ , gives us the state after the splitter via its solution,

$$|\psi(t)\rangle = e^{i\Omega t/2(\hat{a}\hat{b}^\dagger + \hat{a}^\dagger\hat{b})} |\psi_0\rangle . \quad (15.190)$$

A 50% beam splitter corresponds to a  $\Omega t = \pi/2$  pulse.

#### 15.6.1.2 Heisenberg picture

We can also describe the beam splitter in the Heisenberg picture. With the commutation rules,

$$[\hat{a}, \hat{a}^\dagger] = 1 = [\hat{b}, \hat{b}^\dagger] \quad , \quad [\hat{a}, \hat{b}] = 0 \quad , \quad (15.191)$$

and the Heisenberg equations,

$$\begin{aligned} \dot{\hat{a}} &= \frac{i}{\hbar} [\hat{H}, \hat{a}] = \frac{i}{2} \Omega [(\hat{a}\hat{b}^\dagger + \hat{a}^\dagger\hat{b}), \hat{a}] = -\frac{i}{2} \Omega \hat{b} \\ \dot{\hat{b}} &= \frac{i}{\hbar} [\hat{H}, \hat{b}] = \frac{i}{2} \Omega [(\hat{a}\hat{b}^\dagger + \hat{a}^\dagger\hat{b}), \hat{b}] = -\frac{i}{2} \Omega \hat{a} \quad , \end{aligned} \quad (15.192)$$

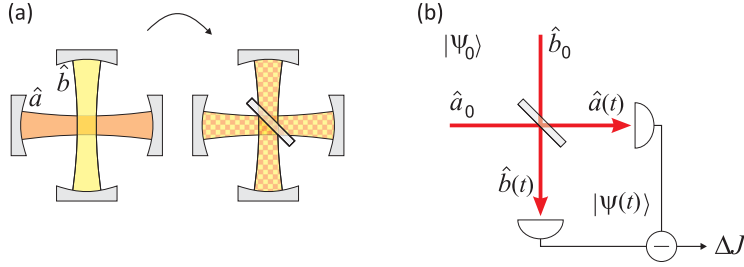


Figure 15.19: (a) Coupling of two cavity modes by insertion of a beam splitter. (b) Beam splitter mixing two propagating modes.

we calculate,

$$\ddot{\hat{a}} = -\frac{1}{4}\Omega^2\hat{a} \quad \text{and} \quad \ddot{\hat{b}} = -\frac{1}{4}\Omega^2\hat{b}, \quad (15.193)$$

the solution of which is,

$$\begin{pmatrix} \hat{a}(t) \\ \hat{b}(t) \end{pmatrix} = \begin{pmatrix} \cos \frac{1}{2}\Omega t & -i \sin \frac{1}{2}\Omega t \\ -i \sin \frac{1}{2}\Omega t & \cos \frac{1}{2}\Omega t \end{pmatrix} \begin{pmatrix} \hat{a}_0 \\ \hat{b}_0 \end{pmatrix}. \quad (15.194)$$

Introducing the abbreviation  $\eta \equiv \cos^2(\Omega t/2)$ , we can describe the evolution as,

$$\boxed{\begin{pmatrix} \hat{a}(t) \\ \hat{b}(t) \end{pmatrix} = \begin{pmatrix} \sqrt{\eta} & -i\sqrt{1-\eta} \\ -i\sqrt{1-\eta} & \sqrt{\eta} \end{pmatrix} \begin{pmatrix} \hat{a}_0 \\ \hat{b}_0 \end{pmatrix}}. \quad (15.195)$$

For a  $\Omega t = \pi/2$  pulse, we get,

$$\begin{pmatrix} \hat{a}(t) \\ \hat{b}(t) \end{pmatrix} = \sqrt{\frac{1}{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \begin{pmatrix} \hat{a}_0 \\ \hat{b}_0 \end{pmatrix}. \quad (15.196)$$

that each the reflected beam suffers a phase shift of  $\pi/2$ <sup>11</sup>. Resolve the Excs. 15.6.8.1 to 15.6.8.4.

### 15.6.1.3 Glauber representation

In the Heisenberg picture, the wavefunctions of the quantum states (and hence the density operator and the Wigner function) remain unchanged during the evolution, i.e.,

$$|\psi\rangle \equiv |\alpha\rangle|\beta\rangle = |\alpha_0\rangle|\beta_0\rangle \equiv |\psi_0\rangle, \quad (15.197)$$

$$\begin{aligned} \rho_{|\psi\rangle} &= \rho_{|\psi_0\rangle}, \\ W_{|\psi\rangle}(\gamma) &= W_{|\psi_0\rangle}(\gamma), \\ P_{|\psi\rangle}(\gamma) &= P_{|\psi_0\rangle}(\gamma), \\ Q_{|\psi\rangle}(\gamma) &= Q_{|\psi_0\rangle}(\gamma), \end{aligned}$$

<sup>11</sup>This fact is a consequence of *time-reversal invariance* at the beam splitter. We will see later that, in fact, only the beam reflected at the surface of an optically denser medium suffers a phase-shift of  $\pi$ , while the beam reflected at an optically thinner medium does not suffer any phase shift.

where the  $|\psi\rangle$  are arbitrary quantum states and the  $|\gamma\rangle$  are Glauber's states. This means that two field modes mixed at a beam splitter do not interfere with phase space, i.e. do not develop quantum correlations. Of course, that would be too easy, indeed; we will soon see in Sec. 3.8, that we need to work a little harder to produce quantum correlations.

Setting  $\theta \equiv \Omega t/2$  and  $\hat{b} \rightsquigarrow -i\hat{b}$  in the propagator of Eq. (15.190), we may define a beam splitting operator in analogy to the displacement operator (3.109),

$$\boxed{\hat{B}(\theta) \equiv e^{\theta(\hat{a}^\dagger \hat{b} - \hat{a} \hat{b}^\dagger)}}, \quad (15.198)$$

which is an equivalent beam splitter description. We find,

$$\boxed{\begin{aligned} \hat{B}(\theta)^\dagger \hat{a} \hat{B}(\theta) &= \hat{a} \cos \theta + \hat{b} \sin \theta \\ \hat{B}(\theta)^\dagger \hat{b} \hat{B}(\theta) &= -\hat{a} \sin \theta + \hat{b} \cos \theta \end{aligned}}, \quad (15.199)$$

as will be shown in Exc. 15.6.8.3<sup>12</sup>.

#### 15.6.1.4 Fock representation

Alternatively, we can describe the beam splitter in the Fock representation<sup>13</sup>. The Hamiltonian of the beam splitter couples two modes of harmonic oscillators. Expanding on a two-dimensional Fock basis via  $|\psi\rangle \equiv (\dots|0\rangle|n_a\rangle\dots|n_b\rangle|0\rangle\dots)$  we can gain more insight:

$$\begin{aligned} \hat{H} &= \frac{\hbar}{2}\Omega(\hat{a}\hat{b}^\dagger + \hat{a}^\dagger\hat{b}) \\ &= \frac{\hbar}{2}\Omega \sum_{n_a, n_b} \sqrt{n_a(n_b+1)}|n_a-1, n_b+1\rangle\langle n_a, n_b| + \sqrt{(n_a+1)n_b}|n_a+1, n_b-1\rangle\langle n_a, n_b| \\ &= \sum_{n_a+n_b} \hat{H}_{a+b}, \end{aligned} \quad (15.200)$$

where,

$$\hat{H}_{a+b} = \frac{\hbar}{2}\Omega \begin{pmatrix} 0 & \sqrt{1n_b} & & & & \\ \sqrt{1n_b} & 0 & \sqrt{2(n_b-1)} & & & \\ & \sqrt{2(n_b-1)} & \ddots & & & \\ & & & \ddots & & \\ & & & & \ddots & \sqrt{n_a 1} \\ & & & & \sqrt{n_a 1} & 0 \end{pmatrix}. \quad (15.201)$$

The sub-spaces with  $n_a + n_b + 1$  photons are completely degenerate, since  $\det(\lambda \mathbb{I}_{a+b} - \hat{H}_{a+b}) = \lambda^{n_a+n_b+1} = 0$ . The degeneracy is removed, when we introduce loss mechanisms into one of the modes. Thus, the Hamiltonian can be understood as a Dicke system with the multiplicity  $\frac{1}{2}(n_a + n_b) = n_a + n_b + 1$ . See also Exc. 15.6.8.5.

<sup>12</sup>Compare to the formulas (3.116), (3.218), and (15.242).

<sup>13</sup>A more in-depth discussion is found in Ref. [429].

**Example 70 (Beam splitter with 0 or 1 photons):** As an example, we consider  $n_a, n_b = 0, 1$ . Then, in the basis  $(|0, 0\rangle \quad |0, 1\rangle \quad |1, 0\rangle \quad |0, 2\rangle \quad |1, 1\rangle \quad |2, 0\rangle \quad \dots)^t$  the matrix of the Hamiltonian becomes,

$$\hat{H} = \frac{1}{2}\Omega \begin{pmatrix} 0 & & & & & & \\ & 0 & 1 & & & & \\ & 1 & 0 & & & & \\ & & & 0 & \sqrt{2} & 0 & \\ & & & \sqrt{2} & 0 & \sqrt{2} & \\ & & & 0 & \sqrt{2} & 0 & \end{pmatrix}.$$

It is easily verified that the matrix of eigenvectors and the matrix of eigenvalues,

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2}\sqrt{2} & -1 & \frac{1}{2}\sqrt{2} \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & -\frac{1}{2}\sqrt{2} & 1 & \frac{1}{2}\sqrt{2} \end{pmatrix} \quad \text{respectively} \quad E = \frac{\hbar}{2}\Omega \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

satisfy  $U^{-1}HU = E$ . Hence,

$$|\psi\rangle = U^{-1}e^{iEt}U|\psi_0\rangle,$$

and we find, that the state  $|1, 1\rangle = (0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0)^T$  is transformed into a superposition,

$$\begin{pmatrix} 0 & 0 & 0 & \frac{1}{\sqrt{2}}i \sin \Omega t & \cos \Omega t & \frac{1}{\sqrt{2}}i \sin \Omega t \end{pmatrix}^T \xrightarrow{\Omega t = \pi/2} \frac{i}{\sqrt{2}}(|0, 2\rangle + |2, 0\rangle).$$

Similarly, we find that the superposition state  $\frac{1}{\sqrt{2}}(|1, 0\rangle + |0, 1\rangle) = (0 \quad 1 \quad -1 \quad 0 \quad 0 \quad 0)^T$  is transformed into,

$$e^{-\frac{1}{2}i\Omega t} \begin{pmatrix} 0 & 1 & -1 & 0 & 0 & 0 \end{pmatrix}^T \xrightarrow{\Omega t = \pi/2} e^{-i\pi/4} \frac{1}{\sqrt{2}}(|1, 0\rangle + |0, 1\rangle).$$

### 15.6.2 Fock and Glauber states at a beam splitter

A beam splitter divides a Fock state containing  $N$  photons into two Glauber states,

$$\begin{aligned} |\psi\rangle &= \frac{1}{2^{N/2}\sqrt{N!}}(\hat{a}_1^\dagger + \hat{a}_2^\dagger)^N|0, 0\rangle = \frac{1}{2^{N/2}\sqrt{N!}} \sum_{n=0}^N \binom{N}{n} (\hat{a}_1^\dagger)^n (\hat{a}_2^\dagger)^{N-n}|0, 0\rangle \quad (15.202) \\ &= \frac{1}{2^{N/2}} \sum_{n=0}^N \sqrt{\binom{N}{n}} |n, N-n\rangle = \sum_{n=0}^N \sqrt{\binom{N}{n}} 0.5^n 0.5^{N-n} |n, N-n\rangle \\ &\simeq \sum_{n=0}^N \sqrt{\frac{(N/2)^n}{n!}} e^{-N/2} |n, N-n\rangle = e^{-|\alpha|/2} \sum_{n=0}^N \frac{\alpha^n}{\sqrt{n!}} |n, N-n\rangle, \end{aligned}$$

approximating the binomial distribution by the Poisson distribution,

$$\binom{N}{n} p^n (1-p)^{N-n} \xrightarrow{N \rightarrow \infty} \frac{(pN)^n}{n!} e^{-pN}. \quad (15.203)$$

and defining  $\alpha \equiv N/2$ . The normalization is  $\langle \psi | \psi \rangle = 1$ . The population in an individual mode is,

$$\begin{aligned} \langle \hat{n}_1 \rangle &= \langle \psi | \hat{a}_1^\dagger \hat{a}_1 | \psi \rangle = \frac{1}{2^N} \langle m, N-m | \sum_{n,m=0}^N \sqrt{\binom{N}{m}} \hat{a}_1^\dagger \hat{a}_1 \sqrt{\binom{N}{n}} |n, N-n\rangle \\ &= \frac{1}{2^N} \sum_{n=0}^N \binom{N}{n} n = \frac{N}{2}. \end{aligned} \quad (15.204)$$

The result (15.202) shows that, ignoring (tracing over) one of the modes, the other mode automatically becomes a Glauber state<sup>14</sup>.

Besides that,

$$\begin{aligned} \langle \hat{n}_1^2 \rangle &= \frac{1}{2^N} \sum_{n=0}^N \binom{N}{n} n^2 = \frac{N}{2^N} \sum_{n=0}^{N-1} \binom{N}{n} (n+1) = \frac{N(N+1)}{4} \\ \langle \hat{n}_1 \hat{n}_2 \rangle &= \frac{1}{2^N} \sum_{n=0}^N \sqrt{\binom{N}{n}} n(N-n) = N \langle \hat{n}_1 \rangle - \langle \hat{n}_1^2 \rangle = \frac{N(N-1)}{4} \end{aligned} \quad (15.205)$$

The squeezing parameter is,

$$\xi_{12} = \frac{\sigma^2(\hat{n}_1 - \hat{n}_2)}{\langle \hat{n}_1 \rangle + \langle \hat{n}_2 \rangle} = \frac{\langle \hat{n}_1^2 - 2\hat{n}_1 \hat{n}_2 + \hat{n}_2^2 \rangle}{N} = \frac{2\langle \hat{n}_1^2 \rangle - 2\langle \hat{n}_1 \hat{n}_2 \rangle}{N} = 1. \quad (15.206)$$

The correlation functions at equal times are,

$$\begin{aligned} g_{11} &= \frac{\langle \hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1 \rangle}{\langle \hat{n}_1 \rangle^2} = \frac{1}{\langle \hat{n}_1 \rangle^2} \frac{1}{2^N} \sum_{n=2}^N \binom{N}{n} n(n-1) = \frac{\langle \hat{n}_1^2 \rangle - \langle \hat{n}_1 \rangle}{\langle \hat{n}_1 \rangle^2} = 1 \\ g_{12} &= \frac{\langle \hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_1 \rangle}{\langle \hat{n}_1 \rangle \langle \hat{n}_2 \rangle} = \frac{1}{\langle \hat{n}_1 \rangle^2} \frac{1}{2^N} \sum_{n=0}^N \binom{N}{n} n(N-n) = \frac{N \langle \hat{n}_1 \rangle - \langle \hat{n}_1^2 \rangle}{\langle \hat{n}_1 \rangle^2} = \frac{N-1}{N} \end{aligned} \quad (15.207)$$

The Cauchy-Schwarz inequality and the quantum inequality are both met,

$$\begin{aligned} g_{12} &\leq \sqrt{g_{11} g_{22}} \\ g_{12} &\leq \sqrt{\left( g_{11} + \frac{1}{\langle \hat{n}_1 \rangle} \right) \left( g_{22} + \frac{1}{\langle \hat{n}_2 \rangle} \right)} \end{aligned} \quad (15.208)$$

<sup>14</sup>This does not mean that the output modes are uncorrelated. For instance, if we measure  $n$  photons in one mode, we know that the other must contain exactly  $N-n$  photons. However, the correlations are so dense in phase space that they are not resolvable or decohere rapidly. In fact, it can be shown that coherent states are the only pure states that produce uncorrelated outputs when mixed by a passive linear-optics device [8, 7].

In comparison, a Glauber state is normally divided,

$$\begin{aligned} |\psi\rangle &= |\alpha_1\rangle|\alpha_2\rangle = e^{-|\alpha_1|^2/2} \sum_n \frac{\alpha_1^n}{\sqrt{n!}} |n\rangle e^{-|\alpha_2|^2/2} \sum_m \frac{\alpha_2^m}{\sqrt{m!}} |m\rangle \\ &= e^{-|\alpha_1|^2/2 - |\alpha_2|^2/2} \sum_{n,m} \frac{\alpha_1^n \alpha_2^m}{\sqrt{n!}\sqrt{m!}} |n\rangle|m\rangle. \end{aligned} \quad (15.209)$$

### 15.6.2.1 Density matrix representation

The density matrix for a pure state is,

$$\hat{\rho} = |\psi\rangle\langle\psi| = \begin{pmatrix} |\langle\psi|1\rangle|^2 & \langle 1|\psi\rangle\langle\psi|2\rangle \\ \langle 2|\psi\rangle\langle\psi|1\rangle & |\langle\psi|2\rangle|^2 \end{pmatrix}. \quad (15.210)$$

The evolution of such a state is described by the von Neumann equation:

$$i\hbar\partial_t\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)]. \quad (15.211)$$

For the beam splitter we obtain,

$$\hat{\rho} = |\psi\rangle\langle\psi| = \begin{pmatrix} |\langle\psi|0,0\rangle|^2 & \langle 0,0|\psi\rangle\langle\psi|0,1\rangle & \langle 0,0|\psi\rangle\langle\psi|1,0\rangle \\ \langle 0,1|\psi\rangle\langle\psi|0,0\rangle & |\langle\psi|0,1\rangle|^2 & \langle 0,1|\psi\rangle\langle\psi|1,0\rangle \\ \langle 1,0|\psi\rangle\langle\psi|0,0\rangle & \langle 1,0|\psi\rangle\langle\psi|0,1\rangle & |\langle\psi|1,0\rangle|^2 \\ & & & \ddots \end{pmatrix}. \quad (15.212)$$

**Example 71 (Density matrix for the beam splitter with 0 or 1 photons):** For the case of the superposition states,  $|\psi\rangle = \frac{1}{\sqrt{2}}(|0,1\rangle \pm |1,0\rangle)$ ,

$$\hat{\rho} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & \pm\frac{1}{2} \\ 0 & \pm\frac{1}{2} & \frac{1}{2} \\ & & & \ddots \end{pmatrix}.$$

Obviously,  $\hat{\rho} = \hat{\rho}^2$ . For the above superposition state,  $\partial_t\hat{\rho}(t) = 0$ .

### 15.6.3 Shot noise

As any quantized degree of freedom, a light mode is subject to intrinsic quantum noise imposed by the Heisenberg uncertainty relation, as we have seen for the harmonic oscillator (3.121). The Heisenberg limit in the quadrature phases of a light field determines the *shot noise* noise in the intensity of the light beam. To measure this noise, we divide the laser beam by a beam splitter into two beams  $\hat{a}$  and  $\hat{b}$  and recombine them with a second beam splitter,

$$\hat{c} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{b}) \quad , \quad \hat{d} = \frac{1}{\sqrt{2}}(\hat{a} - \hat{b}). \quad (15.213)$$

Detected by photodetectors with the gain coefficient  $g$ , these two beams produce currents,

$$\hat{I}_c = g\hat{c}^\dagger\hat{c} \quad , \quad \hat{I}_d = g\hat{d}^\dagger\hat{d}. \quad (15.214)$$



We add and subtract these currents,

$$\hat{I}_+ \equiv \hat{I}_c + \hat{I}_d = g(\hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b}) \quad , \quad \hat{I}_- \equiv \hat{I}_c - \hat{I}_d = g(\hat{a}^\dagger \hat{b} + \hat{b}^\dagger \hat{a}) . \quad (15.215)$$

and,

$$\hat{I}_+^2 = g^2[\hat{n}_a^2 + \hat{n}_b^2 + 2\hat{n}_a \hat{n}_b] \quad , \quad \hat{I}_-^2 = g^2[(\hat{a}^\dagger \hat{b})^2 + (\hat{b}^\dagger \hat{a})^2 + \hat{a}^\dagger \hat{a} + \hat{b} \hat{b}^\dagger + \hat{a} \hat{a}^\dagger + \hat{b}^\dagger \hat{b}] . \quad (15.216)$$

The expectation values are,

$$\begin{aligned} \langle \hat{I}_+ \rangle &= g \langle \hat{n}_a \rangle_a \quad , \quad \langle \hat{I}_+ \rangle = 0 \\ \langle \hat{I}_+^2 \rangle &= g \langle (\hat{a}^\dagger \hat{a})^2 \rangle_a \quad , \quad \langle \hat{I}_-^2 \rangle = g^2 \langle \hat{n}_a \rangle_a . \end{aligned} \quad (15.217)$$

Now, with the definition,  $\langle (\Delta \hat{I})^2 \rangle \equiv \langle \hat{I}^2 \rangle - \langle \hat{I} \rangle^2$ , we get the intensity noise of the field,

$$\langle \Delta \hat{I}_+^2 \rangle = \langle (\Delta \hat{I}_+)^2 \rangle = g^2 \langle (\Delta \hat{n}_a)^2 \rangle , \quad (15.218)$$

and the shot noise,

$$\langle \Delta \hat{I}_-^2 \rangle = g^2 I_a . \quad (15.219)$$

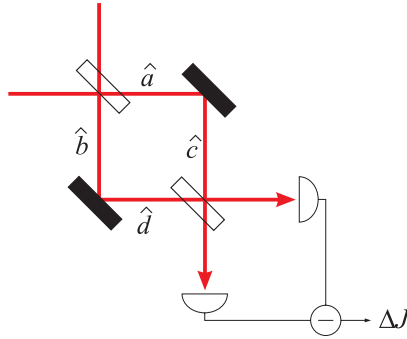


Figure 15.20: Shot noise measurement.

### 15.6.4 Quantum amplifier

We will call in the following as *quantum signals* degrees of freedom subject to quantum noise. Typically a quantum signal will be a mode of an electric field, represented by an annihilation operator  $\hat{a}$ . Such a mode can be enhanced by *quantum amplifier*, which is a device amplifying quantum signals according to the rules of quantum mechanics. Examples include the active elements of lasers and optical parametric amplifiers. A quantum amplifier is characterized by its gain and its own intrinsic quantum noise, which are interdependent parameters; the higher the gain, the larger the uncertainty noise. In the case of lasers, the uncertainty corresponds to the amplified spontaneous emission of the active medium.

Quantum amplification is a unitary transformation  $\hat{U}$ , acting in an initial state  $|in\rangle$  and producing (in the Schrödinger figure) the amplified state,

$$|out\rangle = \hat{U}|in\rangle . \quad (15.220)$$

The amplification depends on the mean value  $\langle \hat{a} \rangle$  of the annihilation operator and its dispersion  $\langle \hat{a}^\dagger \hat{a} \rangle - \langle \hat{a}^\dagger \rangle \langle \hat{a} \rangle$ . A coherent state is a state with minimal uncertainty; when the state is transformed, the uncertainty may increase. This increase can be interpreted as noise in the amplifier. The gain  $G$  can be defined as follows:

$$G = \frac{\langle \hat{a} \rangle_{out}}{\langle \hat{a} \rangle_{in}} . \quad (15.221)$$

The quantum amplifier can also be described in the Heisenberg picture; the changes are attributed to the amplification of the field operator. Thus, the evolution of the operator  $\hat{a}_{out}$  is given by

$$\hat{a}_{out} = \hat{U}^\dagger \hat{a} \hat{U} , \quad (15.222)$$

while the state vector remains unchanged. The gain is then given by,

$$G = \frac{\langle \hat{a}_{out} \rangle_{in}}{\langle \hat{a} \rangle_{in}} . \quad (15.223)$$

In general, the gain  $G$  may be complex, and it may depend on the initial state. For laser applications, the amplification of coherent states is important. Therefore, it is usually assumed that the initial state is a coherent state characterized by a complex-valued initial parameter  $\alpha$ , such that  $|in\rangle = |\alpha\rangle$ . Even with such a restriction, the gain may depend on the amplitude or phase of the initial field.

In the following, the Heisenberg representation is used; all brackets are assumed to be evaluated with respect to the initial coherent state,

$$\text{noise} = \langle \hat{a}_{out}^\dagger \hat{a}_{out} \rangle - \langle \hat{a}_{out}^\dagger \rangle \langle \hat{a}_{out} \rangle - (\langle \hat{a}^\dagger \hat{a} \rangle - \langle \hat{a}^\dagger \rangle \langle \hat{a} \rangle) . \quad (15.224)$$

The expectation values are assumed to be evaluated with respect to the initial coherent state. This quantity characterizes the increase of the uncertainty of the field due to amplification. As the uncertainty of the field operator does not depend on its parameter, the quantity above shows how much output field differs from a coherent state.

#### 15.6.4.1 Linear phase-invariant amplifier

Linear phase-invariant amplifiers may be described as follows. Assume that the unitary operator  $U$  amplifies in such a way that the input  $\hat{a}$  and the output  $\hat{a}_{out} = \hat{U}^\dagger \hat{a} \hat{U}$ , are related by a linear equation,

$$\hat{a}_{out} = c\hat{a} + s\hat{b}^\dagger , \quad (15.225)$$

where  $c$  and  $s$  are c-numbers and  $\hat{b}^\dagger$  is a creation operator characterizing the amplifier. Without loss of generality, it may be assumed that  $c$  and  $s$  are real. The commutator of the field operators is invariant under unitary transformation  $U$ :

$$[\hat{a}_{out}, \hat{a}_{out}^\dagger] = 1 = [\hat{a}, \hat{a}^\dagger] \quad , \quad [\hat{a}_{in}, \hat{a}_{out}^\dagger] = 0 = [\hat{a}_{out}, \hat{a}_{in}^\dagger] . \quad (15.226)$$

From the unitarity of  $U$ , it follows that  $\hat{b}$  satisfies the same commutation relations. The c-numbers are then  $c^2 - s^2 = 1$ . Hence, the phase-invariant amplifier acts by

introducing an additional mode to the field, with a large amount of stored energy, behaving as a boson. Calculating the gain and the noise of this amplifier, one finds  $G = c$ , and

$$\text{noise} = c^2 - 1 . \quad (15.227)$$

The coefficient  $g = |G|^2$  is sometimes called the intensity amplification coefficient. The noise of the linear phase-invariant amplifier is given by  $g - 1$ . The gain can be dropped by splitting the beam; the estimate above gives the minimal possible noise of the linear phase-invariant amplifier. The linear amplifier has an advantage over the multi-mode amplifier: if several modes of a linear amplifier are amplified by the same factor, the noise in each mode is determined independently; that is, modes in a linear quantum amplifier are independent.

To obtain a large amplification coefficient with minimal noise, one may use homodyne detection, constructing a field state with known amplitude and phase, corresponding to the linear phase-invariant amplifier. The uncertainty principle sets the lower bound of quantum noise in an amplifier. In particular, the output of a laser system and the output of an optical generator are not coherent states.

The multiplicative amplifier  $D$  also adds additive noise  $F$ . We have  $DD^\dagger = 1$ ,

$$\begin{pmatrix} \hat{a}_{out}^\dagger \\ \hat{a}_{out} \end{pmatrix} = D \begin{pmatrix} \hat{a}_{in}^\dagger \\ \hat{a}_{in} \end{pmatrix} + \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} . \quad (15.228)$$

### 15.6.5 Homodyne detection and inverse Radon transform

In the method of *homodyne detection* or *phase-sensitive detection* the signal is obtained by superposing the field mode of interest with a local oscillator with a relative phase  $\theta$  at a beam splitter and a subtraction of the photo currents in the two ports of the interferometer:

$$\begin{aligned} \Delta \hat{J} &= \hat{a}_t^\dagger \hat{a}_t - \hat{b}_t^\dagger \hat{b}_t \\ &= (2\eta - 1)(\hat{a}_0^\dagger \hat{a}_0 + \hat{b}_0^\dagger \hat{b}_0) + 2\sqrt{(1-\eta)\eta}(\hat{a}_0^\dagger \hat{a}_0 + \hat{b}_0^\dagger \hat{b}_0) \xrightarrow{\eta \rightarrow 1/2} \hat{a}_0^\dagger \hat{a}_0 + \hat{b}_0^\dagger \hat{b}_0 . \end{aligned} \quad (15.229)$$

If the local oscillator is a classical light field  $\hat{b}_0 = \alpha_{LO} e^{-i\theta}$ ,

$$\begin{aligned} \Delta \hat{J} &= |\alpha_{LO}|(\hat{a}_0 e^{-i\theta} + \hat{a}_0^\dagger e^{i\theta}) \\ &= \sqrt{2}|\alpha_{LO}|\hat{x}_\theta , \end{aligned} \quad (15.230)$$

where the field mode is expressed by the Hermitian quadrature components  $\hat{a}_0 = 2^{-1/2} \cdot (\hat{x}_\theta + i\hat{y}_\theta)$ . The expectation value of  $\Delta \hat{J}$  is afflicted with the Heisenberg uncertainty and can be expressed as the first moment of the Wigner function  $W(\alpha)$ :

$$\begin{aligned} \langle \psi | \Delta \hat{J} | \psi \rangle &= \int W_{|\psi\rangle}(\alpha) \Delta \hat{J} d^2\alpha \\ &= \sqrt{2}|\alpha_{LO}| \int W_{|\psi\rangle}(x_\theta, p_\theta) x_\theta dx_\theta dp_\theta = \sqrt{2}|\alpha_{LO}| \int_{-\infty}^{\infty} w_\theta(x_\theta) x_\theta dx_\theta . \end{aligned} \quad (15.231)$$

Here, the distribution function integrated over a rotated quadrature component  $p_\theta$  is given by,

$$w_\theta(x_\theta) \equiv \int_{-\infty}^{\infty} W_\theta(x_\theta, p_\theta) dp_\theta . \quad (15.232)$$

This is called the *radon transform*. The distribution function  $w_\theta(p_\theta)$  as well as the Wigner function are normalized to 1. Multiple measurements of the expectation value  $x_\theta = \langle \psi | \hat{x}_\theta | \psi \rangle$  now yields a histogram  $H_{|\psi\rangle}(x_\theta)$  reflecting, if normalized,  $w_{|\psi\rangle}(x_\theta) = H_{|\psi\rangle}(x_\theta) / \int H_{|\psi\rangle}(x_\theta)$  exactly the distribution function.

Considering the finite detector efficiency [429]  $w_\theta(x_\theta)$  must be generalized to a convolution with an apparatus function  $\zeta(x)$ :

$$w_\theta^{\text{real}}(\sqrt{\eta}x_\theta) = (w_\theta^{\text{ideal}} \star \zeta) \quad \text{where} \quad \zeta(x) = \frac{1}{\sqrt{\pi(1-\eta)}} e^{-\eta\alpha^2/(1-\eta)}. \quad (15.233)$$

A finite detector efficiency degrades the contrast of the quantum interference structures.

With the procedure of optical *homodyne tomography* or *quantum state endoscopy* the Wigner function for e.g. a Schrödinger cat state can be reconstructed from a set of distribution functions  $w_\theta(x_\theta) = \int W(\alpha e^{i\theta}) dp_\theta$  measured for various phases  $\theta$  [429]. To do this the data set is exposed to an inverse *radon transform*:

$$W(\alpha) = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} \int_0^\pi \int_{-\infty}^{\infty} w_\theta(x_\theta) |\zeta| e^{i\zeta[\text{Re}(2^{-1/2}\alpha e^{-i\theta}) - x_\theta]} dx d\theta d\zeta. \quad (15.234)$$

In contrast to the conventional homodyne detection, where the phase dependency of amplitude noise is recorded, the homodyne tomography allows the complete reconstruction of a quantum state through measurement of the distribution of the amplitude noise power,

$$P_s = \frac{\omega_s}{2\pi} \int_0^{\omega_s/2\pi} dt |\langle I(t) \rangle|^2 \quad (15.235)$$

for various phases.

Alternatively, to the homodyne method, one may reconstruct the photon distribution in field modes from their temporal evolution [705]. Another method could be to use atoms as sensors for the quantum state of a light field in a Jaynes-Cummings type dynamics.

### 15.6.5.1 Homodyne signature of squeezed states

Let us mix squeezed light  $\hat{b}$  with a local oscillator  $\hat{a}$  at a beamsplitter,

$$\begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \begin{pmatrix} \hat{b} \\ \hat{a} \end{pmatrix}. \quad (15.236)$$

The homodyne signal is,

$$\begin{aligned} P_{\text{hody}} &\propto \hat{x}^\dagger \hat{x} - \hat{y}^\dagger \hat{y} \\ &= i\hat{a}^\dagger \hat{b} - i\hat{a} \hat{b}^\dagger \\ &= i(\hat{a}^\dagger - \hat{a})\hat{b}_r - (\hat{a}^\dagger + \hat{a})\hat{b}_p \\ &= 2|\alpha| \left( \hat{b}_r \sin \theta - \hat{b}_p \cos \theta \right), \end{aligned} \quad (15.237)$$

if the local oscillator can be considered as classical,  $\alpha = |\alpha|e^{i\theta}$ . I.e. the phase of the local oscillator permits us to select either one of the quadrature components.

### 15.6.6 Multimode squeezing

Define,

$$\hat{b} = \mu\hat{a} + \nu\hat{c}^\dagger. \quad (15.238)$$

Again using  $\mu^2 - \nu^2 = 1$ , the standard commutation rules for  $\hat{a}$  and  $\hat{c}$  give,

$$\begin{aligned} [\hat{b}, \hat{b}^\dagger] &= 1 \\ [\hat{b}_r, \hat{b}_p] &= \frac{\imath}{2}. \end{aligned} \quad (15.239)$$

The individual variances read,

$$\begin{aligned} \Delta\hat{b}_r^2 &= \langle \hat{b}_r^2 \rangle - \langle \hat{b}_r \rangle^2 \\ &= \frac{1}{4} \langle (\hat{b} + \hat{b}^\dagger)^2 \rangle - \frac{1}{4} \langle \hat{b} + \hat{b}^\dagger \rangle^2 \\ &= \frac{1}{4} \langle (\mu\hat{a} + \mu\hat{a}^\dagger + \nu\hat{c} + \nu\hat{c}^\dagger)^2 \rangle \\ &= \frac{1}{4} \mu^2 + \frac{1}{4} \nu^2 + \frac{1}{2} \mu^2 \langle \hat{a}^\dagger \hat{a} \rangle + \frac{1}{2} \nu^2 \langle \hat{c}^\dagger \hat{c} \rangle + \frac{1}{2} \mu\nu \langle \langle \hat{a} \hat{c} \rangle + \langle \hat{a}^\dagger \hat{c}^\dagger \rangle \rangle. \end{aligned} \quad (15.240)$$

using  $\langle \hat{a} \rangle = \langle \hat{c} \rangle = \langle \hat{a}^\dagger \hat{c} \rangle = 0$ .

Two-mode squeezing can exist even if the individual modes are not squeezed,

$$|r, \phi\rangle = \cosh^{-1} r \sum_n \tanh^n r e^{in\phi} |r, \phi\rangle_a |r, \phi\rangle_b. \quad (15.241)$$

A *two-mode squeezed vacuum state* can be generated by the squeezing operator

$$\hat{S}(\xi) \equiv \exp\left(\frac{\xi^*}{2} \hat{a} \hat{b} - \frac{\xi}{2} \hat{a}^\dagger \hat{b}^\dagger\right). \quad (15.242)$$

Remember that the single-mode squeezing is obtained if  $\hat{a} = \hat{b}$ . In a number state base

$$|r, \phi\rangle = \frac{1}{\cosh r} \sum_n (\tanh r)^n e^{in\phi} |n\rangle_a |n\rangle_b. \quad (15.243)$$

Two-mode relative number squeezing parameter

$$\xi_{i,j} = \frac{\sigma^2(n_i - \langle n_j \rangle)}{\langle n_i \rangle + \langle n_j \rangle}. \quad (15.244)$$

### 15.6.7 Coupled quantum oscillators with/out counter-rotating terms

Here, we are interested in calculating the time evolution of two *coupled oscillators*. We rewrite the Hamiltonian in terms of the *normal modes*. We start from the Hamiltonian with counter-rotating terms [232],

$$\hat{H} = \hbar\omega(\hat{a}^\dagger \hat{a} + \frac{1}{2}) + \hbar\omega(\hat{b}^\dagger \hat{b} + \frac{1}{2}) + \frac{\hbar\Omega}{2}(\hat{a} + \hat{a}^\dagger)(\hat{b} + \hat{b}^\dagger), \quad (15.245)$$

which we rewrite in terms of the quadrature components given by,

$$\begin{pmatrix} \hat{x}_a \\ \hat{p}_a \\ \hat{x}_b \\ \hat{p}_b \end{pmatrix} = X \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \\ \hat{b} \\ \hat{b}^\dagger \end{pmatrix} \quad \text{with} \quad T_{ab} = \sqrt{\frac{\hbar\omega}{2}} \begin{pmatrix} \omega^{-1} & \omega^{-1} & 0 & 0 \\ \imath & -\imath & 0 & 0 \\ 0 & 0 & \omega^{-1} & \omega^{-1} \\ 0 & 0 & \imath & -\imath \end{pmatrix}, \quad (15.246)$$

as

$$\hat{H} = \frac{1}{2}(\hat{p}_a^2 + \omega^2 \hat{x}_a^2) + \frac{1}{2}(\hat{p}_b^2 + \omega^2 \hat{x}_b^2) + \Omega \omega \hat{x}_a \hat{x}_b. \quad (15.247)$$

Setting  $\omega_{\pm} = \sqrt{\omega^2 \pm \Omega \omega}$  allows us to rewrite the Hamiltonian as,

$$\hat{H} = \frac{1}{4}(\hat{p}_a + \hat{p}_b)^2 + \frac{1}{4}\omega_+^2(\hat{x}_a + \hat{x}_b)^2 + \frac{1}{4}(\hat{p}_a - \hat{p}_b)^2 + \frac{1}{4}\omega_-^2(\hat{x}_a - \hat{x}_b)^2. \quad (15.248)$$

Now, we apply the transform,

$$\begin{pmatrix} \hat{x}_A \\ \hat{p}_A \\ \hat{x}_B \\ \hat{p}_B \end{pmatrix} = M \begin{pmatrix} \hat{x}_a \\ \hat{p}_a \\ \hat{x}_b \\ \hat{p}_b \end{pmatrix} \quad \text{with} \quad M = \sqrt{\frac{1}{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} = M^{-1}, \quad (15.249)$$

and rewrite the Hamiltonian again as,

$$\hat{H} = \frac{1}{2}(\hat{p}_A^2 + \omega_+^2 \hat{x}_A^2) + \frac{1}{2}(\hat{p}_B^2 + \omega_-^2 \hat{x}_B^2). \quad (15.250)$$

We go back from the quadrature components to the field mode operators via,

$$\begin{pmatrix} \hat{x}_A \\ \hat{p}_A \\ \hat{x}_B \\ \hat{p}_B \end{pmatrix} = X \begin{pmatrix} \hat{A} \\ \hat{A}^\dagger \\ \hat{B} \\ \hat{B}^\dagger \end{pmatrix} \quad \text{with} \quad T_{AB} = \sqrt{\frac{\hbar}{2}} \begin{pmatrix} 1/\sqrt{\omega_+} & 1/\sqrt{\omega_+} & 0 & 0 \\ i\sqrt{\omega_+} & -i\sqrt{\omega_+} & 0 & 0 \\ 0 & 0 & 1/\sqrt{\omega_-} & 1/\sqrt{\omega_+} \\ 0 & 0 & i\sqrt{\omega_-} & -i\sqrt{\omega_+} \end{pmatrix}, \quad (15.251)$$

and finally obtain,

$$\boxed{\hat{H} = \hbar\omega_+(\hat{A}^\dagger \hat{A} + \frac{1}{2}) + \hbar\omega_-(\hat{B}^\dagger \hat{B} + \frac{1}{2})}. \quad (15.252)$$

The Heisenberg equations of motion for the oscillator modes,

$$\frac{d}{dt} \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} = \begin{pmatrix} \frac{i}{\hbar}[\hat{H}, \hat{a}] \\ \frac{i}{\hbar}[\hat{H}, \hat{b}] \end{pmatrix} = \begin{pmatrix} -i\omega & -\frac{i}{2}\Omega \\ -\frac{i}{2}\Omega & -i\omega \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} + \begin{pmatrix} 0 & -\frac{i}{2}\Omega \\ -\frac{i}{2}\Omega & 0 \end{pmatrix} \begin{pmatrix} \hat{a}^\dagger \\ \hat{b}^\dagger \end{pmatrix}, \quad (15.253)$$

are difficult to integrate. In contrast, the Heisenberg equations for the normal modes,

$$\frac{d}{dt} \begin{pmatrix} \hat{A} \\ \hat{B} \end{pmatrix} = \frac{i}{\hbar} \begin{pmatrix} [\hat{H}, \hat{A}] \\ [\hat{H}, \hat{B}] \end{pmatrix} = -i \begin{pmatrix} \omega_+ & 0 \\ 0 & \omega_- \end{pmatrix} \begin{pmatrix} \hat{A} \\ \hat{B} \end{pmatrix}, \quad (15.254)$$

are easily solved by,

$$\begin{pmatrix} \hat{A}(t) \\ \hat{A}^\dagger(t) \\ \hat{B}(t) \\ \hat{B}^\dagger(t) \end{pmatrix} \quad \text{with} \quad \equiv \Lambda(t) \begin{pmatrix} \hat{A}(0) \\ \hat{A}^\dagger(0) \\ \hat{B}(0) \\ \hat{B}^\dagger(0) \end{pmatrix} \Lambda(t) \equiv \begin{pmatrix} e^{-i\omega_+ t} & 0 & 0 & 0 \\ 0 & e^{i\omega_+ t} & 0 & 0 \\ 0 & 0 & e^{-i\omega_- t} & 0 \\ 0 & 0 & 0 & e^{i\omega_- t} \end{pmatrix}. \quad (15.255)$$

Hence, the oscillator modes evolve as,

$$\begin{pmatrix} \hat{a}(t) \\ \hat{a}^\dagger(t) \\ \hat{b}(t) \\ \hat{b}^\dagger(t) \end{pmatrix} = T_{ab}^{-1} M^{-1} T_{AB} \Lambda(t) T_{AB}^{-1} M T_{ab} \begin{pmatrix} \hat{a}(0) \\ \hat{a}^\dagger(0) \\ \hat{b}(0) \\ \hat{b}^\dagger(0) \end{pmatrix}. \quad (15.256)$$

### 15.6.7.1 Rotating-wave approximation

The rotating-wave approximation is performed via  $\omega_{\pm} \simeq \omega \pm \frac{1}{2}\Omega$ . It leads to the Hamiltonian,

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) + \hbar\omega(\hat{b}^\dagger\hat{b} + \frac{1}{2}) + \frac{\hbar\Omega}{2}(\hat{a}\hat{b}^\dagger + \hat{a}^\dagger\hat{b}). \quad (15.257)$$

In this approximation, we find  $T_{AB}^{-1}MT_{ab} \simeq M$  and the transformation defined in (15.249),

$$\begin{pmatrix} \hat{A} \\ \hat{A}^\dagger \\ \hat{B} \\ \hat{B}^\dagger \end{pmatrix} = M \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \\ \hat{b} \\ \hat{b}^\dagger \end{pmatrix}, \quad (15.258)$$

takes us directly from the Hamiltonian (15.257) to <sup>15</sup>,

$$\hat{H} = (\hbar\omega + \frac{\hbar\Omega}{2})(\hat{A}^\dagger\hat{A} + \frac{1}{2}) + (\hbar\omega - \frac{\hbar\Omega}{2})(\hat{B}^\dagger\hat{B} + \frac{1}{2}). \quad (15.259)$$

Do the Exc. 15.6.8.7.

Note, that two coupled oscillator model becomes *criticality*, when the atom-field coupling strength exceeds the frequencies of the mode and the atomic two-level system.

## 15.6.8 Exercises

### 15.6.8.1 Ex: Conservation law at a beam splitter 1

Show that the beam-split transformation

$$\begin{pmatrix} \hat{c} \\ \hat{d} \end{pmatrix} = \begin{pmatrix} t & -r \\ r & t \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix}$$

preserves the commutations relations and the photon number.

### 15.6.8.2 Ex: Conservation law at a beam splitter 2

Derive from the Hamiltonian (15.189) that  $\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b} = \text{const}$ .

### 15.6.8.3 Ex: Beam splitter

Show that for  $\hat{B} \equiv e^{\theta(\hat{a}\hat{b}^\dagger - \hat{a}^\dagger\hat{b})}$  holds,

$$\hat{B}\hat{a}\hat{B}^\dagger = \hat{a} \cos \theta + \hat{b} \sin \theta \quad \text{and} \quad \hat{B}\hat{b}\hat{B}^\dagger = -\hat{a} \sin \theta + \hat{b} \cos \theta.$$

<sup>15</sup>Note the different behavior of a beam splitter under this transformation,

$$\begin{aligned} \hat{H} &= \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) + \hbar\omega(\hat{b}^\dagger\hat{b} + \frac{1}{2}) + \frac{\hbar\Omega}{2}(\hat{a}\hat{b}^\dagger - \hat{a}^\dagger\hat{b}) \\ &= \hbar\omega(\hat{A}^\dagger\hat{A} + \frac{1}{2}) + \hbar\omega(\hat{B}^\dagger\hat{B} + \frac{1}{2}) + \frac{\hbar\Omega}{2}(-\hat{A}\hat{B}^\dagger + \hat{A}^\dagger\hat{B}). \end{aligned}$$

**15.6.8.4 Ex: Beam splitter**

Show that  $\hat{B}|1, 0\rangle = \cos\theta|1, 0\rangle - \sin\theta|0, 1\rangle$  and  $\hat{B}|0, n\rangle = \sum_{k=0}^{\infty} \sqrt{\binom{n}{k}} \cos^k\theta \sin^{n-k}\theta |n-k, k\rangle$ .

**15.6.8.5 Ex: Elitzur and Vaidman bomb tester**

a. Write down the beam splitter Hamiltonian in the Fock representation for a case of a single photon, diagonalize it, and determine the propagator  $e^{i\hat{H}t/\hbar}$  for a 50/50 beam splitter.

b. Based on the propagator derived in (a) draw an analogy between a Mach-Zehnder interferometer and a resonantly driven two-level system. Interpreting the interferometer as a qubit explain the *Elitzur and Vaidman bomb testing problem*. What is the probability

**15.6.8.6 Ex: Link between entanglement and squeezing**

Prove that, if  $\hat{a}_1$  and  $\hat{a}_2$  are EPR-entangled beams with respect to quadrature components, then beams  $\hat{b}_{1,2} = \frac{1}{\sqrt{2}}(\hat{a}_1 \pm \hat{a}_2)$  are squeezed with respect to two orthogonal quadrature components and vice versa [576, 577, 443].

**15.6.8.7 Ex: Equivalence of the beamsplitter and the coupled oscillators model**

Show that the beamsplitter and the coupled oscillators model are equivalent.

**15.7 Further reading**

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- Z. Ficek et al., *Effect of interatomic interactions on resonance fluorescence of two atoms coherently driven by strong resonant laser field* [DOI]
- J.C. García-Melgarejo et al., *A Numerical Perspective on the Jaynes-Cummings Model Wigner Function* [DOI]
- D.J. Heinzen et al., *Enhanced and Inhibited Visible Spontaneous Emission by Atoms in a Confocal Resonator* [DOI]
- D.J. Heinzen et al., *Vacuum Radiative Level Shift and Spontaneous-Emission Linewidth of an Atom in an Optical Resonator* [DOI]
- K. Nakayama et al., *Precise intensity correlation measurement for atomic resonance fluorescence from optical molasses* [DOI]
- U. Leonhardt et al., *Measuring the quantum state of light* [DOI]
- P. Longo et al., *Far-Field Signatures of a Two-Body Bound State in Collective Emission from Interacting Two-Level Atoms on a Lattice* [DOI]
- R. Loudon et al., *Squeezed light* [DOI]
- L.A. Lugiato et al., *Quantum imaging* [DOI]
- B.R. Mollow et al., *Power spectrum of light scattered by two-level systems* [DOI]
- K. Mølmer et al., *Monte Carlo wave-function method in quantum optics* [DOI]
- F.A. de Oliveira et al., *Properties of displaced number states* [DOI]
- M.D. Reid, *Quantum Correlations of Phase in Nondegenerate Parametric Oscillation* [DOI]
- M.D. Reid, *Demonstration of the Einstein-Podolsky-Rosen paradox using nondegenerate parametric amplification* [DOI]
- D. Stoler, *Equivalence Classes of Minimum Uncertainty Packets* [DOI]
- M. Uria et al., *Deterministic Generation of Large Fock States* [DOI]
- H.P. Yuen et al., *Two-photon coherent states of the radiation field* [DOI]
- M. Schubert et al., *Photon antibunching and non-Poissonian fluorescence of a single three-level ion* [DOI]
- G.S. Agarwal et al., *Inhibition of Decoherence due to Decay in a Continuum* [DOI]
- Ho Trung Dung et al., *Electromagnetic-field quantization and spontaneous decay in left-handed media* [DOI]

### 15.7.1 on second quantization

W.E.Jr. Lamb, *Anti-Photon* [\[DOI\]](#)

### 15.7.2 on the Jaynes-Cummings model

J. Eiselt et al., *Quasiprobability distributions for the Jaynes-Cummings model with cavity damping* [\[DOI\]](#)

M. Brune et al., *Manipulation of photons in a cavity by dispersive atom-field coupling: Quantum-nondemolition measurement and generation of "Schrödinger cat" states* [\[DOI\]](#)

K. Gietka et al., *Quantum-enhanced interferometry with cavity QED-generated non-classical light* [\[DOI\]](#)

M. Mohammad et al., *Cavity quantum electrodynamics with atom-like mirrors* [\[DOI\]](#)

### 15.7.3 on beam splitters

L.E. Estes et al., *Quantum-Mechanical Description of Two Coupled Harmonic Oscillators* [\[DOI\]](#)

U. Leonhardt, *Quantum physics of simple optical instruments* [\[DOI\]](#)



# Chapter 16

## Quantum measurement

Since its foundation, the theory of quantum mechanics was driven by the urge to clarify the relationship between the world and what we can learn about it, that is, between reality and the observer. Scientists such as Bohr, Heisenberg, Schrödinger, and Einstein defended controversial positions and struggled for the correct interpretation of quantum mechanics. The *measurement process* is supposed to provide information about the world out there, but it is not clear whether this information can be complete and accurate, or whether there are limitations or hidden variables. Also, it was unclear, to what extent a measurement can be non-invasive or whether it would always perturb the phenomenon under investigation. The most important step in this question was the *Copenhagen interpretation* formulated by Bohr, Heisenberg and Born in 1927 and elaborated later by von Neumann and Dirac. Although contested many times in the past, its essence still remains valid today.

In this chapter we will study the measurement process from the viewpoint quantum mechanics and discuss some seemingly paradoxical effects, that will allow us to deepen our understanding. Among them are the quantum jump, Schrödinger's cat, the quantum Zeno effect, and the Einstein-Podolski-Rosen paradox.

### 16.1 The observer and the reality

According to the Copenhagen interpretation, theoretical predictions have a probabilistic character. However, this is not an expression of the imperfection of the theory, but of the intrinsically indeterministic character of quantum processes<sup>1</sup>. Moreover, the Copenhagen interpretation desists to attribute to objects of the quantum formalism, such as wavefunctions and operators, an immediate reality. Instead, the objects of the formalism only represent vehicles for a probabilistic prediction of the results of measurements. These results are *only truly real* elements of quantum theory. It is obvious, that the quantum theory and its interpretations are of fundamental importance to the scientific view of the world and our concept of nature.

#### 16.1.1 Schrödinger's cat

In the microscopic world, the relationship between the sample and the observer is very delicate. And this delicacy is at the origin of quantum effects that seem paradoxical

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<sup>1</sup>Note that it is problematic to identify unpredictability and indeterminism. We may be unable to predict specific events, without having to assume that these events occur in a random manner.

through our classical concept of the world. It is, thus, not surprising that one of the most fascinating areas of investigations is the *interface* between the classical and the quantum, the macroscopic and the microscopic worlds. For the pioneers of quantum mechanics the most important questions were of the type: 'How is it possible that a microscopic particle flies simultaneously through two slits?' Nowadays, we are accustomed to such paradoxes, and we simply accept the fact that we have to consider a particle as a wave. Nevertheless, we still do not understand very well, why the classical and the quantum world behave so differently. 'Why does quantum mechanics allow for quantum superpositions states, which are absolutely forbidden in classical physics?', 'Why are the fundamental laws of the quantum world invariant to the arrow of time, while the macroscopic world always evolves from the past to the future?', 'How can it be that quantum mechanics allows for effects having no cause, like spontaneous emission, while the everyday world seems to be deterministic?'



Figure 16.1: Double slit.

Quantum mechanics must, in some limit, clearly encompass classical physics. But in spite of *Ehrenfest's correspondence principle*, this fact is far from being trivial. Some predictions of classical and quantum physics are fundamentally different and, in some cases, even contradictory. The famous *Schrödinger cat* states are the epitome of this fact: In one version of this paradox, a particle crosses a double slit. Behind one of the slits is a detector which, as soon as it registers a particle, actuates a device killing a cat. We know that in quantum reality the particle crosses both slits in a superposition state, so that the cat should be in a superposition state as well. Hence, quantum cats can be in a superposition of 'dead' and 'alive'.

We believe nowadays that the answers to the above questions are somehow buried in processes that destroy the quantum superposition of Schrödinger cats during the transition from the microscopic to the macroscopic world. However, the details of these quantum coherence destruction processes, called *decoherence*, are very compli-

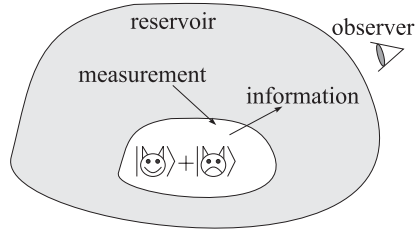


Figure 16.2: The measurement of a quantum system presupposes the interaction of the system with a reservoir, which disturbs its dynamics.

cated and the subject of serious efforts in contemporary research. It is one of the motivations for trying to create in laboratories the largest possible (quasi-macroscopic) quantum systems, bring them in Schrödinger cat-like superposition states and study their decoherence <sup>2</sup>.

### 16.1.1.1 Quantum measurement

Every unperturbed system follows the Schrödinger equation. Once its Hamiltonian has been determined, the formal solution,

$$|\psi\rangle = e^{-i\hat{H}t/\hbar}|\psi_0\rangle, \quad (16.1)$$

allows to calculate the time evolution, that is, the trajectory of the wavefunction. The evolution is *coherent and reversible* in time.

Now, the process of measuring a pure quantum state includes –according to the Copenhagen interpretation and as discussed in Sec. 2.2.7– two consecutive steps: In the *first step*, the interaction of the quantum sample with the measuring device (which from now on we will call *meter*) destroys all coherences and projects the pure state into a statistical mixture of eigenstates of the meter. Following von Neumann, the impact of the meter on the quantum system is so strong, that its coherent evolution is interrupted and it is projected onto the degree of freedom that the apparatus wants to measure, e.g. its position or its momentum, but not both in the same time. The projection transforms a pure quantum state  $|\psi\rangle$  into a statistical mixture  $\rho$  of eigenstates,

$$\hat{\rho}_{sample} = |\psi(t)\rangle\langle\psi(t)| \rightsquigarrow \hat{\rho}_{proj} = \sum_k |\langle\psi|k\rangle|^2 |k\rangle\langle k|. \quad (16.2)$$

This process is irreversible, that is, it separates the past from the future. The projection is *not* described by the Schrödinger equation. Instead, the sudden reduction of the state must be postulated, as done by von Neumann’s famous axiom.

In a *second step*, the observer looks at the measuring device and confirms one of the possible results. Thus, he transforms the state into a eigenstate of the device <sup>3</sup>:

$$\hat{\rho}_{proj} \rightsquigarrow \hat{\rho}_{meter} = |k\rangle\langle k|. \quad (16.3)$$

<sup>2</sup>There are attempts to introduce the concept of the time arrow also in the microscopic world: ‘In an isolated system, spontaneous processes occur in the direction of increasing entropy.’ [486].

<sup>3</sup>We note that, only if *all* commuting observables of the system are measured *and* acknowledged,  $\hat{\rho}_{meter}$  becomes a pure state. Otherwise  $\rho_{meter}$  remains a partial mixture.

From this moment, we can again leave the quantum system alone until the next measure.

From the viewpoint of the quantum system, the evolution of the measurement process appears *discontinuous*, because it destroys all possible coherences between its states. In fact, the problem comes from the non-ideal behavior of the measuring device (symbolized by  $|\uparrow\rangle$  before the measurement). An ideal non-invasive measurement<sup>4</sup> would leave the quantum state  $|\psi\rangle$  unchanged:

$$|\psi\rangle|\uparrow\rangle \xrightarrow{H} |\psi\rangle|\nearrow\rangle, \quad (16.4)$$

while the measuring device changes to a state ( $|\nearrow\rangle$  after the measurement) indicating the current state of the system. However, this is normally impossible without previously established correlation between  $|\psi\rangle$  and  $|\uparrow\rangle$ . In a real meter device, the coupling between  $|\psi\rangle$  and  $|\uparrow\rangle$  requires that the meter and the system to be non-orthogonal.

### 16.1.1.2 Measurement-induced decoherence

A more modern view of the quantum measurement is the following: When the outer world (called reservoir, observer or meter) *reads* a quantum system, it causes, due to this transfer of information, an irreversible demolition of coherence. Consequently, the density operator condenses to its diagonal. On the other hand, the system as a whole (including the sample and the reservoir) always evolves coherently according to the von Neumann equation with the Hamiltonian of everything  $\hat{H}_{all}$ :

$$\dot{\hat{\rho}} = \frac{i}{\hbar}[\hat{\rho}, \hat{H}_{all}]. \quad (16.5)$$

If  $\hat{H}_{sample}$  is the small quantum system under investigation, a complete description of the measurement process requires the inclusion of the observer, that is, the total Hamiltonian is,

$$\hat{H} = \hat{H}_{sample} \otimes \hat{H}_{meter} = \begin{pmatrix} \text{sample} & 0 \\ 0 & \text{meter} \end{pmatrix}. \quad (16.6)$$

Ideally, the system evolves independently without being disturbed by the meter. Unfortunately, this also means that the meter evolves independently, that is, it is not influenced by the system and thus does not provide information about the system. To allow a transfer of information, we need to couple the respective spaces by an interaction  $\Omega$ , such that,

$$\hat{H} = \begin{pmatrix} \text{sample} & \Omega \\ \Omega & \text{meter} \end{pmatrix}. \quad (16.7)$$

Tracing over all degrees of freedom of the universe *except* those of the quantum system, the von Neumann equation (16.5) turns into a master equation,

$$\dot{\hat{\rho}}_{sample} = \frac{i}{\hbar}[\hat{\rho}, \hat{H}_{sample}] + \mathcal{L}_{reserv}\rho. \quad (16.8)$$

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<sup>4</sup>See the discussion of the *quantum non-demolition measurement*.

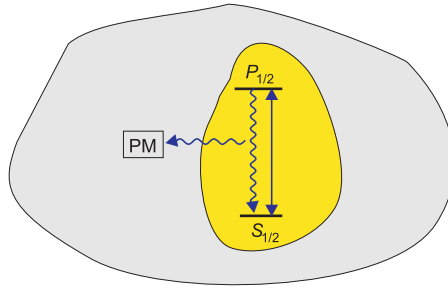


Figure 16.3: Spontaneous emission can be seen as a coupling of the system under investigation to an external meter, because it delivers information to the meter, even if only to tell us: 'The system was in an excited state, but now it's in a ground state.'

**Example 72 (Quantum measurement in a two-qubit system):** To discuss this at an example, we consider the simplest imaginable system: Two two-level atoms, the first one representing the quantum system under investigation and the second the meter. We introduce the following basis:

$$|1\rangle \equiv |\downarrow\rangle|\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |2\rangle \equiv |\uparrow\rangle|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |3\rangle \equiv |\downarrow\rangle|\uparrow\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |4\rangle \equiv |\uparrow\rangle|\uparrow\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

The Hamiltonian of independent atoms is,

$$\hat{H} = |\downarrow\rangle\langle\downarrow| \otimes |\uparrow\rangle\langle\uparrow|.$$

The discussion about the correct interpretation of the measurement process is still ongoing. Modern theories describe the state reduction in terms of *quantum decoherence* due to interactions of the system with the environment. Other interpretations involve *decoherent histories* or assume *multiple worlds* [537]. On the practical side, the current interest in quantum decoherence is motivated by the fact that this phenomenon may turn out to be the fundamental factor limiting the useful operation of quantum computers. Another interesting area where quantum mechanics meets classical physics is the phenomenon of quantum chaos.

### 16.1.2 The quantum jump

Obviously, the whole quantum measurement process, including the discontinuity of the state projection, could be fully understood within a grand model of the complete system, which would include the measuring device. In practice, this is illusory, because of the excessive number of degrees of freedom of the classical measuring device (e.g. a Schrödinger cat).

On the other hand, many characteristics of quantum measurement can be illustrated in a simple *three-level atom* with a weak transition representing the quantum sample and a strong transition representing the meter. The assertion defended in



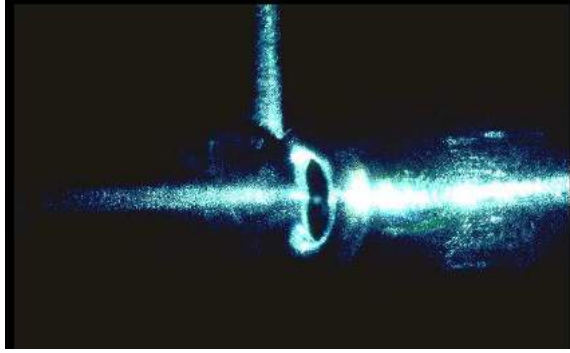


Figure 16.4: One of the first pictures of a single  $\text{Ba}^+$  ion.

the following is, that this three-level system, called *quantum amplifier*, gives a deep insight into what happens during the process of state reduction and, therefore, can be considered as paradigmatic for theories on quantum measurement.

To be able to discuss the dynamics of this system on a firmer ground, we will first introduce the quantum Monte Carlo wavefunction simulation method (MCWF).

### 16.1.2.1 Quantum Monte-Carlo wavefunction simulation of a two-level system

The possible occurrence of spontaneous emission produces a dynamics called *quantum trajectory*, which can be described by a non-hermitian *effective Hamiltonian*,

$$\hat{H}_{eff} = \hbar\Delta\sigma_z + \hbar\Omega\sigma^+ + c.c. - \frac{\imath}{2}\Gamma\sigma_z = \begin{pmatrix} 0 & \Omega \\ \Omega & \Delta - \imath\frac{\Gamma}{2} \end{pmatrix}, \quad (16.9)$$

aiming at including energy dissipation processes. The problem with this Hamiltonian is that, for being non-hermitian,  $[\hat{H}_{eff}, \hat{H}_{eff}^\dagger] \neq 0$ , it also generates a non-unitary dynamics,  $e^{-\imath\hat{H}_{eff}t} \neq e^{\imath\hat{H}_{eff}^\dagger t}$ . This means that the mere *possibility* of spontaneous emission prevents the reversibility of the dynamics. We observe a temporal decrease of the norm  $\langle\psi(t)|\psi(t)\rangle$  indicating a loss of energy,

$$\langle\psi|\psi\rangle = \langle\psi_0|e^{-\imath\hat{H}t}e^{\imath\hat{H}t}|\psi_0\rangle \longrightarrow e^{-\Gamma t}. \quad (16.10)$$

The loss of normalization during the evolution, until the next quantum jump occurs, is due to the dissipation of energy toward the reservoir,

$$\text{Tr } \rho_{sample} \rightarrow 0 \quad \text{while} \quad \text{Tr} \begin{pmatrix} \rho_{sample} & 0 \\ 0 & \rho_{reserv} \end{pmatrix} = 1, \quad (16.11)$$

and represents a measure of the probability that an irreversible process has occurred during the evolution time.

Dissipative processes can be simulated by playing dices with random numbers  $\zeta$ . We divide time into small intervals  $dt$  and propagate the wavefunction from  $\psi(t)$  to  $\psi(t+dt)$ . After each interval we evaluate the probability  $p = 1 - \langle\psi(t)|\psi(t)\rangle$

accumulated during the time period  $[0, t + dt]$  that a dissipative process (such as spontaneous emission) has occurred. Now, we generate a random number  $\zeta$ , uniformly distributed between 0 and 1, which we compare to probability the probability  $p$ . In case,  $\zeta > 1 - \langle \psi(t) | \psi(t) \rangle$ , we conclude that there was no dissipative process, and we let the system proceed in peace, only renormalizing the wavefunction to compensate for the losses [484, ?]. Otherwise, if  $\zeta < 1 - \langle \psi(t) | \psi(t) \rangle$ , we conclude that there was a dissipative process, and the system is projected into the eigenstate  $\psi_0$ . This projection is abrupt and called *quantum jump*. Now, the evolution restarts from zero, ruled by the effective Hamiltonian. The simulation implemented via,

$$|\psi(t)\rangle \rightsquigarrow |\psi(t + dt)\rangle \equiv \begin{cases} \frac{(1 - i\hat{H}dt)|\psi(t+dt)\rangle}{\sqrt{\langle \psi(t) | \psi(t) \rangle}} & \text{if } \zeta > 1 - \langle \psi(t) | \psi(t) \rangle \\ |\psi_0\rangle & \text{if } \zeta < 1 - \langle \psi(t) | \psi(t) \rangle \end{cases}. \quad (16.12)$$

This is the method called *quantum Monte Carlo wavefunction simulation*.

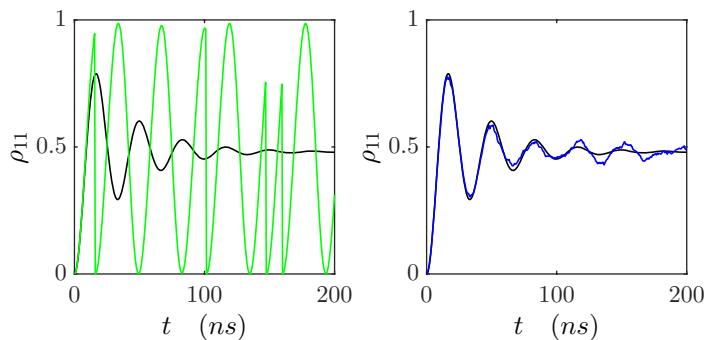


Figure 16.5: (code) a) Quantum Monte Carlo wavefunction simulation. It is important to be aware, that a trajectory generated by a MCWF simulation (16.12) only represents *one* of many possible trajectories of the system. (b) The evolution of the density matrix  $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$  (blue curve) is nothing else, than the average (black curve) over all possible MCWF trajectories for the system. A movie of this simulation can be watched here ([watch movie](#)).

The effective two-level Hamiltonian (16.9) dissipates via spontaneous emission, which is included in the dynamics through the *possibility* for the system to suffer a *state reduction*. The modification of  $|\psi(t)\rangle$  by *non-observation* of spontaneous emission, reduces the population of the state excited by  $1 - \frac{1}{2}\Gamma dt$ , while the ground state population remains unchanged. Every quantum jump projecting the system into the ground state constitutes a measurement, because it corresponds to a detected fluorescence photon.

### 16.1.2.2 Three-level systems: The epitome of quantum measurement

Let us now return to the mysterious interaction between the sample and the meter, which we want to unravel by comparing two possible procedures: 1. treating the sample and the meter separately and explain the extraction of information following the von Neumann postulate; 2. treating the sample and the meter by a global theory.

As said above, the inclusion of the meter in a global theory is, in general, difficult. For this reason, to perform the comparison, we choose the simplest imaginable system: the *three-level system* with two transitions connecting to a common ground state and excited by radiation fields. As shown in Fig. 16.6(a) this three-level system can be an atom with a strong transition and a weak transition, for example, the dipolar transition  $S_{1/2} - P_{1/2}$  and the forbidden quadrupolar transition  $S_{1/2} - D_{5/2}$  in a single  $\text{Ba}^+$  ion. We will now name the 'strong transition' as *meter* and the 'weak transition' as *sample* and show that this system allows to study the von Neumann measurement process including the direct observation of quantum jumps<sup>5</sup>. At the same time, the system is simple enough for a complete theoretical description. In this sense, the three-level system becomes the *epitome of a quantum measurement device*.

We turn our attention to the three-level atom: Obviously, the atom will preferentially scatter photons on its strong dipolar transition. However, at times when the valence electron is 'shelved' in the metastable state excited by the quadrupole transition, no fluorescence can be observed on the strong transition.

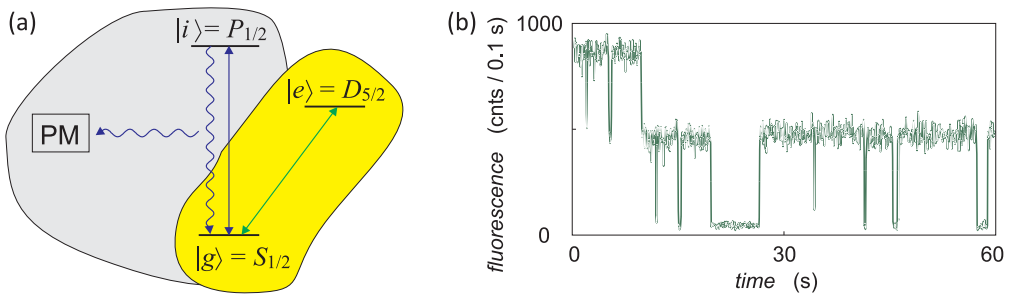


Figure 16.6: (a) Quantum measurement at the example of a three-level atom incorporating a weak (sample) transition and a strong (meter) transition. (b) *Random Telegraph signal* in the resonance fluorescence due to quantum jumps.

Quantum jumps were experimentally observed in single trapped ions, whose lowest energies form a three-level systems [516, 606, 607, 66].

### 16.1.2.3 Quantum Monte-Carlo wavefunction simulation of the quantum amplifier

When both lasers driving the weak and the strong transition are irradiated simultaneously, the coherence on the weak transition is easily perturbed by the dynamics of the strong transition. To resolve this problem *Dehmelt* invented what he called the *quantum amplifier*. The idea consists in alternately irradiating the *sample* laser (at stage  $S - D$  in Fig. 16.7) and the *meter* laser (at stage  $S - P$  in Fig. 16.7)<sup>6</sup>.

<sup>5</sup>The observability of quantum jumps as manifestations of sudden state reductions has been the object of long-standing debates: 'If we have to go on with these damned quantum jumps, then I'm sorry that I ever got involved with quantum mechanics.' [619].

<sup>6</sup>The absence of the 'meter' laser during the 'sample' stage avoids saturation broadening and light-shifts of the ground state. Since the ground state is shared by both transitions, its broadening would reduce the spectral overlap between the 'sample' transition and the driving laser and therefore the probability to excite the metastable level. This inhibition of the coherent dynamic by too strong or too frequent measurements is known as *quantum Zeno effect*: The more an observer tries to

The alternating irradiation of the lasers  $S - D$  and  $S - P$  can also be treated by the Monte Carlo quantum wavefunction simulation method (16.12) using the effective Hamiltonian,

$$\hat{H}_{eff} = \begin{pmatrix} 0 & \frac{1}{2}\Omega_{sp} & \frac{1}{2}\Omega_{sd} \\ \frac{1}{2}\Omega_{sp} & -\Delta_{sp} - \frac{i}{2}\Gamma_{sp} & 0 \\ \frac{1}{2}\Omega_{sd} & 0 & -\Delta_{sd} \end{pmatrix}, \quad (16.13)$$

where the Rabi frequencies  $\Omega_{sd}$  and  $\Omega_{sp}$  are switched on alternately.

In the simulation 16.7 the quantum jumps to the shelved metastable state  $D_{5/2}$  appear as long periods without population in the  $P_{1/2}$  level (first period  $S - P$ , where the population of  $S_{1/2}$ , illustrated by the red curve, gradually tends to 0 for long times). The reduction of the system to the shelved state actually occurs by *non-observation* of fluorescence on the strong transition. The projection needs a finite time, simply because we can not be sure whether the non-observation is actually due to shelving or the incidental absence of scattering events on the  $S - P$  transition: After all, it is not predictable, when the next photon will be spontaneously emitted, even though the lifetime of the excited state is short. But for longer observation times it becomes increasingly unlikely that the absence of photons is *not* due to shelving. It is this unlikeliness, which lets the population rapidly converge towards the metastable state. In the second  $S - P$  period, Fig. 16.7 shows fast transitions to the  $P_{1/2}$  followed by sudden decays to the ground state. These processes correspond to photon absorption and spontaneous reemission by the strong transition. The succession of the photon scattering events is so fast, that the signal recorded by photodetectors appears as a continuous fluorescence. The sudden transitions between bright and dark periods shown in Fig. 16.6(b), which occur totally randomly, are interpreted as quantum jumps.

#### 16.1.2.4 Comparison with Bloch equations and interpretation of quantum jumps

We already mentioned in Fig. 16.5, that a trajectory generated by a MCWF simulation (16.12) represents *one* possible evolution of the system. In Chp. 14.6.1 we got to know an alternative way of predicting the evolution of a system, based on density operator obeying a *master equation*, which in the context of atomic excitation levels is called Bloch equation. Comparing MCWF trajectories (red curves in Fig. 16.7) with Bloch vector evolutions (green curves) it becomes apparent, that the Bloch vector evolution does not produce quantum jumps, but is always smooth and continuous.

In most cases, our knowledge about the actual state of an atom comes from the collection of spontaneously emitted photons. The observation of a photon projects the atomic state into the ground state. However, this concept is not included in the Bloch equations, as we just saw in Fig. 16.7. So, as it seems, we have to take back our statement, that the three-level Bloch equation describe the complete system, although they somehow contain spontaneous emission.

Let us go one step back and ask, where the Bloch equations came from. In fact, as we learned in Sec. 15.4 and will deepen in Sec. 16.2, they are derived from a von Neumann equation for the three-level system *plus* the degrees of freedom of the

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extract information from a system, the more he inhibits its evolution. We will discuss this effect in more detail in Sec. 34.3.2.2.

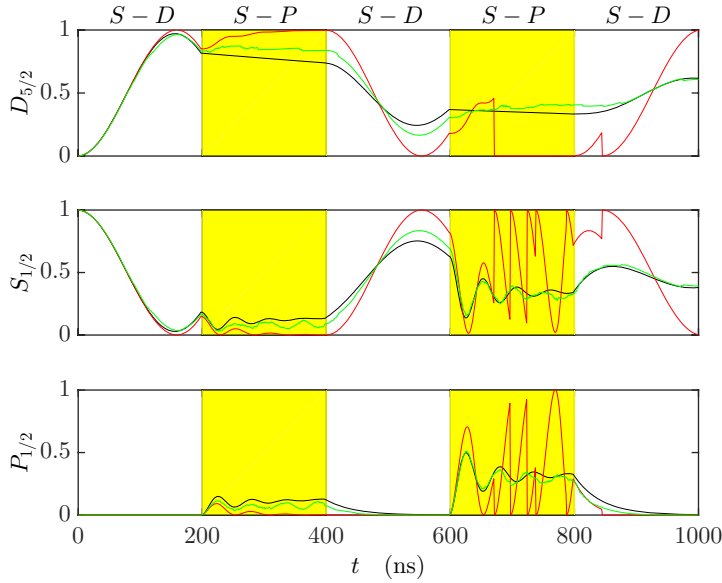


Figure 16.7: (code) Quantum amplifier comparing Monte-Carlo quantum simulations (red lines) and Bloch equations (black lines), which coincide well with the averages over 100 Monte-Carlo trajectories (green lines). The periods  $S - D$  (white background) represent the free evolution of the quantum system, the periods  $S - P$  (yellow background) represent the measurement periods.

vacuum modes receiving the spontaneously emitted photons by *tracing over the latter ones*.

We will not be able to handle all degrees of freedom. However, we can generalize the Bloch equations in the following way [495, 752]. We project the total density operator  $\rho_{AFR}$  of the atom plus the driving field plus the reservoir of vacuum modes into the subspace of the atom and the driving field consisting of exactly  $n$  photons,

$$\rho^{(n)} = \text{Tr}_R (P^{(n)} \rho_{AFR}) , \quad (16.14)$$

and derive, from the von Neumann equation, the master equation for the atomic state  $\rho^{(n)}$  under the constraint of a fixed number of photons  $n$  in the field. The master equation differs only in one term from the usual Bloch equations: The expression  $\Gamma_{12}\rho_{22}^{(n)}$ , which describes the spontaneous decay of the population of the excited state of the meter transition, is replaced by the expression  $\Gamma_{12}\rho_{22}^{(n-1)}$ :

$$\frac{d}{dt}\rho^{(n)} = (\mathcal{L}|1\rangle\Gamma_{12}\langle 2|)\rho^{(n)} + |1\rangle\Gamma_{12}\langle 2|\rho^{(n-1)} , \quad (16.15)$$

The substate with of  $n$  photons violates the trace condition,  $\sum_j \rho_{jj}^{(n)} \neq 1$ . The physical explanation for this is the following: While induced emission and absorption maintain the number of photons in the combined light-atom system (like in the Jaynes-Cummings model), spontaneous emission decreases the number of photons, leading to an irreversible loss of energy. The quantum jump observed in MCWF model

corresponds, in the modified equations (16.15), to a collapse of the subspace described by  $\rho^{(n)}$  with the time constant  $\Gamma_{12}$  and a birth of another subspace  $\rho^{(n-1)}$ , whose evolution is guided by another (analogous) Bloch equation, now for  $n - 1$  photons. Each fluorescence detection at time  $t = 0$  determines the initial condition for the future development of the system:  $\rho^{(n)}(0) = 0$  and  $\rho^{(n-1)}(0) = |1\rangle\langle 1|$ . The probability density  $c(t)$  for a new observation of spontaneous emission at time  $t$  with detection efficiency  $\eta$ , or in other words, the histogram of the durations of dark periods in the fluorescence signal is related to the solution  $\rho^{(n)}$  of the homogeneous part of the equation (16.14) via,

$$c(t) = \eta\Gamma_{12}\tilde{\rho}_{22}^{(n)}(t) = \eta \sum_{j=1}^4 \frac{d}{dt} \tilde{\rho}_{jj}^{(n)}(t) , \tag{16.16}$$

The second step immediately follows from the homogeneous part of equation (16.15).

### 16.1.2.5 Kraus operator for position measurement

As a canonical example of a Kraus operator [46, 125] we take  $\hat{H} = \hat{x} \otimes \hat{p}$ , where the position and the momentum satisfy the commutation relation,  $[\hat{x}, \hat{p}] = i$ . The initial state of the ancilla be a Gaussian distribution,

$$|\phi\rangle = \frac{1}{(2\pi\sigma^2)^{1/4}} \int dq' e^{-q'^2/4\sigma^2} |q'\rangle . \tag{16.17}$$

The position wavefunction of the ancilla is,

$$\phi(q) = \langle q|\phi\rangle = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-q^2/4\sigma^2} . \tag{16.18}$$

The Kraus operators are (compared to the previous discussion, we now let  $\lambda = 1$ ),

$$M(q) = \langle q|e^{-i\hat{x}\otimes\hat{p}}|\phi\rangle = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-(q-x)^2/4\sigma^2} , \tag{16.19}$$

since the operator  $e^{-i\hat{x}\otimes\hat{p}}$  makes a spatial translation when applied to the degree of freedom of the position. The corresponding POVM elements are,

$$E(q) = M_q^\dagger M_q = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(q-x)^2/2\sigma^2} , \tag{16.20}$$

which obey  $\int dq E(q) = \mathbb{I}$ .

Calculate  $\langle \psi_q|\psi_q\rangle = \langle \psi'|M(q)^\dagger M(q)|\psi'\rangle$ .

Note that  $\lim_{\sigma \rightarrow 0} E(q) = |x = q\rangle\langle x = q|$ . That is, in a particular limit, these operators converge to a strong measurement of position. For  $\sigma \rightarrow \infty$ , we speak of weak measurement.

Another example would be the three-level atom of Dehmelt's quantum amplifier.

### 16.1.3 *Welcher Weg* information

#### 16.1.3.1 The Elitzur and Vaidman bomb testing problem

Mixing the concepts of particles and waves we sometimes arrive at seemingly paradoxical conclusions. One example is Elitzur and Vaidman's *bomb testing problem*. They imagined a Mach-Zehnder interferometer with the particularity that the reflecting mirror of one of the arms be connected to a device measuring the photonic recoil. That is, when a photon passes through this arm, the mirror undergoes a small acceleration, which is sufficient to activate an explosive bomb.

Now, we distinguish two cases: 1. The recoil detector *does not work*, i.e. the bomb is not armed. 2. The bomb is *armed*. We now adjust the interferometer in a way to produce destructive interference in one of the two interferometer output ports. If, having sent many photons through the interferometer, we never saw any photons in the 'dark' port, we can be almost sure that the bomb is *not operational*.

In case the bomb is operational, the observation of a photonic recoil destroys the interference pattern at the interferometer outputs. It *has* to do so, because the exploding bomb informs us, in which arm the photon has passed. However, with an operational bomb the interference pattern is *also* destroyed, when the photon passes through the other arm, since the fact that the bomb didn't explode tells us, that the photon went the other way.

The funny conclusion is now, that it may happen, that a photon traverses the interferometer in the arm that does *not* contain the bomb and exits through the 'dark port'. The probability of this happening is only 25%, but nevertheless the observation of a photon in the 'dark port' informs us that the pump is operative without ever having interacted with it <sup>7</sup>.

### 16.1.4 Exercises

#### 16.1.4.1 Ex: Dispersive quantum jumps

Consider a three-level system in V-configuration, as depicted in Fig. 14.6(b), with an unstable state  $|1\rangle$ , a ground state  $|2\rangle$ , and a metastable state  $|3\rangle$ . Discuss whether the atom shelved in state  $|3\rangle$  is sensitive to light-shift and power broadening induced by a laser resonant to the  $|1\rangle - |2\rangle$  transition. E.g. will power-broadening only effect the transition rate  $|1\rangle \rightarrow |3\rangle$  or also  $|3\rangle \rightarrow |1\rangle$ ?

## 16.2 Open systems and the master equation

Let us now derive the master equation for an open quantum system. We assume that the environment (also called *bath* or *reservoir*) and the system under consideration are quantum systems in the sense that (1) the relevant degrees of freedom are completely characterized by state vectors (or density matrices), and (2) the temporal evolution of the total system is unitary  $U(t) = e^{-i\hat{H}t}$ . The total Hamiltonian,  $\hat{H} = \hat{H}_{sys} + \hat{H}_{res} + V$  is assumed to be independent of time and consists of three parts, namely the Hamiltonian of the system  $\hat{H}_{sys}$ , the Hamiltonian of the bath  $\hat{H}_{res}$ , and the

<sup>7</sup>See [https://www.thorlabs.com/newgrouppage9.cfm?objectgroup\\_id=6635](https://www.thorlabs.com/newgrouppage9.cfm?objectgroup_id=6635)

interaction  $V$  between the system and the bath. The purpose of the master equation is to find the dynamics of the system by tracing over all degrees of freedom of the bath. This is not always possible, and we will assume that the interaction  $V$  is sufficiently weak, so that perturbation theory is applicable.

In the interaction representation the evolution of the total density matrix  $\hat{\rho}_{tot}$  becomes,

$$\boxed{i\hbar \frac{d\tilde{\rho}_{tot}}{dt} = [\tilde{V}(t), \tilde{\rho}_{tot}]} . \quad (16.21)$$

where  $\tilde{\rho}_{tot}(t) \equiv U_0^\dagger \rho_{tot} U_0$  and  $\tilde{V}(t) \equiv U_0^\dagger V U_0$  and  $U_0 = e^{-i(\hat{H}_{sys} + \hat{H}_{res})t/\hbar}$ . This evolution is, for the time being, very general, and the solution can be formally written,

$$\tilde{\rho}_{tot}(t) = \tilde{\rho}_{tot}(0) + \frac{1}{i\hbar} \int_0^t dt_1 [\tilde{V}(t_1), \tilde{\rho}_{tot}(t_1)] . \quad (16.22)$$

Iterating once again:

$$\tilde{\rho}_{tot}(t) = \tilde{\rho}_{tot}(0) + \frac{1}{i\hbar} \int_0^t dt_1 [\tilde{V}(t_1), \tilde{\rho}_{tot}(0)] + \frac{1}{(i\hbar)^2} \int_0^t dt_1 \int_0^{t_1} dt_2 [\tilde{V}(t_1), [\tilde{V}(t_2), \tilde{\rho}_{tot}(t_2)]] . \quad (16.23)$$

In the following, we will call several approximations to simplify the calculations, in particular, the Born approximation, the assumption that the initial state is a product state and, later-on, the Markov approximation.

### 16.2.1 Born approximation for weak coupling

We will now assume the interaction  $\tilde{V}$  to be weak. We can then expect that, repeating the iterative process, the series will converge and write the general solution as,

$$\tilde{\rho}_{tot}(t) = \tilde{\rho}_{tot}(0) + \sum_{n \geq 1} \frac{1}{(i\hbar)^n} \int_0^t dt_1 \dots \int_0^{t_{n-1}} dt_n [\tilde{V}(t_1), \dots, [\tilde{V}(t_n), \tilde{\rho}_{tot}(0)]] . \quad (16.24)$$

This way of terminating an iterative equation by  $\rho_{tot}(0)$  is generally known as the *Born approximation*. Here, we will just go to second order in  $\tilde{V}$ . Tracing over the bath,

$$\tilde{\rho}_{sys}(t) = \text{Tr}_{res} \tilde{\rho}_{tot}(t) , \quad (16.25)$$

we extract the density matrix for only the system,

$$\begin{aligned} \tilde{\rho}_{sys}(t) &= \tilde{\rho}_{sys}(0) + \frac{1}{i\hbar} \int_0^t dt_1 \text{Tr}_{res} [\tilde{V}(t_1), \tilde{\rho}_{tot}(0)] \\ &+ \frac{1}{(i\hbar)^2} \int_0^t dt_1 \int_0^{t_1} dt_2 \text{Tr}_{res} [\tilde{V}(t_1), [\tilde{V}(t_2), \tilde{\rho}_{tot}(0)]] . \end{aligned} \quad (16.26)$$

### 16.2.2 Assumption of an initial product state

Next, we need to make the quite important assumption, that the initial state between the system and the environment are not correlated, or mathematically speaking, they can be written as product states,

$$\tilde{\rho}_{tot}(0) = \tilde{\rho}_{sys}(0) \otimes \rho_{res}(0) . \quad (16.27)$$



Another assumption, which is not essential but often valid, is that  $\text{Tr}_{res}[\tilde{V}(t_1), \tilde{\rho}_{tot}(0)] = 0$ . If this is the case, then the first-order term will vanish. In second order, we can write,

$$\tilde{\rho}_{sys}(t) = e^{\mathcal{M}(t)} \tilde{\rho}_{sys}(0) \quad (16.28)$$

where  $\mathcal{M}(t)\chi \equiv \frac{1}{(i\hbar)^2} \int_0^t dt_1 \int_0^{t_1} dt_2 \text{Tr}_{res} \left[ \tilde{V}(t_1), [\tilde{V}(t_2), \chi \otimes \rho_{res}] \right]$ ,

is a *superoperator* acting on the operator density of the system. Taking the temporal derivative, we have the explicit master equation,

$$\boxed{\begin{aligned} \frac{d\tilde{\rho}_{sys}(t)}{dt} = \mathcal{L}\rho_{sys}(t) &= \frac{d}{dt} (\mathcal{M}(t)\tilde{\rho}_{sys}(t)) \\ &= \frac{1}{(i\hbar)^2} \int_0^t d\tau \text{Tr}_{res} \left[ \tilde{V}(t), [\tilde{V}(\tau), \tilde{\rho}_{sys}(t) \otimes \rho_{res}] \right] \end{aligned}} \cdot \quad (16.29)$$

The superoperator  $\mathcal{L}$  is called *Lindblad operator*.

### 16.2.3 Markov approximation for short memory

Here, we have to evaluate the terms involving the average with respect to the thermal bath, which is assumed to have a short memory, in the sense that the correlation time is very short. Mathematically,

$$\begin{aligned} \int_0^t d\tau \text{Tr}_{res} \left( \tilde{V}(t)\tilde{V}(\tau)\rho_{res} \right) &= \int_0^t d\tau \text{Tr}_{res} \left( \tilde{V}(t-\tau)\tilde{V}(0)\rho_{res} \right) \\ &\simeq \int_0^\infty d\tau \text{Tr}_{res} \left( \tilde{V}(t-\tau)\tilde{V}(0)\rho_{res} \right) \end{aligned} \quad (16.30)$$

In other words, the two-point correlation function is significant only, when  $t \simeq \tau$ , and it is valid to extend the upper bound to infinity. This is the *Markov approximation*.

### 16.2.4 Example: Damped harmonic quantum oscillator

As an example, we let us consider the master equation for the *Brownian motion of a quantum harmonic oscillator*. It can be written,

$$\frac{d\tilde{\rho}_{sys}}{dt} = \frac{1}{(i\hbar)^2} \int_0^t d\tau \text{Tr}_{res} \left\{ \begin{array}{l} \tilde{V}(t)\tilde{V}(\tau)\tilde{\rho}(t) \otimes \rho_{res} - \tilde{V}(t)\tilde{\rho}_{sys}(t) \otimes \rho_{res}\tilde{V}(\tau) \\ -\tilde{V}(\tau)\tilde{\rho}_{sys}(t) \otimes \rho_{res}\tilde{V}(t) + \tilde{\rho}_{sys}(t) \otimes \rho_{res}\tilde{V}(\tau)\tilde{V}(t) \end{array} \right\} \cdot \quad (16.31)$$

The coupling of the system to the bath is assumed to be of the form,

$$\tilde{V} = \hbar \left( \hat{a}^\dagger \hat{\Gamma}(t) e^{i\Omega t} + \hat{a} \hat{\Gamma}^\dagger(t) e^{-i\Omega t} \right), \quad (16.32)$$

where  $\hat{\Gamma}(t) = \sum_k g_k \hat{b}_k e^{-i\omega_k t}$ , the bosonic operators  $\hat{a}$  and  $\hat{b}_k$  act, respectively, on the system (with the frequency  $\Omega$ ) and the bath (with the frequency  $\omega_k$ ). Here,  $g_k$

characterizes the coupling force between the oscillators of the system and the bath. Hence,

$$\frac{d\tilde{\rho}_{sys}}{dt} = - \int_0^t d\tau \text{Tr}_{res} \left\{ \begin{array}{l} (a^\dagger \Gamma(t) e^{i\Omega t} + a \Gamma^\dagger(t) e^{-i\Omega t}) (a^\dagger \Gamma(\tau) e^{i\Omega \tau} + a \Gamma^\dagger(\tau) e^{-i\Omega \tau}) \tilde{\rho}(t) \otimes \rho_{res} \\ - (a^\dagger \Gamma(t) e^{i\Omega t} + a \Gamma^\dagger(t) e^{-i\Omega t}) \tilde{\rho}(t) \otimes \rho_{res} (a^\dagger \Gamma(\tau) e^{i\Omega \tau} + a \Gamma^\dagger(\tau) e^{-i\Omega \tau}) \\ - (a^\dagger \Gamma(\tau) e^{i\Omega \tau} + a \Gamma^\dagger(\tau) e^{-i\Omega \tau}) \tilde{\rho}(t) \otimes \rho_{res} (a^\dagger \Gamma(t) e^{i\Omega t} + a \Gamma^\dagger(t) e^{-i\Omega t}) \\ + \tilde{\rho}(t) \otimes \rho_{res} (a^\dagger \Gamma(\tau) e^{i\Omega \tau} + a \Gamma^\dagger(\tau) e^{-i\Omega \tau}) (a^\dagger \Gamma(t) e^{i\Omega t} + a \Gamma^\dagger(t) e^{-i\Omega t}) \end{array} \right\} \quad (16.33)$$

Let's take a closer look at one of the terms,

$$\begin{aligned} T &\equiv - \int_0^t d\tau \text{Tr}_{res} \{ a^\dagger \Gamma(t) e^{i\Omega t} a \Gamma^\dagger(\tau) e^{-i\Omega \tau} \tilde{\rho}(t) \otimes \rho_{res} \} \\ &= -a^\dagger a \tilde{\rho}(t) \int_0^t d\tau \langle \Gamma(t) \Gamma^\dagger(\tau) \rangle_{res} e^{i\Omega t} e^{-i\Omega \tau} . \end{aligned} \quad (16.34)$$

We will have to evaluate quantities such as

$$\text{Tr}_{res} (V(t)V(s)\rho_{res}) = \hbar^2 a^\dagger a \langle \Gamma(t) \Gamma^\dagger(t) \rangle_{res} e^{i\Omega(t-s)} + \hbar^2 a a^\dagger \langle \Gamma^\dagger(t) \Gamma(t) \rangle_{res} e^{-i\Omega(t-s)} , \quad (16.35)$$

where  $\langle \Gamma(t) \Gamma^\dagger(t) \rangle_{res} \equiv \text{Tr}_{res} [\Gamma(t) \Gamma^\dagger(t) \rho_{res}]$ , and for the thermal bath,  $\langle b_j^\dagger b_k \rangle = \delta_{jk} n_k$  and  $\langle b_j b_k^\dagger \rangle = \delta_{jk} (1 + n_k)$  and  $n_k = (e^{\beta \hbar \omega_k} - 1)^{-1}$ . Hence,

$$\begin{aligned} T &= -a^\dagger a \tilde{\rho}(t) \sum_{j,k} g_j g_k \langle b_j b_k^\dagger \rangle_{res} \int_0^t d\tau e^{i(\omega_j t - \omega_k \tau)} e^{i\Omega(t-\tau)} \\ &\simeq -a^\dagger a \tilde{\rho}(t) \sum_k g_k^2 n_k \int_0^\infty d\tau e^{i(\omega_k - \Omega)(t-\tau)} . \end{aligned} \quad (16.36)$$

Then we will have to use the relationship,

$$\int_0^\infty d\tau e^{\pm i\varepsilon \tau} = \pi \delta(\varepsilon) \pm iPV , \quad (16.37)$$

where  $PV$  denotes Cauchy part of the principal value. These correspond to a 'Lamb shift' and a 'Stark shift' of the frequency, which are considered to be small in comparison to  $\Omega$  and should be neglected here,

$$\begin{aligned} T &= -a^\dagger a \tilde{\rho}(t) \sum_k g_k^2 (e^{\beta \hbar \omega_k} - 1)^{-1} \int_0^\infty d\tau e^{i(\omega_k - \Omega)(t-\tau)} \\ &= -a^\dagger a \tilde{\rho}(t) \sum_k g_k^2 (e^{\beta \hbar \omega_k} - 1)^{-1} \pi \delta(\omega_k - \Omega) \\ &= -a^\dagger a \tilde{\rho}(t) \sum_k g_k^2 (e^{\beta \hbar \Omega} - 1)^{-1} \pi = -\pi N a^\dagger a \tilde{\rho}(t) \sum_k g_k^2 \delta(\omega_k - \Omega) = N a a^\dagger \tilde{\rho}(t) \pi \frac{\gamma}{2} . \end{aligned} \quad (16.38)$$

where  $N \equiv (e^{\beta \hbar \Omega} - 1)^{-1}$ . We define  $\frac{\gamma}{2} \equiv \sum_k g_k^2 \delta(\omega_k - \Omega)$ . The procedure can be repeated for all terms in the master equation. We then obtain the master equation for a damped harmonic oscillator,

$$\frac{d\tilde{\rho}}{dt} = \frac{\gamma}{2} (N + 1) (2a\tilde{\rho}a^\dagger - a^\dagger a \tilde{\rho} - \tilde{\rho} a^\dagger a) - \frac{\gamma}{2} N (2a^\dagger \tilde{\rho} a - a a^\dagger \tilde{\rho} - \tilde{\rho} a a^\dagger) . \quad (16.39)$$

### 16.2.5 Deriving the Heisenberg-Langevin from the master equation

The Heisenberg-Langevin equation for the operators  $\hat{A}$  of a system subject to dissipation with rates  $\gamma_k$  via the degrees of freedom  $\hat{L}_k$  and the *master equation* for the density operator  $\hat{\rho}$  are equivalent descriptions for the time-evolution of a system,

$$\begin{aligned} \frac{d\hat{\rho}}{dt} &= \mathcal{L}\hat{\rho} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \sum_k \gamma_k \left( \hat{L}_k \hat{\rho} \hat{L}_k^\dagger - \frac{1}{2} \hat{L}_k^\dagger \hat{L}_k \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{L}_k^\dagger \hat{L}_k \right) \\ \frac{d\hat{A}}{dt} &= \mathcal{L}^\dagger \hat{A} = \frac{i}{\hbar}[\hat{H}, \hat{A}] + \sum_k \gamma_k \left( \hat{L}_k^\dagger \hat{A} \hat{L}_k - \frac{1}{2} \hat{L}_k^\dagger \hat{L}_k \hat{A} - \frac{1}{2} \hat{A} \hat{L}_k^\dagger \hat{L}_k \right), \end{aligned} \quad (16.40)$$

as we will show in Exc. 16.2.6.2. The former stresses the Schrödinger picture and the latter the Heisenberg picture. In particular, the dissipative *Lindblad terms* are equivalent.

### 16.2.6 Exercises

#### 16.2.6.1 Ex: Master equation for cavities

Be  $\kappa$  the loss rate for photons by transmission through the mirrors of a cavity. Show that the master equation gives,

$$\frac{d\hat{\rho}}{dt} = \frac{\kappa}{2}(\bar{n} + 1) (2\hat{a}\hat{\rho}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}) - \frac{\kappa}{2}\bar{n} (2\hat{a}^\dagger\hat{\rho}\hat{a} - \hat{a}\hat{a}^\dagger\hat{\rho} - \hat{\rho}\hat{a}\hat{a}^\dagger),$$

where the density operator is defined by  $\rho \equiv \sum_{m,n} P_{m,n} |m\rangle\langle n|$  and  $\bar{n}$  is the number of thermal photons.

#### 16.2.6.2 Ex: Deriving the Heisenberg-Langevin from the master equation

Derive the Heisenberg-Langevin from the master equation including the dissipative Lindblad terms.

## 16.3 Repeated measurements

### 16.3.1 The quantum Zeno effect

A famous problem raised by the Greek philosopher (490-430 AC) *Zeno* goes like this: Achilles and a turtle organize a race. The arrogant Achilles leaves a 100-meter lead to the turtle. The race begins. Achilles soon covers the 100 meters, only to find out that meanwhile the turtle has advanced by 10 meters. He continues running to cover the 10 meters, only to find out that meanwhile the turtle has advanced by 1 meter, and so on <sup>8</sup>. A presentation on the subject is available at [\(watch talk\)](#).

<sup>8</sup>In another version of his paradox, Zeno questions the possibility of motion at the example of a flying arrow: At any instant of time it occupies a space equal to its size. That is, at any particular moment of its flight, it is at rest, in a space that does not move. That is, any kind of motion is impossible. Nowadays, we know that this paradox is false, because time and motion are not discrete. But this can only be understood on the basis of infinitesimal calculus [490].

Interestingly, Zeno’s problem has a counterpart in quantum mechanics. Let us do the following Gedankenexperiment: A laser beam passes through a dense series of  $n$  polarizers, each one being rotated by an angle  $\frac{\pi}{2n}$  with respect to the preceding one. Each polarizer performs a local measurement of beam polarization. The result of this arrangement is that, in the limit of an infinitely dense series, the continuous measurement of the system completely governs its evolution and rotates the polarization by an angle of  $\pi/2$  <sup>9</sup>.

In every version of the *Zeno effect*, the system is inhibited from evolving freely, because of too frequent measurements of its current state. Achilles would surely be able to overtake the turtle, if he did not always check on her to assess the remaining distance [356] <sup>10</sup>.

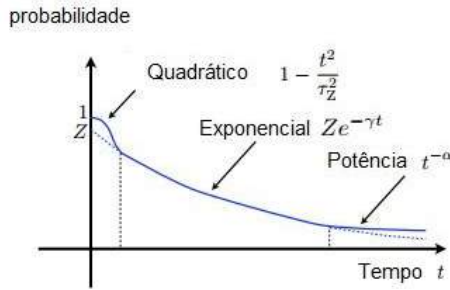


Figure 16.8: Quadratic time dependence of an excited state population.

The temporal evolution of the wavefunction of a system described by the Hamiltonian  $\hat{H}$  is  $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi_0\rangle$ . We can then calculate the amplitude and probability for the system to stay in the initial state,

$$\langle\psi_0|\psi(t)\rangle = \langle\psi_0|e^{-i\hat{H}t/\hbar}|\psi_0\rangle \quad \text{and} \quad P(t) = |\langle\psi_0|\psi(t)\rangle|^2. \quad (16.41)$$

For short times we can expand,

$$\langle\psi_0|\psi(\delta t)\rangle = |\psi_0\rangle - \frac{i}{\hbar}\hat{H}\delta t|\psi_0\rangle - \frac{1}{2\hbar^2}\hat{H}^2\delta t^2|\psi_0\rangle + \dots = |\psi_0\rangle + |\delta\psi\rangle, \quad (16.42)$$

such that,

$$\langle\psi_0|\psi(\delta t)\rangle \simeq 1 - \frac{i}{\hbar}\hat{H}\delta t - \frac{1}{2\hbar^2}\hat{H}^2\delta t^2 \quad \text{and} \quad P(\delta t) \simeq 1 - \frac{1}{\hbar^2}(\langle\hat{H}^2\rangle_0 - \langle\hat{H}\rangle_0^2)\delta t^2. \quad (16.43)$$

In this way we can extract the Zeno time from the above equations,  $\tau_Z = \hbar^2/\sqrt{\langle\hat{H}^2\rangle_0 - \langle\hat{H}\rangle_0^2}$ . We now make  $N$  successive von Neumann measurements within a time  $t$ , which leads to a measurement frequency of  $\tau^{-1}$ . The measurements are conceived as to verify,

<sup>9</sup>An analogous experiment can be imagined by a series of Stern-Gerlach measurements of the spin of an atom.

<sup>10</sup>The quantum Zeno effect was often used to justify the physical relevance of the state reduction postulate. It was shown, however, that this postulate is not essential for understanding the quantum Zeno effect [54]. The effect already follows directly from the Schrödinger equation and therefore has a purely dynamical nature. This shows that the projection is a purely mathematical construct without physical reality (see Sec. 16.1.2).

whether the system is still in its initial state, but each measurement projects our system back to its initial state, from where it has to start the transition process from scratch. Under these conditions, the population of the initial state will evolve like,

$$P^{(N)}(\tau) = P^{(N)}(t/N)^N . \quad (16.44)$$

Fig. 16.9 shows the evolution for five measurements separated by time intervals  $\tau$ . In comparison with the evolution, when no measurements are taken (dashed line), the evolution with measurements inhibits the depletion of the initial state. Extrapolating the number of measurements to infinity, the probability (16.44) converges to 1,

$$\left[ 1 - \left( \frac{t}{N\tau_Z} \right)^2 \right]^N \xrightarrow{N \text{ large}} e^{-t^2/N\tau_Z^2} \xrightarrow{N \rightarrow \infty} 1 . \quad (16.45)$$

See Excs. 16.3.4.1 and 16.3.4.2.

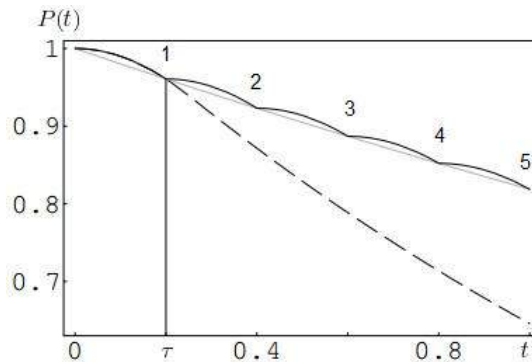


Figure 16.9: Inhibition of the decay of a state by repeated measurements (here  $N = 5$ ). The dashed (solid) line represents the survival probability with (without) measurements. The gray line represents an exponential interpolation function.

Suppression of the evolution of a quantum system due to the quantum Zeno effect was observed experimentally [356] using beryllium ions. Nevertheless, the discussion about the correct interpretation of this effect and its relationship to trivial power broadening is not closed. Some works have even proposed the possibility of an anti-Zeno effect [13, 702], where observation would accelerate the evolution of the system. Currently the quantum Zeno effect is also studied for possible applications in metrology, computation, and quantum information [394].

When the quantum Zeno effect was proposed for the first time, it was considered a paradox: How could an unstable particle never decay, just by being continually observed? And what would happen to Schrödinger's cat, whose live depends on state of the particle? Could we save it from its cruel fate just by observing it?

Another interesting question concerns the quantum nature of the quantum Zeno effect. Is it really non-classical? On one hand, the quantum Zeno effect supposes the complete reduction of the system to an eigenstate. However, we can imagine classical measurements that also reduce the state (such as the above-mentioned measurement of the polarization of a beam of light).

### 16.3.2 Quantum projection noise

The intrinsic indeterminism of quantum mechanics has serious consequences for metrology. To show this, we consider the example of a system of two levels  $|+\rangle$  and  $|-\rangle$ . This system can be in a superposition state  $|\psi\rangle$ . The probability<sup>11</sup> to find the system in one of the two states  $|\pm\rangle$  is,

$$p_{\pm} = \langle \hat{P}_{\pm} \rangle = |\langle \psi | \pm \rangle|^2 = 1 - p_{\mp} , \quad (16.46)$$

where  $\hat{P}_{\pm}$  is the projection operator. The result of a measurement of the population is afflicted by an inherent uncertainty expressed by the variance,

$$(\Delta p_{\pm})^2 = \langle \hat{P}_{\pm}^2 \rangle - \langle \hat{P}_{\pm} \rangle^2 = \langle \pm | \psi \rangle \langle \psi | \psi \rangle \langle \psi | \pm \rangle - (\langle \pm | \psi \rangle \langle \psi | \pm \rangle)^2 = p_{\pm}(1 - p_{\pm}) . \quad (16.47)$$

In other words, the random projection of the system on the eigenstate basis induces a noise called *quantum projection noise*<sup>12</sup>. This noise inhibits the determination of the probabilities  $p_{\pm}$  in a single measurement. On the other hand, by measuring populations on a sample of  $N$  atoms or by repeating the measurement  $N$  times with a single atom under identical conditions, we can reduce the uncertainty. The probability of finding an atom  $r$  times in the state  $|+\rangle$  is [355],

$$P_{N,r,+} = \binom{N}{r} p_+^r (1 - p_+)^{N-r} . \quad (16.48)$$

The expectation value and variance of this binomial distribution are [355],

$$\bar{r} = \sum_{r=0}^N r P_{N,r,+} = N p_+ \quad , \quad (\Delta r)^2 = \sum_{r=0}^N (r - N p_+)^2 P_{N,r,+} = N p_+ (1 - p_+) . \quad (16.49)$$

Thus, the standard deviation decreases with the number of atoms or measurements,

$$\sigma = \frac{\Delta r}{\bar{r}} \sim \frac{1}{\sqrt{N}} . \quad (16.50)$$

The increase of knowledge on the population of a two-level system by repeated measurements can be illustrated by a simple simulation exhibited in Fig. 16.10(a). Experiments are performed by comparing  $p_2$  with a random number  $\eta$ . Two outcomes are possible  $r = 0, 1$ . The histograms narrow as the number of experiments increases. In practice, a measurement is performed using the quantum amplifier method illustrated in Fig. 16.6 [347].

#### 16.3.2.1 Rabi experiments

The method of repeated measurements can be extended to map time-dependent dynamics of the two-level system. Under the influence of a radiation field, the population

<sup>11</sup>We adopt here the viewpoint of the Copenhagen interpretation of the quantum state reduction, but we note that a discussion based on statistical mixtures described by density matrices gives the same results.

<sup>12</sup>Projection noise can be interpreted as *shot noise*. However, the optical shot noise in photodetectors is generated by the repartition of the field energy into discrete photons, the projection noise is the consequence of the discretization of the electronic excitation levels.

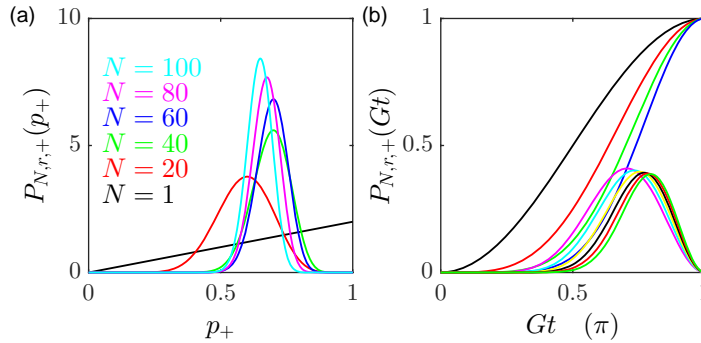


Figure 16.10: (code) (a) Simulation of the increase of knowledge on the population of a two-level system by repeated measurement,  $P_{N,r,+}(p_+)/\int_0^1 P_{N,r,+}(p_+)dp_+$ . The population of the state  $|+\rangle$  was set to  $p_+ = 0.2$ . (b) Determination of the most likely Rabi pulse length  $Gt = 2 \arcsin(r/N)^{1/2}$ .

of the two-level system (which we assume free of spontaneous emission) performs Rabi oscillations,  $\rho_{++}(t) = \frac{\Omega^2}{G^2} \sin^2 \frac{Gt}{2}$ , where  $G = \sqrt{\Delta^2 + \Omega^2}$ . The probability of finding the system in state  $|2\rangle$ , therefore, varies in time,  $p_+(t) = \rho_{++}(t)$ , and the binomial distribution (16.48) becomes,

$$P_{N,r,+}(t) = \binom{N}{r} \left(\frac{\Omega}{G}\right)^{2N} \sin^{2r} \frac{Gt}{2} \cos^{2N-2r} \frac{Gt}{2}. \quad (16.51)$$

When we increase the number of measurements,  $N \rightarrow \infty$ , this function condenses around a narrow peak at the position  $Gt = 2 \arcsin \sqrt{r/N}$ . The width of the peak evolves like  $2 \arccos(2^{-1/2N})$ . Fig. 16.10(b) shows a simulation demonstrating how repeated measurements gradually pin down the pulse area  $\Omega t$ .

In summary, even for perfectly efficient population measurements (e.g. using the microwave-optical double resonance method) it is impossible to measure the probability  $p_+$  with a single atom in a single experiment. As such an observation only admits two possible results, 'fluorescence observed' or 'fluorescence not observed', i.e.  $\rho_{++} = 1$  or  $\rho_{++} = 0$ , a whole range of possible populations between 0 and 1 is excluded. Therefore, a single observation only provides 'partial' information, which can be gradually improved with each consecutive observation.

A presentation on this topic is available here [\(watch talk\)](#).

### 16.3.2.2 Ramsey experiments

The Ramsey experiment is basically equivalent to the Rabi experiment described above except for an additional rotation in configuration space allowing for the measurement of the phase precession of the coherence between the Ramsey pulses via population spectroscopy. The Ramsey fringes are approximated by  $p_+ = 0.5(1 + \cos[(\omega - \omega_0)T])$ . The interesting magnitude is the frequency uncertainty,

$$\frac{\Delta r}{(\partial r / \partial \omega)|_{(\omega - \omega_0)T = \pi/2}} = \frac{\sqrt{N p_+(1-p_+)}}{N(\partial p_+ / \partial \omega)} = \frac{1}{T\sqrt{N}}. \quad (16.52)$$

### 16.3.2.3 Spin squeezing and the Heisenberg limit

The above considerations apply to *independent measurements*. When the atoms are maximally correlated they occupy EPR-like states,  $|\psi\rangle = p_+|++\dots\rangle + p_-|---\dots\rangle$ , such that it is sufficient to measure a single atom to know the state of all others. This means that the ratio  $\Delta r/\bar{r}$  is just the one of a single measurement, but the signal strength and hence the signal-to-noise ratio increase by the factor  $N$ . Thus the standard deviation scales with  $1/N$  rather than with  $1/\sqrt{N}$ . This is the so-called *Heisenberg limit*. For Ramsey interferometers we get [724, 87, 99, 480],

$$\frac{\Delta r}{(\partial r/\partial\omega)|_{(\omega-\omega_0)T=\pi/2}} = \frac{1}{TN} . \quad (16.53)$$

**Example 73 (Interferometry with condensates):** It is an interesting question, whether condensates can improve metrology and enhance the precision of atomic clocks. The answer is *no*, if we only replace the thermal atomic cloud by a condensate! To see this, we consider an interferometer in configuration space measuring a phase (and therefore a frequency shift) by the method of Ramsey spectroscopy. The states are coupled by a radiation adjusted for  $\pi/2$  pulses. The condensate *Fock state* factorizes the Schrödinger equation with the Hamiltonian  $\hat{H} = \sum_{i=1}^N (H^{(i)} + V_{12}^{(i)})$  into  $N$  identical equations for every single atom. The dynamic evolution of this state will be the same as the one for a thermal state. However, this is not true for two Fock state condensates in both entrance channels of the interferometer.

The first radiative beamsplitter divides  $N_1$ . This division produces an atom number uncertainty in each state, which come together with a well-defined phase relationship between the two states. By providing at the second port of the interferometer another Fock state  $N_2$ , one increases the atom number uncertainty and therefore (because entropy must be conserved in coherent processes) the phase precision. It's a bit like a massive parallel computing for every possible repartition of the populations of both states. Of course the two Fock states cannot be obtained by dividing a single condensate in two in a coherent manner, except if the repartition is measured afterward.

The Fock state is a maximally *spin-squeezed state* (sub-Poissonian statistics). The beam-splitters (which only perform unitary rotations) create starting from the Fock state a quantum entanglement, which is the deeper reason for the improvement of the resolution of the interferometer up the the Heisenberg limit by reducing the *quantum projection noise* [99].

Quantum correlations and spin-squeezed states are the same phenomena seen in different bases. Often the term of *quantum entanglement* is used in an energy bases, while spin squeezing is described in a Dicke state bases.

We may also consider real space interferometers. This allows us to use for creating the Fock states the recently discovered method of transforming BECs into *Mott insulator* states. Of course it is important to use condensates. First of all, we need Fock states, i.e. states with strong on-site quantum correlations with well-defined phase relations between every pair of atoms from the same site. Furthermore, Mott insulators have thus far only been seen with CBEs.



### 16.3.3 Quantum non-demolition measurements

#### 16.3.4 Exercises

##### 16.3.4.1 Ex: The quantum Zeno effect

Discuss the quantum Zeno effect at the example of a laser beam passing through a birefringent medium. Compare the situations without polarizers and with an infinite number of vertical polarizers.

##### 16.3.4.2 Ex: The quantum Zeno effect

A two-level atom resonantly driven by a laser can be described by the Hamiltonian:

$$H = \begin{pmatrix} 0 & \frac{1}{2}\Omega \\ \frac{1}{2}\Omega & 0 \end{pmatrix}.$$

The solution of the Schrödinger equation gives,

$$|\psi(t)\rangle = e^{-it\hat{H}/\hbar}|\psi_0\rangle = \begin{pmatrix} \cos \frac{1}{2}\Omega t & i \sin \frac{1}{2}\Omega t \\ i \sin \frac{1}{2}\Omega t & \cos \frac{1}{2}\Omega t \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

provided the atom is initially in the ground state  $\langle\psi_0| = (1 \ 0)$ . A measurement of the ground state population can only be done by a projection of the wavefunction, that is, the measurement yields the result  $\| |1\rangle\langle 1|\psi(t)\rangle \|^2$ . What is the final state of the atom,

- when the ground state population is measured once after an evolution time of  $t = \pi/\Omega$ ;
- when the ground state population is measured once after  $n$  time intervals  $t_n = \pi/n\Omega$ ;
- when the ground state population is measured  $n$  times after evolution times of  $t_n = \pi/n\Omega$ ;
- when  $n \rightarrow \infty$ .

##### 16.3.4.3 Ex: The quantum Zeno effect

Consider a system described by a time-independent Hamiltonian  $\hat{H}$ .

- Calculate the probability  $P(t)$  of the system to remain in its initial state  $|\Psi_0\rangle$  in the short time approximation, that is, considering until the second-order expression expansion term for the probability. Use the simplification:

$$\tau_z = \frac{\hbar}{\sqrt{\langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2}},$$

where the term  $\tau_z$  is called the Zeno time.

- If  $N$  measurements are performed during a time  $t$ , we have the time interval  $T = t/N$  between measurements. When a measurement is performed, the system is projected on the initial state and the temporal evolution must start from zero. Thus, after  $N$  measurements, the probability of the system remaining in the initial state is given by  $[P(T)]^N$ . Show that for an infinite number of measurements,  $N \rightarrow \infty$ , the

system remains in the initial state without loss of probability:  $[P(T)]^N = 1$ . Interpret the result.

c. One of the simplest imaginable systems, a laser-driven two-level system executing Rabi oscillation, is described by the Hamiltonian:

$$\hat{H} = \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix} .$$

Find the expression for  $\tau_z$  as a function of the Rabi frequency  $\Omega$  for the initial state  $(1 \ 0)^\dagger$ .

d. Choosing the evolution time  $t = 0.01\tau_z \ll \tau_z$  and performing  $N = 5$  measurements during this time interval, how likely is the system to remain in the initial state?

e. Let us now include a decay channel for the state  $(0 \ 1)^\dagger$  with  $\Gamma = 4\gamma$ , such as to simulate a system with continuous measurement. The system is initially prepared in the state  $(1 \ 0)^\dagger$ . If we now observe emission by decay, it means that the system *left* the initial state. We now have the effective Hamiltonian:

$$\hat{H} = \begin{pmatrix} 0 & \Omega \\ \Omega & -2i\gamma \end{pmatrix} .$$

For this system, the probability amplitude for the initial state is:

$$\langle \Psi_0 | \Psi(t) \rangle = \frac{1}{2} \left( 1 + \frac{\gamma}{\Delta} \right) e^{-(\gamma-\Delta)t/\hbar} + \frac{1}{2} \left( 1 - \frac{\gamma}{\Delta} \right) e^{-(\gamma+\Delta)t/\hbar} ,$$

with  $\Delta = \sqrt{\gamma^2 - \Omega^2}$ . For a decay rate  $\gamma \ll \Omega$ , calculate the probability that the system remains in the initial state. Interpret the result.

**Formulas:**

$$e^x = 1 + x + \frac{x^2}{2} + \mathcal{O}(x^3) \quad , \quad (1-x)^N = 1 - Nx + \mathcal{O}(x^2)$$

$$\cos^2(x) = 1 - x^2 + \mathcal{O}(x^3) \quad , \quad \hat{H} = \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix} \rightarrow e^{-i\hat{H}t/\hbar} = \begin{pmatrix} \cos \frac{\Omega t}{\hbar} & -i \sin \frac{\Omega t}{\hbar} \\ -i \sin \frac{\Omega t}{\hbar} & \cos \frac{\Omega t}{\hbar} \end{pmatrix} .$$

## 16.4 Geometric and topological phases

We consider a Hamiltonian  $\hat{H}(\mathbf{R}(t))$ , which only depends implicitly on time, that is, via some time-dependent parameter  $\mathbf{R}(t)$ . Then the Hamiltonian evolves by developing a *non-measurable* dynamic phase and additionally accumulates a *geometric phase* (also called *topological phase* or *Berry phase*. This geometric phase, which *depends on the trajectory*, is adiabatically followed in parameter space. Let us consider the time-evolution of a state  $|\psi(t)\rangle$  [68],

$$\hat{H}|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle , \tag{16.54}$$

assuming that at any instant of time the system stays in a eigenstate  $|n(\mathbf{R})\rangle$ ,

$$\hat{H}|n(\mathbf{R})\rangle = E_n(\mathbf{R})|n(\mathbf{R})\rangle . \tag{16.55}$$

When  $\hat{H}$  moves along a trajectory  $C : t \rightarrow \mathbf{R}(t)$ , then we see from,

$$\boxed{|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar} \int_0^t E_n(\mathbf{R}(t')) dt'\right] \exp(i\gamma_n(C)) |n(\mathbf{R}(t))\rangle}, \quad (16.56)$$

that, while the first exponential describes the standard dynamical phase, the phase  $\gamma_n : C \rightarrow \gamma_n(C)$  is not integrable, i.e.  $\gamma_n$  cannot be expressed as a function of  $\mathbf{R}(t)$  and is not single-valued meaning that from  $\mathbf{R}(T) = \mathbf{R}(0)$  we cannot infer  $\gamma_n(T) = \gamma_n(0)$ . Substituting (16.56) in (16.54), we find,

$$\hat{H}(\mathbf{R}(t))|\psi(t)\rangle = i\hbar|\dot{\psi}(t)\rangle = \left(E_n + i\hbar\dot{\gamma}_n(t) + i\hbar\dot{\mathbf{R}}(t) \cdot \nabla_{\mathbf{R}}\right) |\psi(t)\rangle. \quad (16.57)$$

Since for a particular eigenstate,

$$\hat{H}(\mathbf{R}(t))|n(\mathbf{R}(t))\rangle = E_n|n(\mathbf{R}(t))\rangle, \quad (16.58)$$

we infer,

$$\dot{\gamma}_n(t) = i\dot{\mathbf{R}}(t) \cdot \langle n(\mathbf{R}(t)) | \nabla_{\mathbf{R}} | n(\mathbf{R}(t)) \rangle. \quad (16.59)$$

The integrated phase change upon evolution of the state from  $|\psi(0)\rangle$  to  $|\psi(T)\rangle$  around a closed loop is then,

$$\boxed{\gamma_n(C) = i \oint_C \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle \cdot d\mathbf{R} \equiv \oint_C \vec{\mathcal{A}}(\mathbf{R}) \cdot d\mathbf{R}}, \quad (16.60)$$

where  $\vec{\mathcal{A}}$  is known as *Berry connection*.

The condition of adiabaticity is essential for emergence of geometric phases. The system always remains in an eigenstate (fixed quantum numbers) when we vary parameters of the environment more slowly than all characteristic constants of the system, even when the Hamiltonian is time-dependent (variable eigenvalues).

## 16.4.1 Properties of the Berry phase

### 16.4.1.1 Gauge invariance

We have seen in 2.5.3 that the gauge transformation (2.199),  $U_{ci}(\xi) = e^{-i\xi(\mathbf{R})}$ , leaves the Schrödinger equation invariant. Applied to an eigenstate,

$$|\tilde{n}(\mathbf{R})\rangle = e^{-i\xi(\mathbf{R})} |n(\mathbf{R})\rangle, \quad (16.61)$$

the Berry connection becomes,

$$\vec{\tilde{\mathcal{A}}}(\mathbf{R}) = i \langle e^{i\xi(\mathbf{R})} n(\mathbf{R}) | \nabla_{\mathbf{R}} | e^{-i\xi(\mathbf{R})} n(\mathbf{R}) \rangle = \vec{\mathcal{A}}(\mathbf{R}) + \nabla_{\mathbf{R}} \xi(\mathbf{R}). \quad (16.62)$$

It is apparently gauge-dependent, so that the local Berry connection  $\vec{\mathcal{A}}_n(\mathbf{R})$  can never be physically observable. On the other hand, the Berry phase is,

$$\tilde{\gamma}_n(C) = \gamma_n(C) + \int_C \nabla_{\mathbf{R}} \xi \cdot d\mathbf{R} = \gamma_n(C) + \xi(T) - \xi(0). \quad (16.63)$$

For a *closed loop*, continuity of the gauge field requires  $\xi(T) - \xi(0) = 2\pi m$ . Hence, up to an integer multiple of  $2\pi$ , *closed loop Berry phases remain gauge-invariant* under arbitrary gauge transformation and may be related to physical observables.

### 16.4.1.2 Berry curvature

It is often advantageous to convert the path integral (16.60) into a surface integral using Stokes' theorem. Defining the Berry curvature as,

$$\vec{\mathcal{V}}_n(\mathbf{R}) \equiv \nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R}) , \quad (16.64)$$

we obtain,

$$\gamma_n(C) = \iint_S \vec{\mathcal{V}}_n(\mathbf{r}) \cdot d\mathbf{S} . \quad (16.65)$$

The Berry curvature can be expressed as [68],

$$\mathbf{V}_n(\mathbf{r}) = \text{Im} \sum_{m \neq n} \frac{\langle n(\mathbf{r}) | \nabla_{\mathbf{r}} \hat{H}(\mathbf{r}) | m(\mathbf{r}) \rangle \cdot \langle m(\mathbf{r}) | \nabla_{\mathbf{r}} \hat{H}(\mathbf{r}) | n(\mathbf{r}) \rangle}{(E_m(\mathbf{r}) - E_n(\mathbf{r}))^2} . \quad (16.66)$$

This will be shown in Exc. 16.4.3.1.

**Example 74 (Geometric phase in a two-level system):** We consider the following state [575],

$$n_{\pm}(\mathbf{r}) = \cos \theta |g\rangle \pm e^{\pm i\phi} \sin \theta |e\rangle .$$

Now, we want to calculate the geometric phase,

$$\gamma_{\pm} = \oint_C i \langle n_{\pm}(\mathbf{r}) | \nabla_{\mathbf{r}} | n_{\pm}(\mathbf{r}) \rangle d\mathbf{r} .$$

Applying the gradient in spherical coordinates,

$$\nabla_{\mathbf{r}} = \hat{\mathbf{e}}_{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\mathbf{e}}_{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} + \hat{\mathbf{e}}_r \frac{\partial}{\partial r}$$

to the function  $|n_{+}\rangle$ , we find,

$$\nabla_{\mathbf{r}} |n_{+}(\mathbf{r})\rangle = -\hat{\mathbf{e}}_{\theta} \frac{\sin \theta}{r} |g\rangle + \hat{\mathbf{e}}_{\theta} \frac{e^{\pm i\phi} \cos \theta}{r} |e\rangle + \hat{\mathbf{e}}_{\phi} \frac{ie^{\pm i\phi}}{r} |e\rangle ,$$

and,

$$i \langle n_{\pm}(\mathbf{r}) | \nabla_{\mathbf{r}} | n_{\pm}(\mathbf{r}) \rangle = i \hat{\mathbf{e}}_{\phi} \frac{i \sin \theta}{r} .$$

Finally,

$$\gamma_{+} = \oint_C \frac{-\sin \theta}{r} \hat{\mathbf{e}}_{\phi} d\mathbf{R} = \oint_C \frac{-\sin \theta}{r} r \sin \theta d\phi = \oint_C \sin^2 \theta \dot{\phi} dt .$$

**Example 75 (Berry phase on the Bloch sphere):** We consider the example of a two-level system without decay described by the Bloch vector  $\vec{\rho}$  defined in (??) and whose evolution is governed by the Hamiltonian (??),

$$\hat{H} = \frac{1}{2} \mathbf{G} \cdot \boldsymbol{\sigma} \equiv \begin{pmatrix} \text{Re } \Omega \\ \text{Im } \Omega \\ \Delta/2 \end{pmatrix} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} .$$

Now, we change the parameters regrouped in  $\mathbf{G}$  adiabatically. It is easy to see that,

$$E_{\pm} = \pm R/2 \quad \text{and} \quad \nabla_{\mathbf{G}} \hat{H} = \vec{\sigma}/2 ,$$

such that,

$$\mathbf{V}_n(\mathbf{r}) = \text{Im} \frac{\langle n_{\pm}(\mathbf{G}) | \nabla_{\mathbf{G}} \hat{H}(\mathbf{G}) | n_{\mp}(\mathbf{G}) \rangle \cdot \langle n_{\mp}(\mathbf{G}) | \nabla_{\mathbf{G}} \hat{H}(\mathbf{G}) | n_{\pm}(\mathbf{G}) \rangle}{(E_+(\mathbf{G}) - E_-(\mathbf{G}))^2} = \pm \frac{\mathbf{G}}{2G^3} .$$

The geometric phase accumulated on a closed loop  $C = \partial S$  surrounding an area  $S = 4\pi\Omega_S$  on the surface of the Bloch sphere is,

$$\gamma_n(C) = \mp \oint_C \frac{dS}{2G^2} = 4\pi \mp \oint_C dR = \mp \frac{\Omega_S(C)}{2}$$

and thus equal to half the enclosed solid angle  $\Omega_S$ . The Berry phase can be measured in Ramsey experiments, as discussed in Exc. 16.4.3.2.

### 16.4.1.3 Generalization of the Berry phase according to Aharonov

We will now drop the conditions imposed to the Hamiltonian with regard to its adiabatic behavior and request that the state must be a eigenstate [139]:

$$\hat{H}|\psi(t)\rangle = i\hbar|\dot{\psi}(t)\rangle . \quad (16.67)$$

A process is cyclic, when there is a  $\tau$ , such that,

$$|\psi(\tau)\rangle = e^{i[f(\tau)-f(0)]}|\psi(0)\rangle . \quad (16.68)$$

Defining the space of radii by  $|\tilde{\psi}(t)\rangle = e^{-if(t)}|\psi(t)\rangle$ , we obtain,

$$|\tilde{\psi}(\tau)\rangle = |\tilde{\psi}(0)\rangle , \quad (16.69)$$

and from the Schrödinger equation we obtain,

$$f(t) - f(0) = -\frac{1}{\hbar} \int_0^t \langle \psi(t) | \hat{H}(t) | \psi(t) \rangle dt + \int_0^t \langle \tilde{\psi}(t) | i \frac{d}{dt} | \tilde{\psi}(t) \rangle \equiv \delta + \beta . \quad (16.70)$$

Therefore, in the space of radii we have a closed curve:

$$\begin{aligned} C : [0, \tau] &\longrightarrow \psi(t) \in \mathcal{H} \\ &\downarrow e^{-if(t)} \\ C' : [0, \tau] &\longrightarrow \tilde{\psi}(t) \in \mathcal{P} . \end{aligned} \quad (16.71)$$

The dynamic phase  $\delta$  can be zeroed by an appropriate choice of  $\hat{H}(t)$ , but not the topological phase  $\beta$ .  $\beta$  does not depend on  $\hat{H}(t)$ , but is a geometric property of the curve, which projects  $\mathcal{H}$  onto  $\mathcal{P}$ . In contrast to  $e^{i\beta}$ , the phase  $\beta$  is only determined modulo  $2\pi n$ .

### 16.4.2 Aharonov-Bohm effect

A particular case for topological phases is the *Aharonov-Bohm effect*, which we will discuss in the following. The only observables of electromagnetism are the forces of Coulomb and Lorentz which, in the theory of electrodynamics, are described by electric and magnetic fields. Electromagnetic potentials can be introduced to simplify calculations, but they are not observables with a physical reality. In contrast, in quantum mechanics, electromagnetic potentials are more fundamental than electromagnetic fields. This is demonstrated by the Aharonov-Bohm effect.

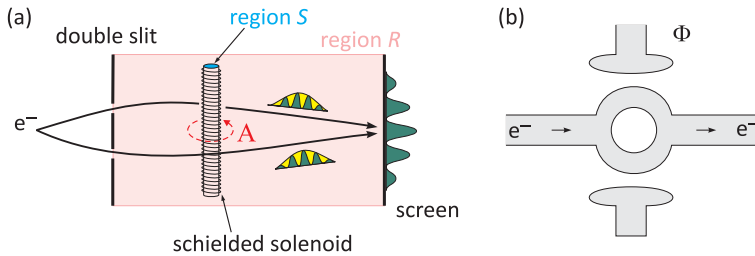


Figure 16.11: (a) Scheme for measuring the Aharonov-Bohm effect. The electrons propagate as wavepackets whose centers-of-mass are not subject to forces, but whose de Broglie waves are phase-shifted by the vector potential. (b) Aharonov-Casher effect: the electrodes  $\Phi$  do not produce electric fields inside the conductors; even so, one observes constructive or destructive interference at the output of the interferometer, depending on the applied potential.

The idea of this effect is schematized in Fig. 16.11. An electron beam is coherently divided into two arms (e.g. by a double slit) passing both sides of an infinitely extended and perfectly shielded solenoid. In this way the magnetic field  $\vec{B}$  vanishes in the region outside the solenoid, but there must exist nonetheless a potential vector  $\mathbf{A}$ , because we observe on the screen an interference pattern of the two arms of the electronic interferometer. When pass a current through the solenoid, we observe a displacement of the interference pattern.

#### 16.4.2.1 Aharonov-Bohm effect and gauge transformation

Let  $R$  and  $S$  be two disconnected spatial regions. Suppose that the electric and magnetic fields are kept zero in region  $R$ . Then, it is *classically impossible* to measure some change in the dynamics of a body confined to the region  $R$  resulting from a change of the magnetic field confined to the region  $S$ . The Aharonov-Bohm effect shows that the *opposite* is true: Electrons in the magnetic field-free region  $R$  do sense magnetic field fluxes in a region  $S$ , despite the regions  $R$  and  $S$  having no intersection!

In the classical theory of electromagnetism, in a region of empty space (except for electric charges and electric currents), the electric  $\vec{E}(\mathbf{r}, t)$  and magnetic fields  $\vec{B}(\mathbf{r}, t)$  are related to the electric charge  $\rho(\mathbf{r}, t)$  and current densities  $\mathbf{j}(\mathbf{r}, t)$  according to the *Maxwell equations*. When we know for a spatial region the sources  $\rho$  and  $\mathbf{j}$  and the

boundary conditions that the fields  $\vec{\mathcal{E}}$  and  $\vec{\mathcal{B}}$  must fulfill, we can determine the fields as solutions of Maxwell's system of partial differential equations.

In classical electrodynamics, observed from some inertial frame, the electromagnetic force  $\mathbf{F}_{em}$  acting on a point-like body with charge  $q$ , at position  $\mathbf{r}$ , and with velocity  $\mathbf{v}$ , is given by the Lorentz force:

$$\mathbf{F}_{em}(\mathbf{r}(t), t) = q\vec{\mathcal{E}}(\mathbf{r}(t), t) + q\mathbf{v}(t) \times \vec{\mathcal{B}}(\mathbf{r}(t), t) . \quad (16.72)$$

Electrodynamic theory affirms the existence of two functions  $\Phi(\mathbf{r}, t)$  and  $\mathbf{A}(\mathbf{r}, t)$ , such that,

$$\vec{\mathcal{B}}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t) \quad \text{and} \quad \vec{\mathcal{E}}(\mathbf{r}, t) = -\nabla\Phi(\mathbf{r}, t) - \frac{\partial\mathbf{A}(\mathbf{r}, t)}{\partial t} . \quad (16.73)$$

Thus, we can use the equations (16.73) to rewrite the Maxwell equations.

The so-defined potentials  $\Phi$  and  $\mathbf{A}$  are not unique, but any  $\Phi$  and  $\mathbf{A}$  leading to the same fields  $\vec{\mathcal{E}}$  and  $\vec{\mathcal{B}}$ , and thus to the same physics, are equivalent. We will, however, fix  $\Phi$  and  $\mathbf{A}$  adopting an additional condition that must be obeyed, i.e. we will adopt a particular gauge. For the discussion of the Aharonov-Bohm effect, we will adopt the *Lorentz gauge* defined by,

$$\nabla \cdot \mathbf{A}(\mathbf{r}, t) + \frac{1}{c^2} \frac{\partial\Phi(\mathbf{r}, t)}{\partial t} = 0 , \quad (16.74)$$

where  $c$  is the propagation velocity of light in vacuum.

#### 16.4.2.2 Equation for quantum particle exposed to a vector potential $\mathbf{A}$

Assume a particle (without spin) of mass  $m$  and charge  $q$ , whose wavefunction is confined to a region  $R$  (connected by paths). We demand  $\Phi = 0$  and  $\vec{\mathcal{E}} = 0 = \vec{\mathcal{B}}$ , but we let  $\mathbf{A} \neq 0$ , that is,  $\nabla \times \mathbf{A}(\mathbf{r}, t) = 0$ . Note that along with (16.73) this forces  $\mathbf{A}$  to be stationary. According to quantum mechanics the wavefunction  $\Psi$  of the particle must obey the following Schrödinger equation:

$$\frac{1}{2m} \left( \frac{\hbar}{i} \nabla - q\mathbf{A}(\mathbf{r}) \right)^2 \Psi(\mathbf{r}, t) + V(\mathbf{r})\Psi(\mathbf{r}, t) = i\hbar \frac{\partial\Psi(\mathbf{r}, t)}{\partial t} . \quad (16.75)$$

In (16.75) the potential vector  $\mathbf{A}$  is present, even if  $\phi$ ,  $\vec{\mathcal{E}}$ , and  $\vec{\mathcal{B}}$  are kept zero throughout the region  $R$ .

Since the rotation  $\mathbf{A}$  vanishes in  $R$ , considering that the integral can be calculated for any path contained in  $R$  that is deformable to a (arbitrarily chosen) point  $O \in R$ , we can define the following scalar field:

$$g(\mathbf{r}) \equiv \frac{q}{\hbar} \int_0^{\mathbf{r}} \mathbf{A}(\mathbf{x}) \cdot d\mathbf{x} . \quad (16.76)$$

From (16.76) we have:

$$\nabla g(\mathbf{r}) = \frac{q}{\hbar} \mathbf{A}(\mathbf{r}) . \quad (16.77)$$

Now, we have already shown in Sec. 2.5.3, that the wavefunction

$$\psi(\mathbf{r}, t) \equiv e^{-ig(\mathbf{r})} \Psi(\mathbf{r}, t) \quad (16.78)$$

corresponds to the gauge transform (2.199) and, given the condition (2.198), satisfies the same Schrödinger equation as  $\Psi(\mathbf{r}, t)$ . We showed this explicitly in Exc. 16.4.3.3. Thus, the presence of a potential vector in the region  $R$ , even in the absence of fields, causes a phase shift  $e^{ig(\mathbf{r})}$  of the wavefunction. An interesting issue studied in Exc. 16.4.3.4 is, whether this implies that the freedom of choice of the gauge field is lost.

**Example 76 (Observation of the Aharonov-Bohm effect):** Imagine an electron beam passing through a double-slit, as shown in Fig. 16.11(a). The electronic wavefunction diffracts through both slits, which produces an interference pattern on a subsequent screen. Now, just after the double-slit, in the shade of the region separating the two slits, we place an ideal infinitely long solenoid traversed on its axis by a constant, however, adjustable flux of magnetic field. The magnetic (and also the electric) field of the solenoid is confined to a region  $S$ , and the confinement can be guaranteed, e.g. with layers of shielding materials, including superconductors. On the other hand, the wavefunctions of the electrons are manifestly zero in this  $S$  region. In the  $R$  region, where the electronic wavefunction may be non-zero, the fields are kept zero.  $R$  and  $S$  have no overlap, both  $R$  and  $S$  are *separately* connected by paths.

We will show that the flux of the magnetic field in  $S$  can be measured through the electronic dynamics in the region  $R$ , although the electron is *never* in the region  $S$ , but confined to the field-free region  $R$ . This is the Aharonov-Bohm (magnetic) effect.

The field  $\vec{B}$  in the inner region of the solenoid is given by ( $I$  is the electric current in the wire,  $N$  is the density of windings),

$$\vec{B}(\mathbf{r}, t) = \mu_0 IN \hat{\mathbf{e}}_z .$$

Outside the solenoid, that is, for  $\rho > a$ , we have,

$$\mathbf{A}(\mathbf{r}, t) = \frac{\Phi_B}{2\pi\rho} \hat{\mathbf{e}}_\phi ,$$

where  $\Phi_B = \pi a^2 B(0, t)$  is the magnetic field flux  $\vec{B}$  through the cross section of the solenoid.

At a point  $\mathbf{r}_{sim}$  of the screen, located in the plane of symmetry of the system, we calculate  $g(\mathbf{r}_{sim})$  from Eq. (16.76) for two different paths: both starting at the source and ending at the screen, but one going through the left slit, the other through the right slit:

$$g(\mathbf{r}_{sim}) = \frac{q}{\hbar} \int_0^{\mathbf{r}_{sim}} \mathbf{A}(\mathbf{x}) \cdot d\mathbf{x} = \frac{q\Phi_B}{2\pi\hbar} \int \left( \frac{1}{\rho} \hat{\phi} \right) \cdot (\rho \hat{\phi} d\phi) = \pm \frac{q\Phi_B}{2\hbar} .$$

The + sign means, that the integration was done in the sense parallel to  $\mathbf{A}$ , and thus in the sense of  $I$  in the solenoid. The sign - holds for the other integration path. The phase difference, at point  $\mathbf{r}_{sim}$ , between these two paths will be:

$$\delta = \frac{q\Phi_B}{\hbar} .$$

That is, the phase difference (experimentally observable via a shift of the interference pattern) is directly proportional to the magnetic field flux  $\vec{B}$ , even though the wavefunction is zero in the region  $S$ , where the  $\vec{B}$  field is confined. Let us also imagine another situation: Instead of an electron source producing



a beam, let us confine an electronic wavefunction on a closed path circling the solenoid at a distance  $b$ , but inside the region of  $R$ . That is, the electron follows a field line  $BA \propto \hat{\mathbf{e}}_\phi$ . Then it can be shown, that the flow  $\Phi_B$  removes the degeneracy of the energy levels of the electron:

$$E_n = \frac{\hbar^2}{2mb} \left( n - \frac{q\Phi_B}{2\pi\hbar} \right)^2,$$

with integer, that is,  $n = 0, \pm 1, \pm 2, \dots$  [286].

The *Aharonov-Bohm phase* is a (topological) *Berry-phase* [68]. This is shown explicitly in Exc. 16.4.3.5.

### 16.4.2.3 Generalizations of the Aharonov-Bohm effect

The Aharonov-Bohm effect can be generalized to the internal degrees of freedom of a single atom, that is, from real space to configuration space. Let us imagine a Mach-Zehnder interferometer, where one of the arms crosses a constant homogeneous field region. The corresponding Lorentz force  $\mathbf{F} = \int d^3r \rho(\mathbf{r})\vec{\mathcal{E}}(\mathbf{r}) + \mathbf{j}(\mathbf{r}) \times \vec{\mathcal{B}}(\mathbf{r})$  vanishes, but the de Broglie wave undergoes a phase shift  $\chi = \int \hat{H}_{int} dt$ :

scalar potentials		
$\chi = - \int e\phi dt$	$\nabla\phi = 0$	for $e^-$
$- \int \mathbf{d} \cdot \vec{\mathcal{E}} dt$	$\nabla \times \vec{\mathcal{E}} = \nabla \cdot \vec{\mathcal{E}} = 0$	Mg, Yb <sup>+</sup>
$- \int \vec{\mu} \cdot \vec{\mathcal{B}} dt$	$\nabla \times \vec{\mathcal{B}} = \nabla \cdot \vec{\mathcal{B}} = 0$	n, Yb <sup>+</sup>
vector potentials		
$- \oint e\mathbf{A} d\mathbf{r}$	$\nabla \times \mathbf{A} = 0$	$e^-$ , (ABE)
$- \oint d \times \vec{\mathcal{B}} d\mathbf{r}$		?
$- \oint \mu \times \vec{\mathcal{E}} d\mathbf{r}$		n, Ca, (ACE)

**Example 77 (Topological phase in configuration space):** We consider a temporal Ramsey experiment with a single trapped ion by exciting a hyperfine transition. Between the pulses we apply a magnetic field for a time  $t$ . The accumulated phase will be  $\phi = (\vec{\mu} \cdot \vec{\mathcal{B}}/\hbar)t$ . This phase corresponds to the precession of the dipole moment excited by the first Ramsey pulse. The phase can be interpreted in analogy to Aharonov-Bohm effect, considering that 1. the magnetic field is homogeneous, and 2. despite this fact still acts on the spin, not exerting a force, but causing a phase shift.

## 16.4.3 Exercises

### 16.4.3.1 Ex: Derivation of the Berry curvature

Derive the expression (16.66) for the Berry curvature.

### 16.4.3.2 Ex: Measurement of the Berry phase in a two-level system

Discuss how the Berry phase in a two-level system can be measured via a Ramsey experiment.

**16.4.3.3 Ex: The Aharonov-Bohm effect as a gauge transform**

Show explicitly that the wavefunction transformed by a gauge transformation (16.78) satisfies the Schrödinger equation.

**16.4.3.4 Ex: Aharonov-Bohm effect and gauge transformation**

The phase of the interference pattern in the Aharonov-Bohm effect is fixed by the magnetic flux through the solenoid. Does that mean, that we lose the freedom of choosing an arbitrary gauge potential?

**16.4.3.5 Ex: Aharonov-Bohm effect as a geometric phase**

Show that the Aharonov-Bohm effect represents a particular case of a geometric phase.

## 16.5 Frequency metrology and sensing in quantum mechanics

Absolute space and time do not exist. According to the restricted and the general theory of relativity they are interconnected by velocity and they depend on the presence of masses exerted gravitational forces. These relationships and the question how quantum mechanics can be harnessed to improve measurements of time and forces, in particular gravity, will be treated in the following sections.

### 16.5.1 Atomic clocks

Before we start talking about clocks, we should spend a few words on the physical quantity they are supposed to measure: *time*. In the same way as it is meaningless to talk about space with nothing in it, time is only there, because things are happening. Space is the distance between things and time is nothing else than the distance between events.



Figure 16.12: (left) 'Time persistence' by Salvatore Dali. (center) Recurrent events. (right) Periodic astronomical cycles.

In our current physical understanding of the universe the most elementary events are collisions between (real or virtual) particles. Obviously, our universe is full of time. In order to bring any succession of such events into a logical and causal order, a reference time line is needed. It allows for historical book keeping of sequences of events, that we may call *histories*. And in order to facilitate a comparison between different histories, this reference time line should follow a simple deterministic rule, e.g. be periodic or exponentially decaying. In fact, both types of processes are currently used for time measurements. E.g. exponential processes, such as radioactive decay is commonly used in radioactive dating.

The most common practical approach to the measurement of time, however, is based on the observation of recurrent phenomena that we think of being periodic, such as a day on Earth, the dripping of a water pipe, or the oscillation of a pendulum or of an atomic excitation. Assuming the time intervals separating the recurrent phenomena as being all the same, we build a ruler for time which we call *clock*.

But now comes a tricky question: How do we know whether a clock is really periodic? In fact, we never know for sure whether the time intervals are really all the same. We only know that some clocks deserve a greater degree of confidence based on the fact that *more care has been taken in their design and construction*, or based on the observation that clocks built in a certain manner tend to deviate less from each other than clocks built in a different manner. The other approach would be to compare several totally *independent* clocks and to give preference to those who deviate less from each other.

An important criterion for a useful clock concerns its duty cycle. The shorter the cycling time, the faster we can extract information from the clock, and the higher is the accuracy we can reach in a given integration time. Ancient time standards had been link to the periodic motion of celestial bodies, e.g. the revolution time of the Earth around the sun. Therefore, clocks with smaller duty cycles have been engineered, such as the clepsydra or the hour glass. But their calibration to periodical astronomical cycles remained tedious and slow. Historically, the development of ever precise clocks has been motivated by navigation. Indeed, 1 minute of inaccuracy in the clock generates an uncertainty of 28 km in global positioning. And this motivation still prevails nowadays, although, meanwhile, atomic clocks are reaching uncertainties of below  $10^{-18}$  and extremely short duty cycles on the order of femto-seconds.

The left part of Fig. 16.13 shows the basic idea of any human-made clock, which consists in locking an oscillating mechanism, whose time constant can be manipulated, for instance a pendulum or a laser, by a very precise periodic process, that we call *resonance*. This resonance can be an astronomic period or the transition of an atomic between two states of excitation. Expressing the stability of a clock that can be obtained in a given integration time as,

$$\sigma = \frac{\Gamma_{nat} + \Gamma_{pert}}{\omega} \frac{1}{S/N_{noise}}, \quad (16.79)$$

we see that we better look for oscillators and resonances operating at high frequencies  $\omega$ , having very narrow widths  $\Gamma_{nat}$ , being subject to very weak perturbations and line broadenings  $\Gamma_{pert}$ , and delivering a good signal-to-noise ratio. The right part of Fig. 16.13 shows the concept of a cesium beam atomic clock. A microwave oscillator operating at  $\omega/2\pi = 9.1$  GHz excites cesium atoms passing through a microwave

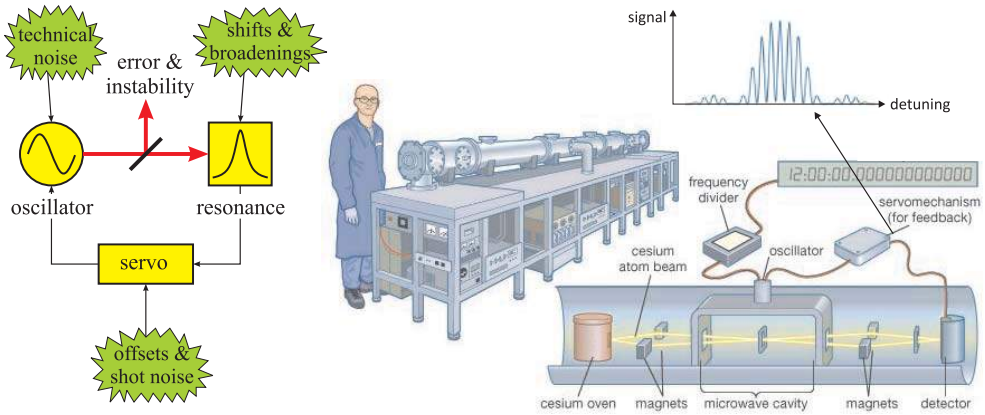


Figure 16.13: (left) Principle of any clock and possible perturbations. (right) Cesium beam atomic clock and Ramsey interference fringes.

cavity thus generating in a detector a frequency-dependent error signal which can be used to correct the oscillator frequency.

### 16.5.2 Gravitational redshift

Clocks and gravimeters are intrinsically related the gravitational redshift. The *gravitational redshift* is that phenomenon in which electromagnetic waves or photons traveling out of a gravitational well (seem to) lose energy. This loss of energy corresponds to a decrease in the wave frequency and increase in the wavelength. Gravitational redshift can be interpreted (i) as a consequence of the equivalence principle stating that gravity and acceleration are equivalent and the redshift is caused by the Doppler effect. It can also be understood (ii) as a consequence of the mass-energy equivalence stating that 'falling' photons gain energy (though there are numerous subtleties that complicate a rigorous derivation). Finally, it can be understood (iii) in terms of gravitational time dilation at the source of the radiation: an oscillator (producing electromagnetic radiation) will seem to 'tick' faster when exposed to a stronger gravitational potential.

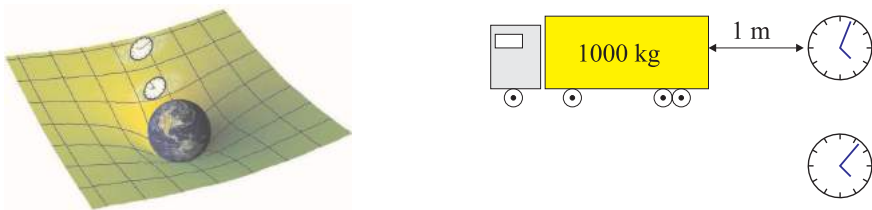


Figure 16.14: Gravitational redshift is due to the dilation of time near heavy masses.

To first approximation, the gravitational redshift is proportional to the difference

in gravitational potential. In a homogeneous field,

$$\frac{\Delta\nu}{\nu} = \frac{\Delta\lambda}{\lambda} \simeq \frac{g\Delta z}{c^2}, \quad (16.80)$$

where  $\Delta z$  is the change in height. Accounting for the accompanying gravitational time dilation affecting the atomic clock in the satellite is crucially important for accurate navigation. For this reason, *metrology* of time and *gravimetry* are closely interrelated. Do the Exc. 16.5.4.1.

**Example 78 (Prediction by the equivalence principle and general relativity for a uniform gravitational field or acceleration):** Einstein's theory of general relativity incorporates the equivalence principle, which can be stated in various different ways. One such statement is that gravitational effects are locally undetectable for a free-falling observer. Therefore, in a laboratory experiment at the surface of the earth, all gravitational effects should be equivalent to the effects that would have been observed if the laboratory had been accelerating through outer space at  $g$ . One consequence is a gravitational Doppler effect. If a light pulse is emitted at the floor of the laboratory, then a free-falling observer says that by the time it reaches the ceiling, the ceiling has accelerated away from it, and therefore when observed by a detector fixed to the ceiling, it will be observed to have been Doppler shifted toward the red end of the spectrum. This shift, which the free-falling observer considers to be a kinematic Doppler shift, is thought of by the laboratory observer as a gravitational redshift. Such an effect was verified in the 1959 Pound-Rebka experiment. Since this prediction arises directly from the equivalence principle, it does not require any of the mathematical apparatus of general relativity, and its verification does not specifically support general relativity over any other theory that incorporates the equivalence principle.

### 16.5.3 Quantum sensing

Let us first define what we mean by a *sensor* in general before discussing what quantum mechanics has to do with it. A *sensor* is a device, module, machine, or subsystem whose purpose is to detect events or changes in its environment and send the information to other electronics, frequently a computer processor. Progress in engineering, science, medicine, and other disciplines is unavoidably conditioned to sensing: What you cannot measure, you cannot improve! In many areas of applications, however, conventional sensing techniques have met fundamental limitations, and novel disruptive approaches are required in order to reach higher sensitivity and precision.

In many cases, limitations are imposed by the macroscopic, i.e. *classical*, nature of the sensor, and much can be gained by using microscopic sensors. These however, follow different rules of physics given by *quantum mechanics*. Nuclear magnetic resonance spectroscopy (NMR), magnetic resonance imaging, and the development of transistors, LEDs, solar panels, and lasers are examples of technologies developed during the first so-called quantum revolution in the 20th century, which was based on the exploitation of the particle-wave duality. However, the full potential of quantum mechanics goes much further. Today *quantum sensing* is, together with quantum

computation and quantum communication (see Sec. ??), one of the key technologies anticipated to drive the quantum revolution 2.0.

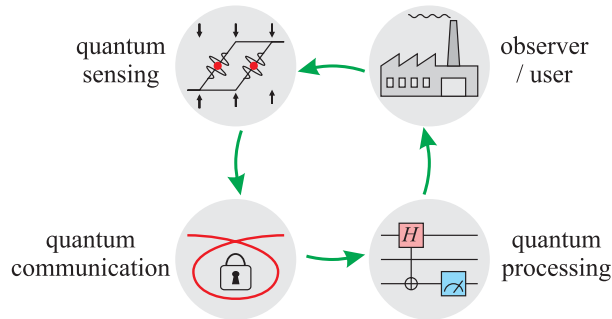


Figure 16.15: Key technologies of the second quantum revolution.

Let us discuss the disruptive role of quantum mechanics at the example of an *atom*, which is a paradigmatic example for a sensor subject to quantum laws. The reasons for this are numerous: (i) Because all atoms of a given species are strictly identical (that is, indistinguishable in the quantum statistical sense) they can be used in different sensing devices, places and countries. We do not need to duplicate reference standards, such as the Original Meter or the Original Kilogram safely kept in Paris. We simply recommend to people wishing to construct their own clock standard to gather cesium atoms (wherever you can find them) and try to excite the 9.1 GHz hyperfine transition (with whatever technique you prefer). In the end, you just need to prove that your clock is sufficiently good. (ii) Some atomic species have ultra-narrow transitions outperforming any imaginable artificial device by many orders of magnitude, which makes them ideal candidates for clock resonances. (iii) Atoms can easily be moved in space with extremely high precision, which makes them suitable for matter wave interferometers, which are useful for the measurement of distances and the sensing of forces.

The main reason, however, for the superiority of atoms (and other quantum devices, such as SQUIDS, quantum dots or nitrogen-vacancy (NV) centers in diamond) with respect to classical objects in sensing applications is, that they can exist in superposition states (of their internal excitation or of their center-of-mass motion) whose evolution delicately depends on external parameters, such as forces. We can now define a *quantum sensor* as a measurement device exploiting quantum correlations in order to enhance sensitivity and resolution, f.ex. quantum superpositions or entanglement [179]. Typically its core is a single atomic two-level system (or any other kind of qubit), whose superposition states (i) are sensitive to some environment parameter, (ii) can be manipulated in a controlled way, and (iii) can be read out.

In fact, quantum sensors already exist since the invention of atomic clocks and matter wave interferometers, which build on the control and detection of quantum states in individual qubits, even though in practice, most of these device are operated with large incoherent ensembles of qubits. Even if perturbations related to uncontrolled inter-qubit interactions (collisions, thermal excitations, etc.) can be avoided, the sensitivity that can be reached with such ensembles is bound to the standard quantum limit imposed by quantum projection noise (see Secs. 16.3.2 and ??). Novel

approaches investigate the possibilities of overcoming these limits via the creation of strong interparticle correlations via entanglement, spin-squeezing [724], or superradiant lasing [538]. Such correlations have been created with atoms, which therefore qualify as building blocks of quantum computers or sensing devices capable of overruling the standard quantum limit.

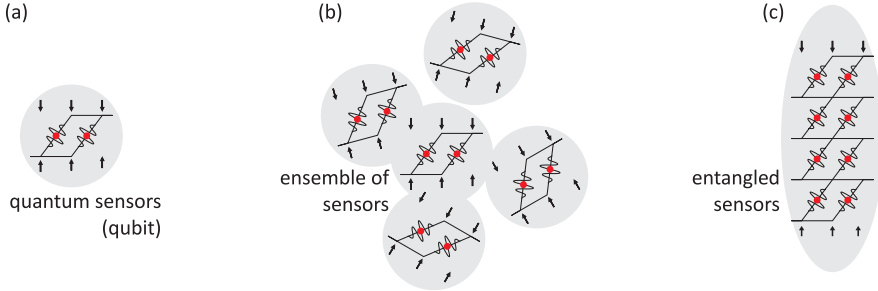


Figure 16.16: (left) Single qu-bit. (center) Larger signals can be observed using ensemble of qu-bits. (right) Collective manipulations on entangled qu-bits allow precisions beyond the standard quantum limit.

### 16.5.3.1 Working principle of a quantum sensor

As mentioned above, in order to measure a weak force it is not sufficient to sense it, one also has to read the result. In the field of atom optics, this can conveniently be done with light fields taking the information from an atom isolated in a vacuum chamber to the macroscopic world. In order not to lose information already at the level of the light-atom interaction, one generally tries to avoid dissipation and keep the interaction coherent<sup>13</sup>.

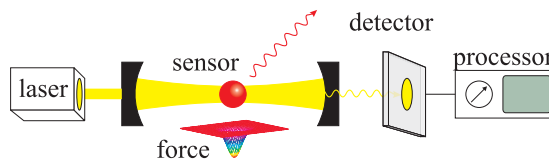


Figure 16.17: Taking information from the sensor to the detector.

A typical quantum sensor can be described by the generic Hamiltonian [179],

$$\hat{H}(t) = \hat{H}_{qbit} + \hat{H}_{ctrl}(t) + \hat{H}_{int}(t), \quad (16.81)$$

composed of a (known) internal Hamiltonian  $\hat{H}_{qbit}$ , a control Hamiltonian  $\hat{H}_{ctrl}$  allowing to manipulate or tune the sensor, and a signal Hamiltonian  $\hat{H}_{int}$  allowing to pass information about the state of the system to the outside world.

<sup>13</sup>E.g. by using two-level systems not subject to motion, collisions, spontaneous emission, etc.. Sometimes spontaneous emission can be controlled by confining both, the atom and the interrogating light field, in a cavity.

Typically, the internal Hamiltonian is static and defines the energy eigenstates  $|0\rangle$  and  $|1\rangle$ ,

$$\hat{H}_{qbit} = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1|. \quad (16.82)$$

The qubit internal Hamiltonian may contain additional interactions, such as couplings to other qubits or time-dependent stochastic terms due to interactions with an environment.

Many quantum sensing protocols require to manipulate the qubit either before, during, or after the sensing process. This is achieved via a control Hamiltonian, which allows implementing a sequence of appropriate quantum gates, such as the Hadamard gate or Pauli  $X$  and  $Y$  gates. These gates are nothing else than what, in the language of atom interferometry is known as  $\pi/2$  or  $\pi$ -pulses around different axes. Advanced sensing schemes employing more than one sensor qubit may further require conditional gates, especially controlled-NOT gates to generate entanglement, swap gates to exploit memory qubits, and controlled phase shifts in quantum phase estimation (see Sec. ??). Finally, the control Hamiltonian can include control fields for systematically tuning the transition frequency  $\hbar\omega_0 = E_1 - E_2$ .

Finally, the signal Hamiltonian represents the coupling between the sensor qubit and a signal  $V(t)$  to be measured. When the signal is weak (which is assumed here)  $\hat{H}_{int}$  adds a small perturbation to the internal Hamiltonian. The signal Hamiltonian can then be separated into two qualitatively different contributions,

$$\hat{H}_{int} = \hat{H}_{int,\parallel} + \hat{H}_{int,\perp}, \quad (16.83)$$

where  $\hat{H}_{int,\parallel}$  is the parallel (commuting) and  $\hat{H}_{int,\perp}$  the transverse (non-commuting) components, respectively. The two components can quite generally be captured by,

$$\begin{aligned} \hat{H}_{int,\parallel} &= \frac{\gamma}{2}V_{\parallel}(t)[|1\rangle\langle 1| - |0\rangle\langle 0|] \\ \hat{H}_{int,\perp} &= \frac{\gamma}{2}[V_{\perp}(t)|1\rangle\langle 0| + V_{\perp}^{\dagger}(t)|0\rangle\langle 1|], \end{aligned} \quad (16.84)$$

where  $\gamma$  is the coupling or transduction parameter of the qubit to the signal  $V(t)$ . Examples of coupling parameters include the Zeeman shift parameter or the Stark shift parameter of electric dipoles in an electric field. The parallel and transverse components of a signal have distinctly different effects on the quantum sensor. A commuting perturbation  $\hat{H}_{int,\parallel}$  leads to shifts of the energy levels and an associated change of the transition frequency  $\omega_0$ . A non-commuting perturbation  $\hat{H}_{int,\perp}$ , by contrast, can induce transitions between levels, manifesting through an increased transition rate. Most often, this requires the signal to be time-dependent (resonant with the transition) in order to have an appreciable effect on the quantum sensor.

An important class of signals are vector signal  $\mathbf{V}(t)$ , in particular, those provided by electric or magnetic fields. The interaction between a vector signal and a qubit can be described by the signal Hamiltonian,

$$\hat{H}_{int} = \gamma\mathbf{V}(t) \cdot \hat{\boldsymbol{\sigma}}, \quad (16.85)$$

where  $\hat{\boldsymbol{\sigma}}$  is the vector of Pauli matrices (2.47). For a vector signal, the two signal functions  $V_{\parallel}(t)$  and  $V_{\perp}(t)$  are,

$$\begin{aligned} V_{\parallel}(t) &= V_z(t) \\ V_{\perp}(t) &= V_x(t) + iV_y(t), \end{aligned} \quad (16.86)$$



where the  $z$ -direction is defined by the qubit's quantization axis. The corresponding signal Hamiltonian,

$$\hat{H}_V(t) = \gamma \hat{\sigma}_x \text{Re } V_{\perp}(t) + \gamma \hat{\sigma}_y \text{Im } V_{\perp}(t) + \gamma \hat{\sigma}_z V_{\parallel}(t), \quad (16.87)$$

is just the one of the Rabi model extensively discussed in Sec. 14.2.

### 16.5.3.2 Sensing forces by matter wave interferometry

Matter wave interferometry is ideal for sensing weak forces or sensing strong forces with high precision. Many interferometers employ the Ramsey scheme, which consists in sandwiching the sensing Hamiltonian between two  $\pi/2$ -control Hamiltonian pulses  $\hat{H}_{ctrl}$  preparing and reading out the atomic coherence. Between the pulses (or interaction zones), the atomic coherence is influenced by the parallel part of the sensing Hamiltonian  $\hat{H}_{int,\parallel}$ .

The basic idea is the following: One takes a matter wave and lets it fall in the Earth's gravitational field. But before that, apply a laser pulse separating the matter wave into two parts taking different paths. Thus, the Broglie waves of the two parts will accumulate different phases, which results in an interference pattern when the waves are superimposed again. As illustrated in Fig. 16.18, the matter wave interferometry works similarly to the Ramsey method used in atomic clocks with the difference that in the former the trajectories of the atomic center-of-mass motion must be separated in real space as much as possible (see Sec. 14.2.5 on Ramsey pulses and NMR, Sec. 3.1.3 on gravity with Excs. 2.4.7.4 and 2.4.7.5, Sec. 28.2.2 on Bragg interferometry and photon echos with Excs. 28.2.4.1)<sup>14</sup>.

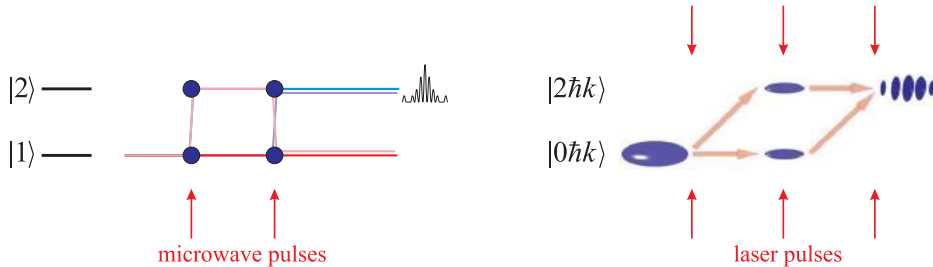


Figure 16.18: Difference between clocks and interferometers. (left) Ramsey-type clock. (right) Ramsey-Bordé interferometer.

A particularly smart way to do matter wave interferometry is via the observation of Bloch oscillations of matter waves in a periodic lattice (see Sec. 5.2.2). The Bloch oscillations can be understood in the following picture: A resting atom has infinite de Broglie wavelength. Being constantly accelerated by gravity, the matter wave reduces its de Broglie wavelength from  $\infty$  to a value, where it becomes commensurate with the periodicity of the standing light wave potential. At this moment Bragg scattering comes into play, reflecting the atomic motion back into upward direction, and the process starts over again. The atoms evolve like jumping on a trampoline with a

<sup>14</sup>See also Sec. 31.5 and 32.5 on interferometric and spectroscopic techniques.

frequency given,

$$\nu_{blo} = \frac{mg}{2\hbar k_{lat}} . \quad (16.88)$$

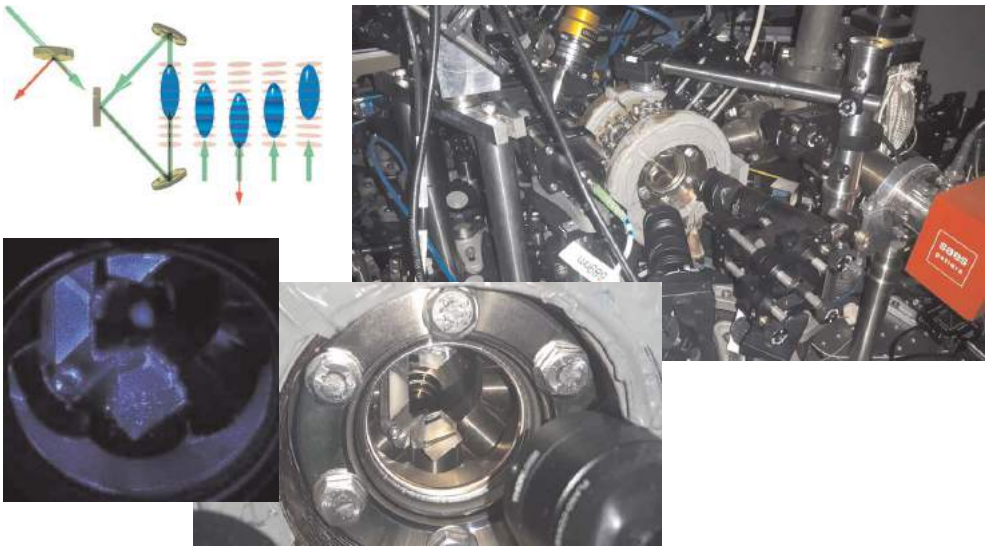


Figure 16.19: Working principle and pictures of the Sr Bloch oscillation interferometer constructed at the IFSC, USP.

## 16.5.4 Exercises

### 16.5.4.1 Ex: Red-shift of sun light and on Earth

- Calculate the gravitational redshift of light escaping from the sun.
- Calculate the blue-shift of navigational signals from GPS satellites orbiting at 20000 km altitude with respect to the surface of Earth. Compare it to the Doppler shift resulting from their orbital velocity.
- In astronomy, the magnitude of a gravitational redshift is often expressed as the velocity that would create an equivalent shift through the relativistic Doppler effect. Calculate the sunlight redshift and the GPS signal blue-shift in terms of this velocity.

## 16.6 Further reading

- P.L. Saldanha et al., *Inconsistency of a realistic interpretation of quantum measurements a simple example* [\[DOI\]](#)
- B. Hacker et al., *Deterministic creation of entangled atom-light Schrödinger-cat states* [\[DOI\]](#)

### 16.6.1 on quantum jumps

- A. Schenzle et al., *Macroscopic quantum jump in a single atom* [DOI]
- A. Schenzle et al., *Possibility of quantum jumps* [DOI]
- P. Zoller et al., *Quantum jumps in atomic systems* [DOI]
- T. Erber et al., *Resonance Fluorescence and Quantum Jumps in Single Atoms, Testing the Randomness of Quantum Mechanics* [DOI]
- J. Dalibard et al., *Wave-Function Approach to Dissipative Processes in Quantum Optics* [DOI]
- K. Mølmer et al., *Monte-Carlo Wave-Function Method in Quantum Optics* [DOI]
- Z. K. Mineev et al., *To catch and reverse a quantum jump mid-flight* [DOI]

### 16.6.2 on projection noise

- R.H. Dicke, *Coherence in Spontaneous Radiation Processes* [DOI]
- M. Kitagawa et al., *Spin-squeezed states* [DOI]
- W.M. Itano et al., *Quantum projection noise: Population fluctuations in two-level systems* [DOI]
- D.J. Wineland et al., *Squeezed atomic states and projection noise in spectroscopy* [DOI]
- Ph. Bouyer et al., *Heisenberg-Limited Spectroscopy with Degenerate Bose-Einstein Gases* [DOI]
- R. Huesmann et al., *Single-Atom Interferometry* [DOI]
- L. Salvi et al., *Squeezing on Momentum States for Atom Interferometry* [DOI]

### 16.6.3 on sensing

- A.D. Cronin et al., *Optics and interferometry with atoms and molecules* [DOI]
- L. Pezzè et al., *Quantum metrology with nonclassical states of atomic ensembles* [DOI]
- D. Braun et al., *Quantum-enhanced measurements without entanglement* [DOI]
- J. Kitching et al., *Atomic sensors - A review* [DOI]
- C.L. Degen et al., *Quantum sensing* [DOI]

#### 16.6.4 on geometric phases

M.V. Berry, *Quantal Phase Factors Accompanying Adiabatic Changes* [\[DOI\]](#)

Y. Aharonov et al., *Significance of Electromagnetic Potentials in the Quantum Theory* [\[DOI\]](#)

E. Cohen et al., *Geometric phase from Aharonov-Bohm to Pancharatnam-Berry and beyond* [\[DOI\]](#)



# Chapter 17

## Nonlinear optics

The discipline of *nonlinear optics* studies phenomena that occur as a consequence of modifications of the optical properties of materials by the presence of light. Such modifications are appreciable only, when the interacting light is sufficiently intense, i.e. of the order of the interatomic electric field,

$$E_{at} = \frac{e^2}{4\pi\epsilon_0 a_B^2} \simeq 5.14 \cdot 10^{11} \text{ V/m} , \quad (17.1)$$

which explains that nonlinear effects could only be studied properly after the advent of the laser.

In general, light-matter interaction is expressed through the relationship between the polarization induced in the medium,  $P(\omega)$ , with the optical light field,  $E(\omega)$ . In linear optics this relation can be expressed as,

$$\tilde{P}(\omega) = \epsilon_0 \chi(\omega) \tilde{E}(\omega) . \quad (17.2)$$

But in the perturbative regime of non-linear optics this expression must be generalized to a series of powers of the electric field,

$$\tilde{P}(\omega) = \epsilon_0 [\chi^{(1)}(\omega) \tilde{E}(\omega) + \chi^{(2)}(\omega) \tilde{E}^2(\omega) + \chi^{(3)}(\omega) \tilde{E}^3(\omega) + \dots] , \quad (17.3)$$

so that higher order polarization terms,  $P^{(n)}(\omega) = \epsilon_0 \chi^{(n)} E^N(\omega)$ , are considered. Therefore, the phenomena are non-linear in the sense that they depend non-linearly on the optical field applied to the material. In a more complete treatment, in terms of the optical properties of materials,  $\tilde{P}$  and  $\tilde{E}$  are vector fields and the electric susceptibility is a tensor. However, to simplify the treatment, we consider the fields as scalars and  $\chi^{(n)}$  as constants independent of the frequency  $\omega$ .

Examples of non-linear optical phenomena are: parametric processes of sum and difference frequency generation, as shown in Fig. 17.1, optical parametric oscillation, and the dependence of the refractive index with the optical intensity. Examples of non-parametric processes are: multi-photon absorption, stimulated Raman scattering, and saturated absorption. In the latter example, the absorption coefficient of the material decreases with increasing light intensity:

$$\alpha = \frac{\alpha_0}{1 + I/I_s} . \quad (17.4)$$

Saturated absorption is an example where a perturbative approach is not capable of providing good results, and its most reliable description is given by the approximation of a two-level quantum system.

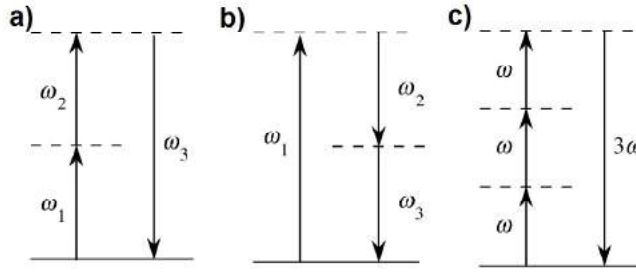


Figure 17.1: Parametric (a) sum and (b) difference frequency generation. (c) Third harmonic generation.

It is also important to emphasize that parametric processes are those, in which the initial and final quantum states of a system are identical. Consequently, the population of an initial state can only be moved to a virtual state, different in energy by  $\Delta E$ , for a short time lapse limited by Heisenberg's uncertainty principle ( $\hbar/\Delta E$ ). Nonparametric processes are those involving population transfer between real energy levels, eigenstates of the system's Hamiltonian. In terms of the electrical susceptibility of the medium,  $\chi^{(n)}$  is a real quantity for parametric and an imaginary one for nonparametric processes.

## 17.1 The nonlinear optical susceptibility

The description of nonlinear optical phenomena can be approached from a variety of perspectives, most of which are semi-classical in the sense that the matter is treated quantum mechanically, while the electromagnetic radiation is treated classically. One possible description explores the wave nature of the radiation, using Maxwell's equations to describe the generation of new spectral components by the nonlinear terms of the polarization. More generally, this description explains how different frequencies can be coupled through their nonlinear interaction with the material. It can be shown that the electromagnetic wave equation in the nonlinear regime is,

$$\nabla \tilde{E} - \frac{n^2}{c^2} \frac{\partial^2}{\partial t^2} \tilde{E} = \frac{1}{\epsilon_0 c^2} \frac{\partial^2}{\partial t^2} \tilde{P}, \quad (17.5)$$

such that  $\tilde{P} = \tilde{P}^{(1)} + \tilde{P}^{nl}$ . In this view,  $\tilde{P}^{nl}$  acts as a source of frequencies, several of that are incident.

Although electromagnetic theory is capable of explaining several aspects of nonlinear optics, it is the quantum description that provides explicit expressions for nonlinear optical susceptibility. There are three main motivations for obtaining quantum expressions:

- They reveal a functional form of the nonlinear optical susceptibility and show how they depend on microscopic parameters of the material, such as transition dipole moments and atomic energy levels.
- They exhibit the intrinsic symmetries of nonlinear susceptibility.

- They can be used to calculate numerically the values of nonlinear susceptibilities.

The numerical predictions of quantum theory for nonlinear optical susceptibilities are particularly accurate in the case of atomic vapors, because the atomic parameters of these are known with sufficient precision for the theory to provide reliable results.

Two quantum mechanical formalisms can be used for the calculation of nonlinear optical susceptibilities. Perturbation theory is used to make predictions on non-resonant systems, i.e. situations where the photon energy is much smaller than the energy separation between two eigenstates of the material. On the other hand, when the interactions are close to resonance, such that it becomes necessary to include relaxation processes, the state-density matrix formalism is used. Although this approach is more complex, it provides better results.

### 17.1.1 Hanle effect

The *Hanle effect* occurs when a magnetic and an optical field compete for the quantization axis. Imagine an atom irradiated by a laser from direction  $\mathbf{k} = k\hat{\mathbf{e}}_x$ , linearly polarized  $\varepsilon = \hat{\mathbf{e}}_y$  and subject to a magnetic field  $\vec{B} = B\hat{\mathbf{e}}_z$ . The fluorescence is detected in direction  $\hat{\mathbf{e}}_y$  through a linear polarizer [186].

If  $B = 0$ , no light is emitted into the detector since the dipole radiation pattern is a torus with symmetry axis  $\hat{\mathbf{e}}_y$ . If  $B$  is now increased, the quantization axis is tilted and the torus slowly precesses about the  $\hat{\mathbf{e}}_x$  axis. Plotting the time-averaged fluorescence as a function of the magnetic field  $B$ , we observe a *dark resonance*. These arguments are rather classical.

Quantum mechanically, Hanle resonances are easily calculated. The transition rates additionally depend on the relative orientation of the laser polarization and the magnetic field direction. This dependence is accounted for by decomposing the polarization vector into the coordinates defined by,

$$\hat{\mathbf{e}}_3 = \frac{\vec{B}}{B} \quad , \quad \hat{\mathbf{e}}_2 = \frac{\hat{\mathbf{e}}_3 \times \hat{\mathbf{g}}}{|\hat{\mathbf{e}}_3 \times \hat{\mathbf{g}}|} \quad , \quad \hat{\mathbf{e}}_1 = \frac{\hat{\mathbf{e}}_2 \times \hat{\mathbf{e}}_3}{|\hat{\mathbf{e}}_2 \times \hat{\mathbf{e}}_3|} \quad , \quad (17.6)$$

where  $\hat{\mathbf{g}}$  is an arbitrarily chosen direction, e.g. gravity. The relative amplitude of the transitions  $\Delta m_J = 0$  is proportional to the projection of the polarization vector on the magnetic field axis  $\zeta_\pi = (\hat{\varepsilon} \cdot \hat{\mathbf{e}}_3)^2$ . To estimate the amplitude of the transitions  $\Delta m_J = \pm 1$ , we must project onto the coordinates,

$$\hat{\mathbf{e}}_\pm = \frac{1}{\sqrt{2}}(\hat{\mathbf{e}}_1 \mp i\hat{\mathbf{e}}_2) \quad , \quad (17.7)$$

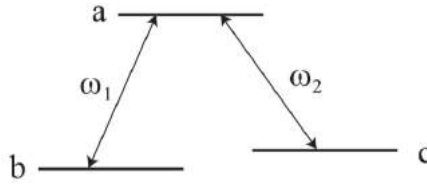
and we obtain  $\zeta_{\sigma\pm} = (\hat{\varepsilon} \cdot \hat{\mathbf{e}}_\pm)^2$ . Resolve the Excs. 17.1.2.1 and 17.1.2.2.

## 17.1.2 Exercises

### 17.1.2.1 Ex: Coherent trapping and dark states

Consider a three-level system  $a$ ,  $b$ , and  $c$  in  $\Lambda$ -configuration interacting with two electromagnetic fields with frequencies  $\omega_1$  and  $\omega_2$ , as shown in the figure. I.e. the two states of lower energy  $b$  and  $c$  are coupled with a more energetic state  $a$ . Assume that





the the transition  $|b\rangle \leftrightarrow |c\rangle$  is forbidden and that the Hamiltonian of the system has the form  $\hat{H} = \hat{H}_0 + \hat{H}_I$ , where,

$$\hat{H}_0 = \hbar\omega_a|a\rangle\langle a| + \hbar\omega_b|b\rangle\langle b| + \hbar\omega_c|c\rangle\langle c|$$

$$\hat{H}_I = -\frac{\hbar}{2}(\Omega_1 e^{-i\omega_1 t}|a\rangle\langle b| + \Omega_1^* e^{i\omega_1 t}|b\rangle\langle a|) - \frac{\hbar}{2}(\Omega_2 e^{-i\omega_2 t}|a\rangle\langle c| + \Omega_2^* e^{i\omega_2 t}|c\rangle\langle a|) .$$

- Assuming that the system's state is described by  $|\psi\rangle = K_a|a\rangle + K_b|b\rangle + K_c|c\rangle$  find the system of equations that describe the dynamics of probability amplitudes  $K_i$  ( $i = a, b, c$ ).
- Rewrite the equations for the case where the frequencies of the applied fields are resonant (that is,  $\omega_1 = \omega_a - \omega_b$  e  $\omega_2 = \omega_a - \omega_c$ ). Simplify the system by writing in terms of the variables  $u_k = C_k e^{i\omega_k t}$  ( $k = a, b, c$ ).
- Assuming the initial condition  $|\psi(0)\rangle = (|b\rangle + |c\rangle)/\sqrt{2}$ , solve the system of equations for the resonant case and interpret the result.

### 17.1.2.2 Ex: Hanle effect in Ca

Simulate the Hanle effect for the Ca 3-level system using optical Bloch equations.

## 17.2 Quantum interference

We have seen earlier that a *dark resonance* in  $\Lambda$ -shaped three-level systems create superposition states between the two stable ground states which allow the adiabatic elimination of the excited state. Dark resonances may be understood as destructively interfering excitation paths at Raman-coherences between inneratomic transitions. Quantum interference is at the origin of various other phenomena which are discussed in the following sections.

### 17.2.1 Lasing without inversion

The question of the necessity of population inversion to construct a laser has been the subject of debates. Indeed, even an ordinary two-level system may exhibit gain with a small frequency interval [494] known as *Mollow gain*. Lasing without population inversion may also result from a splitting of emission and absorption spectra caused by atomic recoil as in the example of CARL [91].

Various schemes of a *laser without inversion* (LWI) have been proposed. Here is one of them [518]. We will discuss an example in Exc. 17.2.3.1.

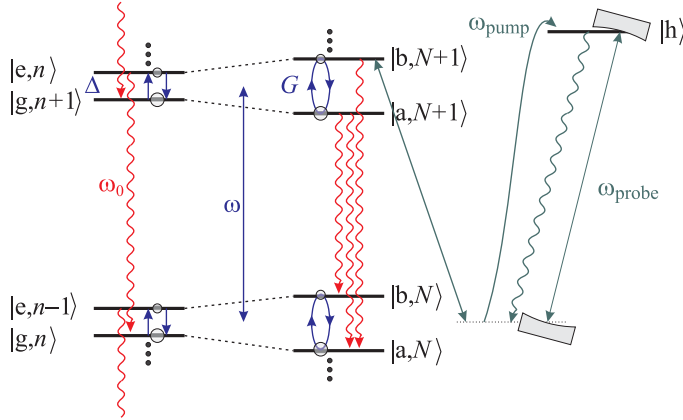


Figure 17.2: Dressed states level scheme for LWI. Quantum interference between two possible Raman transitions (green) leads to a cancellation of the ground state population. When the upper level  $|h\rangle$  is incoherently pumped, gain can be reached for a weak probe field. Inserting the atoms in a cavity one can reach lasing [345].

### 17.2.2 Brillouin scattering

Stimulated scattering of phonons is called *stimulated Brillouin scattering* (SBS). Like *Raman-scattering* (SRS) Brillouin-scattering is a limiting factor for the transmission efficiency in optical fibers. It is used in acousto-optic modulators (AOM). While SBS is based on the exchange of phonons between atoms bound in crystals, SRS is based on the exchange of phonons between atoms bound in molecules.

Raman-scattering (in a restricted historical sense) is very common technique of molecular spectroscopy. The process is Rayleigh-scattering at an electronic transition, but towards a different vibrational substate. Brillouin-scattering also involves the motional state of the scatterer, but its center-of-mass motion rather than some internal degree of freedom. It is also related to *polariton scattering* in solids, which produces optical phonons, rather than acoustic phonons.

If a strong electromagnetic field (pump laser) is irradiated into a medium (typically a crystal or a fluid) it produces a time-varying *electrostrictive strain*, which can be understood as the reaction force of particles dislocated from their equilibrium position. The strain is quantized into *phonons* and may drive a sound wave. This wave modulates the optical dielectric constant  $\epsilon$  and thus create a periodic polarization  $\vec{P}$ . This polarization may now interact with the incident electric field (pump laser  $\omega_2, \mathbf{k}_2, \vec{\mathcal{E}}_2$ ). The resulting energy exchange can, under suitable circumstances, lead to simultaneous amplification of a probe wave ( $\omega_2, \mathbf{k}_2, \vec{\mathcal{E}}_2$ ) and a sound wave ( $\omega_s, \mathbf{k}_s, u_s$ ).

Let us consider a 1D geometry,  $\mathbf{k}_j = k_j \hat{\mathbf{e}}_z$  and  $\vec{\mathcal{E}}_j = \mathcal{E}_j \hat{\mathbf{e}}_x$ . (More general geometries can be considered [742]). The pump field  $E_2(t, z)$  causes a strain  $\partial u_s / \partial z$  via longitudinal displacements  $u_s(z, t)$  of test volumes. This strain produces a modulation of  $\epsilon$  by  $\delta\epsilon = -\gamma \partial u_s / \partial z$ , where  $\gamma$  is the strain coefficient (or coupling strength). The modulation of the dielectric constant  $\delta\epsilon$  now modulates the interaction energy  $\delta U = -\frac{1}{2} \delta\epsilon E_2^2$ , which exerts work  $p \partial u_s / \partial z = \delta U$  against the pressure  $p$ . The pressure modulation creates a force  $F = -\partial p / \partial z = \frac{1}{2} \gamma \partial E_2^2 / \partial z$ . We can now set up a

Fokker-Planck type force equation,

$$\rho \frac{\partial^2 u_s}{\partial t^2} = \frac{\gamma}{2} \frac{\partial E_2^2}{\partial z} - \eta \frac{\partial u_s}{\partial t} + T \frac{\partial^2 u_s}{\partial z^2}, \quad (17.8)$$

where  $\rho$  is the mass density,  $T$  the elastic constant and  $\eta$  acoustic dissipation.  $v_s \equiv \omega_s/k_s = \sqrt{T/\rho}$  is the free propagation velocity of sound. Simultaneously we know that the light wave propagates like,

$$\frac{\partial^2 E_j}{\partial z^2} + \mu \varepsilon \frac{\partial^2 E_j}{\partial t^2} + \mu \frac{\partial^2 P_{NL,j}}{\partial t^2}. \quad (17.9)$$

We insert the ansatz  $E_j(t, z) = \frac{1}{2} E_{0j}(z) e^{i(\omega_j t - k_j z)} + c.c.$  and  $u_s(t, z) = \frac{1}{2} u_{0s}(z) e^{i(\omega_s t - k_s z)} + c.c.$  first into the above equations. We use the approximations  $k_s^2 u_s \gg d^2 u_s / dz^2 \ll k_s du_s / dz$  and  $|\partial(E_2 E_1^*) / \partial z| \ll |k_s E_2 E_1^*|$  and focus on the real parts. Assuming that the pump field  $E_2$  is undepleted, stimulated Brillouin-scattering is described by the following set of equations,

$$\begin{aligned} \frac{dE_1^*}{dz} &= -\frac{\alpha}{2} E_1^* - \frac{\gamma k_1 k_s}{4\varepsilon_1} E_2^* u_s \\ \frac{du_s}{dz} &= -\frac{\eta}{2\rho v_s} u_s - \frac{\gamma}{8\rho v_s^2} E_2 E_1^*. \end{aligned} \quad (17.10)$$

Here  $\rho$  is the mass density, optical losses are described by  $\alpha$ , and  $\eta$  is the dissipation constant for phonons.  $\varepsilon_1 \approx \varepsilon_0$ . The scattering satisfies the *Bragg condition*  $\mathbf{k}_2 - \mathbf{k}_1 = \mathbf{k}_s$ . The above equations describe *exponential gain* and *threshold behavior* for  $E_1$  and  $u_s$ . For backscattering  $\mathbf{k}_1 \mathbf{k}_2 = -k_1 k_2$  the rate of growth for the probe  $E_1$  is influenced by the values of  $E_1$  lying ahead in the direction  $\mathbf{k}_1$ . This is by virtue of the sound beam propagating in opposite direction to  $E_1$  and provides the positive feedback being at the origin of exponential gain.

The equations are reminiscent to the CARL equations. The difference is the nature of the mediating force field: The CARL force is mediated by photons. The mediation is thus instantaneous. Photons do not require a medium in order to propagate. In contrast, the Brillouin-gain is mediated by phonons. Phonons propagate through a gas by collisions. Sound needs a medium to propagate. In dilute gases where CARL is observed, collisions are totally negligible. Brillouin-scattering may lead to bunching, which propagates along  $\mathbf{k}_s$ . But similar to water waves, which do not transport the water molecules, the bunching does not lead to a net transport of atoms.

Just like CARL and the superradiant Rayleigh scattering in BECs SBS can be understood as being mediated by dipole-dipole interactions (i.e. the exchange of real or virtual photons between atoms). In a BECs SBS can be interpreted as phonon-like excitations (smaller momentum transfer) due to dipole-dipole interactions [270], while CARL are particle-like excitations due to dipole-dipole interactions (the nature of scattered particles changes from recoiling atoms to phonons). Note that while ultralow temperatures are necessary, these effects are not base on superfluidity, i.e. binary collisions. Thus the speed of sound is not the Bogolubov sound. The question is whether quantum degeneracy plays a role.

### 17.2.3 Exercises

**17.2.3.1 Ex: Lasing without inversion**

Explain the phenomenon of lasing without inversion in the dressed states picture for a V-type three-level system.

**17.3 Further reading**

- G. Kurizki et al., *Free-electron lasing without inversion by interference of momentum states* [\[DOI\]](#)
- D. Bloch et al., *Atom-wall interaction* [\[DOI\]](#)
- G. Nienhuis, *Nonlinear selective reflection from an atomic vapor at arbitrary incidence angle* [\[DOI\]](#)
- E. Pleghaar, *Quantitative investigation of the effect of resonant absorbers on the Goos-Hänchen shift* [\[DOI\]](#)



# Chapter 18

## Atomic motion in force fields

So far – and especially in Sec. 3.9.2– we analyzed the motion of quantum particles in potential landscapes without specifying the physical origin of the potentials. We know the *gravitational force*, which can be derived from the Earth’s homogeneous attraction,

$$\mathbf{F} = -\nabla V_{grv} = -\nabla(mgz) = -gm\hat{\mathbf{e}}_z . \quad (18.1)$$

Another fundamental force comes from electromagnetism. We have already studied – mainly in Sec. 9.4– the reaction of the electronic shell in atoms subjected to applied electromagnetic fields.

In contrast, the present chapter is devoted to the motion of the *atomic center-of-mass* subject to forces resulting from interactions with *electromagnetic fields*. We will begin, in the first section, with electromagnetic forces of the Coulomb-Lorentz type acting on charges (e.g. ions), permanent electric dipoles (e.g. polar molecules), or permanent magnetic dipoles (e.g. paramagnetic atoms). Also, more complex situations will be discussed, such as the scattering of light by confined atoms, atoms interacting with optical cavities, and adiabatic potentials.

The second section will entirely be devoted to the forces exerted by light beams, in particular the *radiation pressure* and the *optical dipole force*, which are nowadays widely used in atomic cooling and trapping experiments. We will leave the issue of the application of these forces to Chp. 24.7.3 and concentrate here on the (semiclassical or quantum) derivation and the interpretation of the forces. In fact, to understand optical forces acting on atoms, we need to consider their internal degrees of freedom.

Apart from the degrees of freedom related to their center-of-mass motion (kinetic or potential energy), many quantum objects are endowed with internal degrees of freedom, for example, the motion of electrons inside atoms or molecules. In the simplest case, the Hamiltonian of such a system is composed of an outer part, comprising the kinetic and the potential energy, and an inner part counting for the excitation energy  $\hbar\omega_0$  of an internal state  $|e\rangle$ ,

$$\hat{H}_{atm} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) + \hbar\omega_0|e\rangle\langle e| . \quad (18.2)$$

The time scale of the electronic motion is usually very rapid compared to the motion of the nucleus, where (almost) the entire mass of the atom is concentrated. Therefore, the external (nuclear) dynamics decouples from the internal (electronic) one, which allows the separation of the total wavefunction in two parts,

$$|\psi\rangle = |\psi\rangle_{ext}|\psi\rangle_{ele} , \quad (18.3)$$

where for a simple two-level atom,  $|\psi(t)\rangle_{ele} = c_g(t)|g\rangle + c_e(t)|e\rangle$ , with the atomic ground state  $|g\rangle$  and the excited state  $|e\rangle$ . The external states are eigenstates of the momentum in the case of a free particle,  $|\psi\rangle_{ext} = |\mathbf{p}\rangle$ . For particles confined in a potential the external states are the vibrational eigenstates,  $|\psi\rangle_{ext} = |n\rangle$ . The temporal evolutions of the internal and external degrees of freedom are governed by independent Schrödinger equations. For cold atomic clouds the kinetic energy is much smaller than the excitation energy, which allows the separation of the energy scales. That is, the internal degrees of freedom are frozen in the ground state. Many phenomena, for example, Bose-Einstein condensation and the dynamics of condensates are described in this regime.

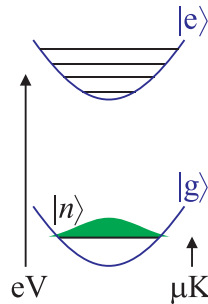


Figure 18.1: The internal degrees of freedom of cold atoms are thermally frozen.

Nevertheless, the fact that it is thermally frozen does not prevent the intentional excitation of the internal degree of freedom by irradiating electromagnetic fields tuned close to resonances and coupling electronic energy levels. In the case of coupling, the external and internal degrees of freedom must both be considered.

## 18.1 Electromagnetic forces

Obviously, in order to allow for forces acting on the atomic center-of-mass, the atomic Hamiltonian must contain terms depending on the center-of-mass coordinates:

$$\mathbf{F} = -\langle \nabla \hat{H}_{int} \rangle. \quad (18.4)$$

We will see shortly that some of terms may be dissipative, other conservative.

The impact of electromagnetic fields on the internal dynamics of atoms has already been studied in the Chp. 9.4. Here, we will focus on the force on the center-of-mass exerted by the gradient of *electromagnetic potentials*, where the Hamiltonian in Eq. (18.4) of a charge interacting with electromagnetic fields is obtained in minimum coupling (9.11) by,

$$\hat{H}_{int} = \frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})^2 + q\Phi \simeq \frac{-\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{m}\mathbf{A} \cdot \nabla + q\Phi. \quad (18.5)$$

From this formula we can, in principle, calculate all electromagnetic forces.

The coupling of external and internal degrees of freedom is mediated by the photonic recoil transferred to the atom during absorption and emission processes. That

is, the feature that the interaction with light simultaneously *excites* the atom and exerts a *force* couples the degrees of freedom. This fact manifests itself in the Hamiltonian of the atom interacting with a light field (15.17) by the appearance of terms joining operators acting on different degrees of freedom,

$$\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a} + \hat{H}_{int} + \hat{H}_{atm} \quad \text{where} \quad \hat{H}_{int} = \hbar\Omega(\hat{\mathbf{r}})e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}\hat{a}^\dagger\hat{\sigma} + c.c. , \quad (18.6)$$

where  $\hat{\sigma} \equiv |g\rangle\langle e|$  and  $\hat{a} \equiv \sum_n |n\rangle\langle n+1|$  and  $\hbar\Omega(\hat{\mathbf{r}}) \equiv \mathbf{d}_{12} \cdot \vec{\mathcal{E}}(\hat{\mathbf{r}})$  is the coupling constant or *Rabi frequency*. The Hamiltonian is that of the Jaynes-Cummings model, except that in addition to the field operators  $\hat{a}$  and the atom transition operators  $\hat{\sigma}$ , appears an operator for the position of the atom  $\hat{\mathbf{r}}$ , whose quantum features we have not taken very seriously so far. It appears in the Rabi frequency and also in the term  $e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}$ . Now, we must remember, that

$$U_{recoil} = e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}} = |\mathbf{p} + \hbar\mathbf{k}\rangle\langle\mathbf{p}| \quad (18.7)$$

is the unitary operator of the photonic recoil in the absorption process. We shall shortly see, that it is precisely this term in the Hamiltonian that gives rise to all phenomena related to light forces on atoms.

The presence of the position operator in the Jaynes-Cummings Hamiltonian introduces a new degree of freedom. With no external potential (that is, the system is invariant to spatial translations), this degree of freedom is simply the atomic center-of-mass momentum, such that the new set of quantum numbers is  $|j, n, \mathbf{p}\rangle$ . Strictly speaking we have to span the whole Hilbert space by an external product,  $\hat{H}_{ele} \otimes \hat{H}_{rad} \otimes \hat{H}_{ext}$ .

### 18.1.1 Forces on charges and electric dipole moments

As shown in Eq. (9.8), the equations (18.4) and (18.5) (obviously) lead to Coulomb-Lorentz forces on charges and currents.

In atomic optics, the Coulomb-Lorentz force is used, for example, to accelerate or trap ions (see Sec. 24.5) and other electrically charged particles.

Atoms naturally do not exhibit *permanent electric dipole moments*, when they are not subject to external electric fields. In contrast, polar molecules (such as heteronuclear dimers), which have permanent electric dipole moments can have their motion be influenced by inhomogeneous electric fields (see Sec. 24.5.3).

### 18.1.2 Forces on magnetic dipole moments

Neutral atoms are insensitive to electric fields. But as we have already seen in Chp. 9.4, the orbital motion of the electrons corresponds to a circular current generating a permanent magnetic dipole moment  $\vec{\mu}$ , which can interact with external magnetic fields. We have already shown in the calculation (9.15) and (9.19) that the interaction energy (18.5) can be written as,

$$\hat{H}_{magn} = -\vec{\mu}_J \cdot \vec{\mathcal{B}} = -\frac{gJ\mu_B}{\hbar} \mathbf{J} \cdot \vec{\mathcal{B}} \longrightarrow -\frac{gJ\mu_B}{\hbar} |\mathbf{J}| \cdot |\vec{\mathcal{B}}| = -gJ\mu_B m_J \mathcal{B} , \quad (18.8)$$



where the *Landé factor* is given by the formula (9.21),

$$g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}. \quad (18.9)$$

Here,  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  is the total angular momentum resulting from the coupling of the total angular orbital momentum and the total spin of all electrons. If the atom has a nuclear spin  $I$  other than zero, then  $\mathbf{F} = \mathbf{J} + \mathbf{I}$  replaces  $\mathbf{J}$  in Eq. (18.8), and the  $g$ -factor generalizes to (9.35)<sup>1</sup>,

$$g_F \simeq g_J \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)}. \quad (18.10)$$

In Sec. 9.2 we used the formula (18.8) to calculate the Zeeman shift of internal energy levels. But, according to the formula (18.4), the interaction also generates a force acting on the center-of-mass of atom,

$$\mathbf{f} = -g_F \mu_B m_F \nabla \mathcal{B}. \quad (18.11)$$

In case of absence of hyperfine structure we simply replace  $F$  by  $J$ .

Obviously, force is conditioned by the existence of a gradient of the absolute value of the magnetic field. It was first used in the famous *Stern-Gerlach experiment*, which led to the discovery of the electron (see Sec. 4.3.3). In atomic optics (see Sec. 24.4), this force is widely used to create *magnetic traps* for cold atoms. Resolve the Excs. 9.2.8.2, 18.1.4.1, and 18.1.4.2.

### 18.1.3 Adiabatic potentials

*Adiabatic potentials* can be used to realize more complicated trapping geometries [154]. To study adiabatic potentials we consider the two-level system  $|\frac{1}{2}, \frac{1}{2}\rangle \leftrightarrow |\frac{1}{2}, -\frac{1}{2}\rangle$  coupled by an incident radiation (e.g. a radiofrequency). A generalization to multilevel systems  $F > \frac{1}{2}$  is simple. The dressed states Hamiltonian of our two-level system is a  $2 \times 2$  matrix,

$$\hat{H}(z) = \begin{pmatrix} \frac{1}{2}\mu_B g_F \mathcal{B}(z) - \frac{1}{2}\hbar\omega & \frac{1}{2}\hbar\Omega \\ \frac{1}{2}\hbar\Omega & -\frac{1}{2}\mu_B g_F \mathcal{B}(z) + \frac{1}{2}\hbar\omega \end{pmatrix}. \quad (18.12)$$

For simplicity, we assume a one-dimensional geometry,  $\mathcal{B} = \mathcal{B}(z)$ , but we can easily generalize to three dimensions. The eigenvalues of  $\hat{H}$  are,

$$E_{\pm}(z) = \pm \frac{1}{2} \sqrt{\hbar^2 \Omega^2 + [\mu_B g_F \mathcal{B}(z) - \hbar\omega]^2}. \quad (18.13)$$

Sufficiently far from resonance,  $\hbar\Omega \ll |\mu_B g_F \mathcal{B}(z) - \hbar\omega|$ , we obtain,

$$E_{\pm}(z) \simeq \pm \frac{1}{2} [\mu_B g_F \mathcal{B}(z) - \hbar\omega] \pm \frac{\hbar^2 \Omega^2}{4[\mu_B g_F \mathcal{B}(z) - \hbar\omega]}, \quad (18.14)$$

<sup>1</sup>Note that the formula only applies to weak fields. For strong fields the Zeeman unfolding changes to the Paschen-Back unfolding of the hyperfine structure.

where the second term can be interpreted as the dynamic Stark shift of the energy levels.

To illustrate the influence of the radiofrequency, we calculate the potential energy and the dressed states assuming a linear 1D magnetic field gradient  $\mathcal{B}(z) \equiv zb$ . Fig. 18.2(a) illustrates the radiofrequency coupling and Fig. 18.2(b) the dressed states for two magnetic substates coupled by a radiofrequency. The minimum emerging in

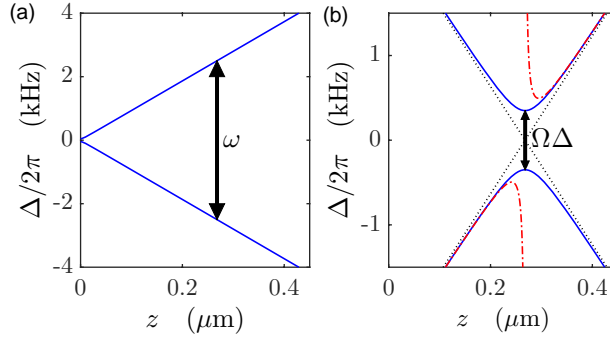


Figure 18.2: (code) (a) Potential energies for a hyperfine structure  $F = \frac{1}{2}$  with a  $g$ -factor of  $g = -\frac{2}{3}$  (as e.g. in the ground state  $^2S_{1/2}$  of  $^6\text{Li}$ ). A radiofrequency (arrow) couples the substates  $m_F = \pm\frac{1}{2}$ . Here,  $b = 200$  G/cm and  $\omega = 2\pi \times 5$  kHz. (b) Uncoupled dressed states (dotted line), coupled dressed states (solid line), and dynamic Stark shifts (dash-dotted) approximated far away from resonance. The Rabi frequency is  $\Omega = 2\pi \times 700$  Hz.

the upper curve of Fig. 18.2(a) may serve as a confinement potential. Using an rf-radiation composed by several frequencies, potential minima can be realized at several distances  $z$ . In Exc. 18.1.4.3 we calculate an example.

In the dressed states basis with the Hamiltonian (18.12), the force is calculated from,

$$\mathbf{F}(\mathbf{r}) = \langle \hat{\mathbf{F}}(\mathbf{r}) \rangle = -\text{Tr}_{atom,laser} \hat{\rho} \nabla_{\mathbf{r}} \hat{H} = - \sum_{n,j} \langle n, j | \hat{\rho} \nabla_{\mathbf{r}} \hat{H} | j, n \rangle. \quad (18.15)$$

We consider only one dimension and disregard the degrees of freedom of the radiation field,

$$\begin{aligned} F(z) &= -\text{Tr}_{atom,laser} \hat{\rho} \partial_z \hat{H} \\ &= - \sum_j \langle j | \hat{\rho} \partial_z \left( \frac{\mu_B g_F \mathcal{B}}{2} |1\rangle\langle 1| - \frac{\hbar\omega}{2} |1\rangle\langle 1| - \frac{\mu_B g_F \mathcal{B}}{2} |2\rangle\langle 2| + \frac{\hbar\omega}{2} |2\rangle\langle 2| + \frac{\hbar\Omega}{2} e^{ikz} \hat{\sigma}^+ + c.c. \right) |j\rangle. \end{aligned} \quad (18.16)$$

Here we neglect any possible position dependence of  $\Omega$ ,

$$F(z) = -\frac{1}{2} \mu_B g_F \partial_z \mathcal{B} \sum_j \langle j | \hat{\rho} (|1\rangle\langle 1| - |2\rangle\langle 2|) |j\rangle = -\frac{1}{2} \mu_B g_F \partial_z \mathcal{B} (\rho_{11} - \rho_{22}). \quad (18.17)$$

If the atoms enter the coupling area adiabatically, the populations of the adiabatic potentials will only depend on  $z$ . This is analogous to the *adiabatic transfer* via adiabatic sweeps or STIRAP pulse sequences. If the atoms are too fast, the populations also depend on history (i.e. the recent trajectory of the atoms), which can result in Landau-Zener transitions to other (possibly untrapped) states.

## 18.1.4 Exercises

### 18.1.4.1 Ex: The Stern-Gerlach effect

Consider initially motionless  $^{87}\text{Rb}$  atoms trapped in a superposition of two the trap-  
 pable Zeeman states  $|F, m_F\rangle = |2, +2\rangle$  and  $|1, -1\rangle$ . Suddenly a magnetic gradient of  
 $\partial_z \mathcal{B} = 100 \text{ G/cm}$  is applied for 2 ms. Calculate the spatial separation of the atoms  
 being in either one of the two states after 10 ms of ballistic expansion.

### 18.1.4.2 Ex: Potential for magnetic trapping

Invent a potential for magnetic confinement.

### 18.1.4.3 Ex: Adiabatic potentials

An *adiabatic potential* can be used to create more complicated trapping potentials  
 [154]. To study these potentials we consider a system of two Zeeman states  $m = \frac{1}{2}$   
 coupled by a radiofrequency radiation  $\hbar\omega$ . The dressed states Hamiltonian of our  
 two-level system is a  $2 \times 2$  matrix,

$$\hat{H} = \begin{pmatrix} \frac{1}{2}\mu_B \mathcal{B} - \frac{1}{2}\hbar\omega & \frac{1}{2}\hbar\Omega \\ \frac{1}{2}\hbar\Omega & -\frac{1}{2}\mu_B \mathcal{B} + \frac{1}{2}\hbar\omega \end{pmatrix},$$

defining the energetic zero in the middle between the states. Now, assume that the  
 magnetic field grows linearly along the axis  $z$ ,  $\mathcal{B}(z) = z\partial_z \mathcal{B}$ , where  $\partial_z \mathcal{B}$  is the gradient.  
 Also assume that the radiofrequency is tuned in resonance with the difference of the  
 energies of the Zeeman states at some distance  $z_0$  such that,  $\hbar\omega = \mu_B z_0 \partial_z \mathcal{B}$ .

- Calculate the eigenenergies of the coupled system as a function of  $z$ .
- Expands eigenenergies around the position  $z_0$ .
- What would be the oscillation frequency of the trapped atoms inside the adiabatic  
 potential?
- Expands the eigenenergies in  $\hbar\Omega$  for locations away from resonance.

## 18.2 Optical forces

Light carries momentum, and the scattering of light by an object produces a force on  
 that object. Although these properties of light are direct consequences of Maxwell's  
 classical theory of electromagnetism, they were only verified in 1933 by *Frisch*, who  
 observed a very small transverse deviation ( $3 \cdot 10^{-5}$  rad) of an atomic sodium beam  
 exposed to the light of a lamp. With the invention of the laser, it became easier to  
 observe the light's mechanical effects, because the more intense and highly directional  
 laser light exerts much larger forces. Although these results sparked the interest in  
 using light forces to control the motion of neutral atoms, the fundamental bases for  
 understanding the physics of light forces were not developed before the late 1970s.  
 Unequivocal experimental demonstrations of cooling and trapping of atoms were not  
 performed before the mid-1980s. In this section we will discuss some fundamental  
 aspects of light forces. Practical schemes used to cool and trap neutral atoms will be  
 presented in Secs. 24.2 and 24.3.

The light force acting on an atom can be of two types: a spontaneous dissipative force and a conservative dipole force. The spontaneous force arises from the recoil experienced by an atom when it absorbs or emits a quantum of light. As we saw in Sec. 1.2.6, when an atom scatters light, the resonant scattering cross section can be written as in Eq. (1.73),  $\sigma_{0a} = \frac{g_2}{g_1} \frac{\lambda_0^2}{2\pi}$ , where  $\lambda_0$  is the resonant wavelength. In the optical region of the electromagnetic spectrum the wavelengths of light are of the order of several hundred nanometers, and the resonant cross sections for scattering become very large, ( $\sim 10^{-9}$  cm<sup>2</sup>). Each absorbed photon transfers a quantum of momentum  $\hbar k$  to the atom in the direction of propagation. Spontaneous emission following an absorption process occurs in random directions and, hence, averaged over many absorption-emission cycles, it cancels to zero. Consequently, the total spontaneous force acts on the atom in the propagation direction of the light, as shown schematically in the diagram of Fig. 18.3. The saturated photon scattering rate via spontaneous emission (the reciprocal value of the excited state's lifetime) sets the upper limit for the magnitude of the force. This force is called *radiation pressure* force.

The *dipolar gradient force* can be easily understood by considering light as a classical wave. It is simply the time-averaged force resulting from the interaction of the transition dipole –induced by the oscillating electric field of the light– with the gradient of the electric field amplitude. The strength of this gradient can be controlled, e.g. by focusing the light beam. By tuning the optical frequency below or above an atomic transition, we can control the sign of the force acting on the atom: Tuning the light below resonance attracts the atom to the center of the light beam, tuning it above resonance repels it. The dipole force is a stimulated process without energy exchange between the field and the atom. Photons are absorbed in one light mode and reappear by stimulated emission in another one. However, conservation of momentum requires that the change in the propagation direction of the scattered photons from an initial mode to a final mode leaves the atom with a recoil. Contrary to spontaneous force, there is, in principle, no upper limit for the magnitude of the dipole force, since it is a function of the field gradient only and the detuning.

Within the theory of electromagnetism we calculate radiative forces on charges via *Maxwell's stress tensor*<sup>2</sup>. The interaction of radiation with atoms having internal degrees of freedom exhibiting resonances can be treated qualitatively by the *Lorentz model*<sup>3</sup>.

In the following, we will show quantitative semi-classical and quantum calculations: The force of a light beam on an atom can be calculated in many different ways, each emphasizing a slightly different aspect: From the classical Lorentz force exerted on an atom by electromagnetic fields we can derive a semi-classical Fokker-Planck equation [663]. In Sec. 18.2.1 we will derive the two contributions (dipole force and radiative pressure) within a semi-classical theory [274]. Wineland *et al.* [726] chose as starting point the cross section for an elementary scattering process (Sec. 18.2.3). Dalibard *et al.* [168] developed a quantum theory using the dressed states representation (Sec. 18.2.2). And Cirac *et al.* [134] showed an approach based on the master equation (Sec. 18.2.3).

<sup>2</sup>See script on *Electrodynamics* (2020), Sec. 6.2.3.

<sup>3</sup>See script on *Electrodynamics* (2020), Sec. 7.2.4.

### 18.2.1 The dipolar gradient force and the radiation pressure force

To compute the forces of light on an atom, we describe the atom as a two-level system: A fundamental level  $|1\rangle$  and an excited level  $|2\rangle$  decaying to the fundamental level with the rate  $\Gamma$ . The energy difference between the levels is  $\omega_0 \equiv E_2 - E_1$ . The light with frequency  $\omega$  is derived from a laser beam, which can be detuned from the atomic transition,  $\Delta \equiv \omega - \omega_0$ . To describe the interaction, we consider the part (18.6) of the total Hamiltonian describing the interaction [168]. Using the semi-classical density operator  $\hat{\rho}$ <sup>4</sup>, we can calculate the force that the light field exerts on the atom,

$$\begin{aligned} \mathbf{F}(\mathbf{r}) &= \langle \hat{\mathbf{F}}(\mathbf{r}) \rangle = -\text{Tr}_{at} \hat{\rho} \nabla_{\mathbf{r}} \hat{H}_{int} \\ &= -\frac{1}{2} \hbar \sum_j \langle j | \hat{\rho} | \nabla_{\mathbf{r}} (\Omega(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r} - i\Delta t} |2\rangle \langle 1| + \Omega(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r} + i\Delta t} |1\rangle \langle 2|) | j \rangle \\ &= -\frac{1}{2} \hbar \nabla_{\mathbf{r}} \Omega(\mathbf{r}) (\langle 1 | \hat{\rho} e^{i\mathbf{k}\cdot\mathbf{r} - i\Delta t} |2\rangle + \langle 2 | \hat{\rho} e^{-i\mathbf{k}\cdot\mathbf{r} + i\Delta t} |1\rangle) \\ &\quad - \frac{i}{2} \hbar \mathbf{k} \Omega(\mathbf{r}) (\langle 1 | \hat{\rho} e^{i\mathbf{k}\cdot\mathbf{r} - i\Delta t} |2\rangle - \langle 2 | \hat{\rho} e^{-i\mathbf{k}\cdot\mathbf{r} + i\Delta t} |1\rangle) . \end{aligned} \quad (18.18)$$

Now, we let the atom be at the position  $\mathbf{r} = 0$ ,

$$\mathbf{F}(\mathbf{0}) = -\frac{1}{2} \hbar \nabla_{\mathbf{r}} \Omega(\mathbf{0}) (\rho_{12} e^{-i\Delta t} + \rho_{21} e^{i\Delta t}) - \frac{i}{2} \hbar \mathbf{k} \Omega(\mathbf{0}) (\rho_{12} e^{-i\Delta t} - \rho_{21} e^{i\Delta t}) . \quad (18.19)$$

The quantities  $\rho_{12} \equiv \langle 1 | \hat{\rho} | 2 \rangle = \rho_{21}^*$  are the coherences, which develop in a two-level system excited by a laser beam. Inserting the stationary solutions of the Bloch equations,

$$\rho_{22} = \frac{\Omega^2}{4\Delta^2 + 2\Omega^2 + \Gamma^2} \quad \text{and} \quad \rho_{12} = \frac{(2\Delta - i\Gamma)\Omega}{4\Delta^2 + 2\Omega^2 + \Gamma^2} e^{-i\Delta t} . \quad (18.20)$$

we obtain

$$\mathbf{F}(\mathbf{0}) = -\frac{1}{2} \hbar \frac{4\Delta\Omega}{4\Delta^2 + 2\Omega^2 + \Gamma^2} \nabla_{\mathbf{r}} \Omega + \hbar \mathbf{k} \frac{\Gamma\Omega^2}{4\Delta^2 + 2\Omega^2 + \Gamma^2} . \quad (18.21)$$

With the definition of the cross section,  $\sigma_a(\Delta) = \sigma_{a0} \frac{\Gamma^2}{4\Delta^2 + 2\Omega^2 + \Gamma^2}$ ,

$$\mathbf{F}(\mathbf{0}) = -\frac{1}{2} \hbar \Delta \nabla_{\mathbf{r}} \ln \left( 1 + \frac{2\Omega^2}{4\Delta^2 + \Gamma^2} \right) + \hbar \mathbf{k} \frac{\Omega^2}{\Gamma} \frac{\sigma_a(\Delta)}{\sigma_{a0}} . \quad (18.22)$$

The resonant cross section for a 'classical' transition is  $\sigma_{a0} = 3\lambda^2/2\pi$ .

Apparently, the force comprises two contributions. The *dipolar gradient force* can be derived from a potential. It is proportional to the intensity gradient and can be interpreted as resulting from absorption processes immediately followed by self-stimulated emission. Near resonance it is dispersive. Far from resonance it can be approximated by,

$$\mathbf{F}_{dp} = \nabla_{\mathbf{r}} \frac{-\hbar\Delta\Omega^2}{4\Delta^2 + \Gamma^2} \xrightarrow{|\Delta| \gg \Gamma} -\nabla_{\mathbf{r}} \frac{\hbar\Omega^2}{4\Delta} . \quad (18.23)$$

<sup>4</sup>Treating the motional and the optical degrees of freedom as classical the density operator only contains the atomic excitation.

The *radiation pressure* force is dissipative. Close to resonance it is absorbing. It is proportional to the phase gradient and the only force exerted by plane waves. It can be interpreted as resulting from absorption processes followed by spontaneous emission. With  $\Omega^2 = \sigma_{a0}\Gamma/\hbar\omega$  we get a formula,

$$\mathbf{F}_{rp} = \hbar\mathbf{k} \frac{I}{\hbar\omega} \sigma_a(\Delta) = \hbar\mathbf{k}\gamma_{sct} \quad , \quad (18.24)$$

which describes the force as a product of the number of photons in the incident beam,  $I/\hbar\omega$ , the absorption cross section,  $\sigma_a(\Delta)$ , and the recoil momentum per photon,  $\hbar k$ .  $\gamma_{sct}$  is the scattering rate. The dipole gradient force (and the associated potential) is

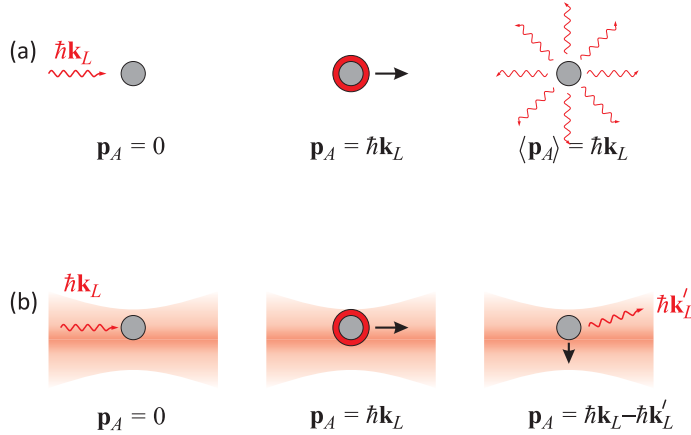


Figure 18.3: (a) An atom with mass  $m$  and velocity  $v_A$  moves to the right and absorbs a photon propagating to the left with momentum  $\hbar k_L$ . Center: An excited atom suffers a change of momentum  $p_A = mv_A - k_L$ . (b) The isotropic reemission of a photon results, averaged over many absorption-emission cycles, in a momentum change for the atom of  $\langle p_A \rangle = mv_A - k_L$ .

often used to spatially confine atoms, and the radiation pressure force is often used to cool them down. Note that we still need to correct Eqs. (18.23) and (18.24) to take into account the square of the average over the possible spatial orientations of the transition matrix element  $d_{12}/3$ .

The saturation parameter,

$$s = \frac{\frac{1}{2}\Omega^2}{\Delta^2 + \frac{1}{4}\Gamma^2} \quad , \quad (18.25)$$

allows to write the dipolar gradient force and the radiative pressure force as,

$$\mathbf{F}_{dp} = -\frac{\hbar\Delta}{6} \frac{1}{1+s} \nabla s = \frac{\hbar\Delta}{6} \nabla \ln[1+s] \quad \text{and} \quad \mathbf{F}_{rp} = \frac{\hbar\mathbf{k}\Gamma}{6} \frac{s}{1+s} \quad . \quad (18.26)$$

Eq. (18.26) shows that the radiation pressure force 'saturates' as  $s$  increases, and is therefore limited by the spontaneous emission rate. The saturation parameter essentially describes the relative importance of terms appearing in the denominator

of the line profile function for the light forces. The spontaneous emission rate is an intrinsic property of the atom, proportional to the square of the atomic transition dipole moment, whereas the square of the Rabi frequency is a function of the incident laser intensity. If  $s \ll 1$ , the spontaneous emission is fast compared to any stimulated process, and the light field is said to be weak. If  $s \gg 1$ , the Rabi oscillation is fast compared to spontaneous emission and the field is considered as strong. The line profile factor indicates a 'power broadening' by saturation of a factor of  $\sqrt{2}$ . Note that the dipolar gradient force and potential, Eqs. (18.26), do not saturate when the intensity of the light field is increased. Usually  $\mathbf{F}_{dp}$  and  $U_{dp}$  are used to manipulate and trap atoms in a laser beam tuned far away from resonance in order to avoid absorption.

Often, the transition moment can be oriented using circularly polarized light. In this case, all previous expressions for  $\mathbf{F}_{dp}$ ,  $\mathbf{F}_{rp}$ , and  $U_{dp}$  should be multiplied by 3. From now on we will abandon the average over the orientations and only use  $d_{12}^2$  for the square of the transition dipole moment. Solve Excs. 18.2.5.1 and 18.2.5.2.

## 18.2.2 Semiclassical calculation of dipole force and radiative pressure

In quantum mechanics we calculate the force from the Heisenberg equation [274],

$$\hat{\mathbf{F}} = \frac{d}{dt} \hat{\mathbf{p}} = \frac{i}{\hbar} [\hat{H}, \hat{\mathbf{p}}] = -\nabla_{\mathbf{r}} \hat{H}_{int} . \quad (18.27)$$

Thus, the force is given by the gradient of the interaction energy between the atom and the light field. Within the dipole approximation the interaction energy is given by  $\mathbf{d} \cdot \vec{\mathcal{E}}(\mathbf{r})$ . The force is now,

$$\begin{aligned} \mathbf{F}(\mathbf{r}) = \langle \hat{\mathbf{F}}(\mathbf{r}) \rangle &= \langle \nabla_{\mathbf{r}} [\mathbf{d} \cdot \vec{\mathcal{E}}(\mathbf{r})] \rangle = \langle (\mathbf{d} \cdot \nabla_{\mathbf{r}}) \vec{\mathcal{E}}(\mathbf{r}) \rangle - \langle \mathbf{d} \times (\nabla_{\mathbf{r}} \times \vec{\mathcal{E}}(\mathbf{r})) \rangle \\ &\equiv \mathbf{F}_C(\mathbf{r}) + \mathbf{F}_L(\mathbf{r}) . \end{aligned} \quad (18.28)$$

The first contribution can be interpreted as the Coulomb force acting on the electron performing rapid oscillations at the position  $\mathbf{r}(t) = \mathbf{r}_0 + e^{-1} \mathbf{P}(\mathbf{r}_0, t)$ . The second term is the time-averaged Lorentz force acting on the oscillating electric dipolar moment [321, 324, 322],

$$\mathbf{F}_C = e \langle \vec{\mathcal{E}} \rangle \quad \text{and} \quad \mathbf{F}_L = -\langle \mathbf{d} \times \partial_t \vec{\mathcal{B}} \rangle = \langle \partial_t \mathbf{d} \times \vec{\mathcal{B}} \rangle . \quad (18.29)$$

The relation between the light-induced electric dipole moment and the polarizability,  $\mathbf{d} = \alpha(\vec{\mathcal{E}}) \vec{\mathcal{E}}$ , where  $\alpha_{\nu\nu} \equiv \alpha_{\nu} + i\beta_{\nu}$  and  $E_{\nu} \equiv \sqrt{I_{\nu}} e^{i\psi_{\nu}}$ , becomes,

$$\mathbf{F} = \sum_{\nu=1}^3 \alpha_{\nu} \nabla I_{\nu} + 2 \sum_{\nu=1}^3 \beta_{\nu} I_{\nu} \nabla \psi_{\nu} . \quad (18.30)$$

## 18.2.3 Force exerted by a quantized radiation field

Photons carry one unit of momentum  $\mathbf{p} = \hbar \mathbf{k}$ , which they transfer to the atom during an absorption or emission process. That is, the light exerts a recoil on the atoms.

Spontaneous emission couples to all radiative modes of the electromagnetic vacuum,  $\hat{H}_{cm-vacuum} = \sum_j \hat{H}_{cm-laser}(\mathbf{k}_j)$ . We can trace over these variables and only keep those of the atom and the laser. Following Cirac *et al.* [726, 134], the randomness of the recoil by spontaneous emission is accounted for by,

$$\hat{\rho} \rightarrow \int_{4\pi\mathbb{R}^2} S(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\rho} e^{-i\mathbf{k}\cdot\mathbf{r}} d\Omega, \quad (18.31)$$

such that the *Lindblad operator* becomes,

$$\mathcal{L}_{atom}\hat{\rho} = -\Gamma\{\hat{\sigma}^\dagger\hat{\sigma}\hat{\rho}(t) - \frac{3}{4\pi} \int S(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\sigma}\hat{\rho}(t)\hat{\sigma}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}} d\Omega + \hat{\rho}(t)\hat{\sigma}^\dagger\hat{\sigma}\} \quad (18.32)$$

$$\mathcal{L}_{cavity}\hat{\rho} = -\kappa\{\hat{a}^\dagger\hat{a}\hat{\rho}(t) - 2\hat{a}\hat{\rho}(t)\hat{a}^\dagger + \hat{\rho}(t)\hat{a}^\dagger\hat{a}\},$$

where  $e^{\pm i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{p}} |\mathbf{p} \mp i\mathbf{k}\cdot\mathbf{r}\rangle \langle \mathbf{p}|$  and  $S(\mathbf{r}) = \frac{1}{2} (1 + (\frac{\mathbf{k}\cdot\mathbf{r}}{kr})^2)$  and  $d\Omega = d\varphi d\cos\vartheta$ . From this they calculate the force and establish a *Fokker-Planck equation* for the *Wigner function*.

### 18.2.4 Refraction of atoms by light and of light by atoms

Non-resonant light acts on the external degrees of freedom of atoms by a *phase shift of the Broglie wave*,  $\exp[i\hbar^{-1} \int U(\mathbf{r}, t) dt]$ , and simultaneously on the internal degrees of freedom by a *dynamic Stark shift* or *light shift* of the energy levels by the value of  $U(\mathbf{r})$ . The Bloch vector defined by,

$$\rho \equiv \begin{pmatrix} \frac{1}{\sqrt{2}} c_g c_e^* \\ \frac{1}{\sqrt{2}} c_g^* c_e \\ |c_e|^2 - |c_g|^2 \end{pmatrix} \quad (18.33)$$

describes, under the influence of the dispersive interaction, a precession around the polar axis. This was discussed in Exc. 14.5.5.7. The Stark shift causes a rotation of  $\hbar^{-1}U(\mathbf{r})t$ . Simultaneously, the atom is subjected to a force, which corresponds to the gradient of the potential  $-\nabla U(\mathbf{r})$ , as illustrated in Fig. 18.4(a). We see that the phase shifts of the Broglie wave and the Bloch vector are equal. Finally, the light mode phase is also shifted by the same amount in an effect called *refraction*. That is, the internal, external, and optical degrees of freedom are entangled.

This fact has a practical use in atomic interferometers, because it is often easier to detect an interference of internal excitation states rather than of Broglie waves. Because of the entanglement, it is sufficient to measure *one* interference pattern to know the *other one*.

By local variations of the potential  $U(\mathbf{r})$ , e.g. induced by a focused laser beam, it is possible to manipulate a Broglie wavefront in the same way that, in classical optics, we manipulate the wavefront of a light beam by lenses or other objects, such as for instance, the refractive index represented by an atomic cloud near resonance, as illustrated in Fig. 18.4(b).

The orientation of the force depends on the light frequency as compared to the resonant frequency. The dipolar force attracts the atom to regions where the light field



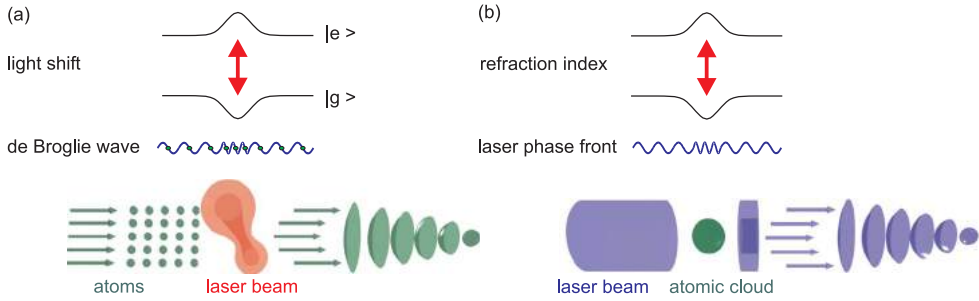


Figure 18.4: Diagram (a) shows product states and dressed states for blue detuning. Note that the population is in the upper level and that the atom is subject to a repulsive weak field seeking force when it enters the laser beam. Diagram (b) is similar, but for red detuning. The population is in the lower level and the atom is subject to an attractive high field seeking force.

is strong, when the frequency is tuned below  $\omega_0$ , and it attracts the atom to regions of weak fields, when tuned above  $\omega_0$ . Integration over the relevant spatial coordinates results in an effective potential or barrier to the atom. The qualitative behavior of the dipolar potential and its effect on the motion of atoms is easily visualized in the dressed states picture. Fig. 18.5 shows what happens when an atom enters a well defined region of an optical field, for example a focused laser beam.

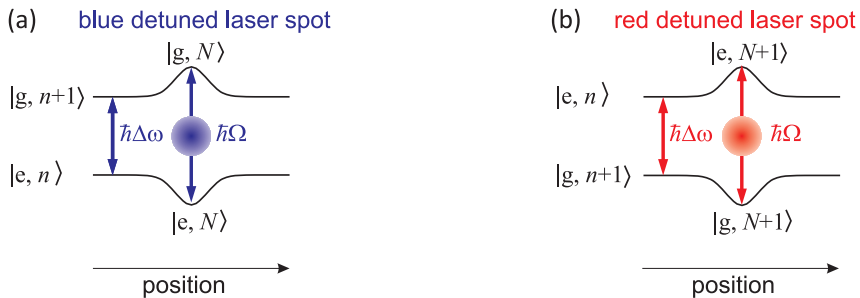


Figure 18.5: Analogy between light optics and atomic optics.

Outside the atom-dipole coupling zone the expression  $\hbar\Omega$  is despicable and the 'dressed states' are just the atom-field product states. When the atom enters the field, this expression becomes nonzero and the atom-field states combine to produce a set of dressed states. The energy levels of the product states 'repel' each other and approach the dressed states levels. Assuming that the laser is sufficiently detuned to maintain the absorption rate negligible, the population remains in the ground state. We see that blue (red) detuning leads to a repulsive (attractive) potential for atoms remaining in the grounded state. In addition, since  $\hbar\Omega$  is directly proportional to the root of the laser intensity, an increase in that intensity (optical power per unit area) obviously amplifies the force on the atom ( $\mathbf{F} \simeq \nabla_R \Omega$ ).

## 18.2.5 Exercises

### 18.2.5.1 Ex: Dipole force for large detunings

Verify that in the limit of large detunings the dipole potential Eq. (18.22) tends to  $\rightarrow \frac{\Omega^2}{4\Delta}$ .

### 18.2.5.2 Ex: Radiation pressure

Calculate the radiation pressure force exerted on a strontium atom by a laser beam in plane wave geometry ( $I = 10 \text{ mW/cm}^2$ ) tuned 50 MHz below the resonance at 461 nm ( $\Gamma/2\pi = 30.5 \text{ MHz}$ ).

## 18.3 Photonic recoil on free and confined atoms

A trap confining the atomic motion can dramatically modify the way in which they interact with light <sup>5</sup>. For instance, a trapping potential may alter the scattering rate, the scattering angle, and the transfer of photonic recoil. However, *potentials do not exist* in microscopic reality, not more than friction forces do. What exists, as we learn in electrodynamics, are *electromagnetic fields* exerting Coulomb and Lorentz forces. When we write down the Hamiltonian  $\hat{H} = \mathbf{p}^2/2m + V(\mathbf{r})$  in quantum mechanics, we already make an important approximation, because the potential  $V(\mathbf{r})$  is an artifact obtained by tracing over all those degrees of freedom, which are necessary to generate a force field that can be approximated by a conservative potential.

In the great majority of situations, the approximation is very good. Problems may however arise, when the momentum conservation comes into play, which is the case e.g. of light scattering from ultracold atoms being accelerated by the photonic recoil and shifting the scattered light via the Doppler effect. We then have to address the issue of photonic recoil conserving (or not) the momentum.

Let us begin with a recapitulation of the classical picture of the scattering process applying the rules of energy and momentum conservation to the elastic collision between a free atom and a photon. This process is known as *Compton scattering*.

### 18.3.1 Recoil- and Doppler-shift in classical mechanics

In classical mechanics we speak of *elastic scattering* when no energy is transferred to internal degrees of freedom of the collision partners, so that *kinetic* energy and momentum stay conserved. This concept can be transferred to quantum particles (e.g. atoms) and photons. In elastic Compton scattering, if the atoms keep their initial internal excitation, the law of momentum conservation requires the transfer of photonic momentum to the scattering atom which, consequently, changes its kinetic energy. To compensate for this kinetic energy change, the frequency of the scattered light must change in order to preserve the total energy, as illustrated in Fig. 18.6(b).

We will calculate in the following the frequency distribution of the light scattered by an atom as a function of its initial velocity  $\mathbf{p}_1$ , of the frequency  $\omega_1$  of the incident

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<sup>5</sup>The interaction also depends on other parameters, such as the geometry of the confinement potential and on cooperative effects (bosonic stimulation), but this will be discussed later.

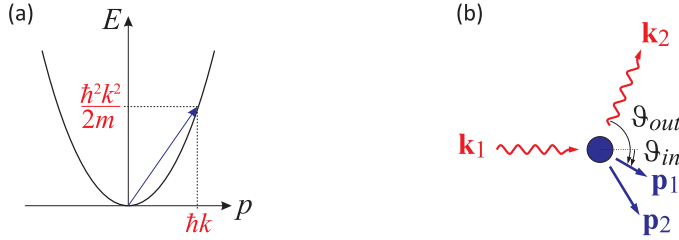


Figure 18.6: (a) Kicking an atom along its dispersion relation. (b) Scheme of the Compton-scattering of light.

light and of the scattering angle, that is, the angle between the modes  $\mathbf{k}_1$  and  $\mathbf{k}_2$ . We begin by writing the laws of conservation of energy and momentum,

$$\begin{aligned} \hbar\mathbf{k}_1 + \mathbf{p}_1 &= \hbar\mathbf{k}_2 + \mathbf{p}_2 & (18.34) \\ \hbar\omega_1 + \frac{p_1^2}{2m} &= \hbar\omega_2 + \frac{p_2^2}{2m} . \end{aligned}$$

Eliminating  $\mathbf{p}_2$  from the second equations, we obtain,

$$\hbar\omega_1 - \frac{\hbar^2 k_1^2}{2m} - \frac{\hbar\mathbf{k}_1 \cdot \mathbf{p}_1}{m} = \hbar\omega_2 + \frac{\hbar^2 k_2^2}{2m} - \frac{(\hbar\mathbf{k}_1 + \mathbf{p}_1) \cdot \hbar\mathbf{k}_2}{m} . \quad (18.35)$$

The photonic recoils of the incident and of the scattered light are almost equal,

$$\omega_{rec} \equiv \frac{\hbar k_1^2}{2m} \simeq \frac{\hbar k_2^2}{2m} , \quad (18.36)$$

such we can approximate,

$$\omega_2 = \omega_1 \frac{1 - \frac{\hbar\omega_1}{mc^2} - \frac{p_1}{mc} \cos \angle(k_1, p_1)}{1 - \frac{\hbar\omega_1}{mc^2} \cos \angle(k_1, k_2) - \frac{p_1}{mc} \cos \angle(p_1, k_2)} , \quad (18.37)$$

using  $\omega_1 = ck_1$ , or also,

$$\omega_2 - \omega_1 = \omega_1 \frac{\frac{\hbar\omega_1}{mc^2} [-1 + \cos(\vartheta_{in} - \vartheta_{out})] + \frac{p_1}{mc} (\cos \vartheta_{out} + \cos \vartheta_{in})}{1 - \frac{\hbar\omega_1}{mc^2} \cos(\vartheta_{in} - \vartheta_{out}) - \frac{p_1}{mc} \cos \vartheta_{out}} , \quad (18.38)$$

where we call the angles  $\vartheta_{in} = \angle(k_1, p_1)$ ,  $\vartheta_{out} = \angle(k_2, p_1)$ , and  $\vartheta = \vartheta_{in} - \vartheta_{out} = \angle(k_1, k_2)$ . For non-relativistic velocities, the denominator is approximately 1:

$$\boxed{\omega_2 - \omega_1 = 2\omega_{rec}(-1 + \cos \vartheta) + k_1 v_1 (\cos \vartheta_{out} + \cos \vartheta_{in})} , \quad (18.39)$$

with  $\mathbf{p}_1 = m\mathbf{v}_1$ . The first term describes the recoil shift and the second term the Doppler shift.

The second term vanishes for initially at resting atoms,  $\mathbf{p}_1 = 0$ , and Eq. (18.39) simplifies to,

$$\omega_2 - \omega_1 = 2\omega_{rec}(-1 + \cos \vartheta) . \quad (18.40)$$

It also vanishes for atoms which have no velocity component in the scattering plane spanned by the wavevectors  $\mathbf{k}_1$  and  $\mathbf{k}_2$ , that is  $\vartheta_{out} = 180^\circ - \vartheta_{in}$ <sup>6</sup>, for which case we get the maximum recoil shift,

$$\omega_2 - \omega_1 = -4\omega_{rec} . \quad (18.41)$$

*The recoil shift is a consequence of momentum conservation.*

The recoil shift is typically on the order of  $\omega_2 - \omega_1 \approx (2\pi) 10$  kHz, which in many situations is negligible (e.g. when we deal with thermal atomic clouds), such that we can consider the scattering as elastic., i.e. the first term can be disregarded. Considering, for simplicity, only backscattering,  $\cos \vartheta_{out} = \cos \vartheta_{in} = 1$ , then Eq. (18.39) simplifies to,

$$\omega_2 - \omega_1 = 2k_1 v_1 . \quad (18.42)$$

Obviously, the frequency shift depends on the initial velocity through the Doppler shift  $k_1 v_1$ . In a thermal gas, the velocities are distributed according to the Maxwell-Boltzmann distribution. Therefore, Rayleigh scattering of light off a cloud of free thermal atoms is subject to Doppler broadening<sup>7</sup>.

### 18.3.2 Kicking a free atom

A conceptual difficulty arises from the incompatibility of scattering picture (generally described in homogeneous space with momentum conservation) and the trapping picture (when it is described in inhomogeneous space without momentum conservation). The difficulty can be avoided by separating the processes into a 'kick' followed by a harmonic oscillation, for which we have to calculate the time-dependence of the states and the observables. We will leave the discussion of such a scattering process to 18.3.3 and for the time being just focus on the time evolution of a harmonic oscillator that just received a kick.

By a 'kicking' an atom we denote a change of momentum within an arbitrarily short amount of time. The shorter the kick-time the larger is, according to Heisenberg's uncertainty relation, the spectrum of possible kinetic energies that can be reached by the kick (see Sec. 6.4.3). However, the spectrum is restricted by the free-particle dispersion relation, as illustrated in Fig. 18.6(a).

The kick is not a realistic physical concept, as it corresponds to an infinitely strong and infinitely short force<sup>8</sup>. In a microscopic scattering process it assumes an infinitely heavy collision partner, while we are more interested in photon scattering. Consequently, in this case the spectrum of reachable energies is determined by the frequency of the photon *and* the free-particle dispersion relation. We will now turn our attention to the (Compton-)scattering of light by free atoms.

<sup>6</sup>This situation is often realized in Bragg scattering from optical lattices [641, 643, 642].

<sup>7</sup>This Doppler broadening is explored e.g. in RIR spectroscopy, where the momentum distribution in  $p_1$  reveals as a frequency distribution  $\Delta\omega = \omega_2 - \omega_1$  of Bragg-scattered light, which can be measured by beating with an irradiated idler mode, which can be chosen as being identical to  $\mathbf{k}_2$ .

<sup>8</sup>which is what allows us to write down a potential

### 18.3.3 (In-)elastic light scattering from a single weakly or strongly confined atom

We mentioned in the last subsection that a scattering process is elastic when none of the collision partners changes its internal excitation energy. The situation becomes, however, more complex when one of the collision partners is confined in a potential, as we will show in the following.

#### 18.3.3.1 Cooperativity in light scattering

In light scattering *cooperativity* means *breaking of the isotropic symmetry* for the angular distribution of scattered modes. In this sense, the anisotropic scattering from an atom confined in an anisotropic trap is cooperative. But there are other cooperative scattering effects messing with isotropy and shaping the density-of-states, like the Purcell effect in the presence of an optical cavity or a photonic band gap concentrating optical modes in a specific solid angles [316]. Another cooperative effect, which is observed in the presence of other atoms, has to do with bosonic stimulation by the optical output mode (as in Bragg scattering [641, 643, 642]) or the momentum sidemode (as in stimulated matter wave 4WM). These effects, which all need to be considered in calculations of the static structure factor ruling the scattering of light, are often strong enough to hide the role of an anisotropic trapping potential. In the following subsections we will disregard all these effects and concentrate on a *single trapped atom*.

The simple picture of Compton scattering presented in Sec. 18.3.1 holds for *free atoms*, whose dynamics is totally understood in terms of their internal electronic excitation ( $\hat{H}_{ele}$ ), the kinetic energy of their center-of-mass ( $\hat{H}_{cm} = \frac{\mathbf{p}^2}{2m}$ ), the radiation field ( $\hat{H}_{rad}$ ) (which may be treated classically under the circumstances discussed here), and the coupling ( $\hat{H}_{int}$ ) of all three degrees of freedom,

$$\hat{H}_{free} = \hat{H}_{ele} + \hat{H}_{cm} + \hat{H}_{rad} + \hat{H}_{int} . \quad (18.43)$$

Transition probabilities are readily calculated using Fermi's Golden rule, because the density-of-states distributions for the final radiation modes receiving the scattered photons (photonic density-of-states) and the recoil modes receiving the scattered atoms (phononic density-of-states) are white, that is, without resonances, and isotropic.

In the presence of an imposed trapping potential, an additional term appears in the Hamiltonian, which has the capacity of dramatically changing the scattering features,

$$\hat{H}_{cm} = \frac{\mathbf{p}^2}{2m} + \hat{V}_{trap}(\mathbf{r}) . \quad (18.44)$$

The confining potential may or may not depend on the internal state of the atom. For ions in a Paul trap it does not depend, but for atoms in magnetic traps it usually depends,

$$\begin{aligned} \hat{H}_{atom} &= |g\rangle \hat{H}_{cm,g} \langle g| + |e\rangle (\hat{H}_{cm,e} + \hbar\omega_0) \langle e| \\ \hat{H}_{cm,j} &= \frac{\hat{p}^2}{2m} + V_j(\mathbf{r}) , \end{aligned} \quad (18.45)$$

where  $\omega_0$  is the frequency of the atomic transition. In the following, however, we will treat potentials that are independent of the internal atomic state.

### 18.3.3.2 Resolved sideband regime

As discussed in Sec. 14.4.5, incident light is absorbed by an atom harmonically oscillating in a trap with frequency  $\omega_{trp}$  on a spectrum of discrete sidebands separated by  $\omega_{trp}$  with amplitudes given by  $J_n(kv_0/\omega_{trp})$ . The modulation index  $kv_0/\omega_{trp} = kx_0 = 2\pi x_0/\lambda$  corresponds to the Lamb-Dicke parameter. When the modulation amplitude is within the so-called *Lamb-Dicke regime*,  $kv_0 \ll \omega_{trp}$ , the first sidebands become smaller than the carrier,  $J_1(kv_0/\omega_{trp}) < J_0(kv_0/\omega_{trp})$  and, therefore, do not contribute to the Doppler width of the frequency distribution. That is, the linear Doppler effect vanishes.

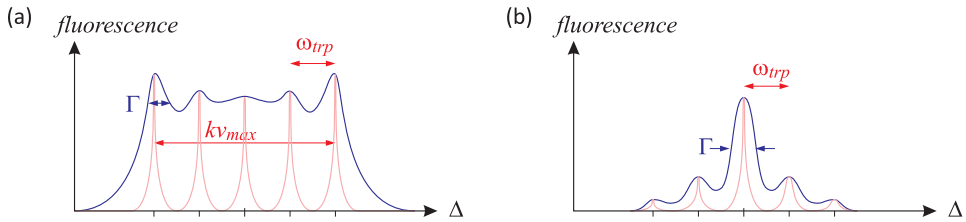


Figure 18.7: Absorption profile in the regimes of (a) weak binding ( $\eta > 1$ ) for the cases of and unresolved sidebands (blue curve) and resolved sidebands (red curve), and (b) strong binding (Lamb-Dicke regime  $\eta < 1$ ) for the same cases as in (a).

The relative size of the characteristic frequencies  $\omega_{rec}$ ,  $\omega_{trp}$ , and  $\Gamma$  define characteristic regimes, as illustrated in the table.

confinement		sidebands	
weak	$\eta > 1$	unresolved	$\frac{\omega_{trp}}{\Gamma} < 1$
strong	$\eta < 1$	resolved	$\frac{\omega_{trp}}{\Gamma} > 1$

### 18.3.3.3 The Mößbauer effect

The role of photonic recoil in the scattering of light by confined atoms has been unraveled by *Mößbauer*, who performed scattering experiments of  $\gamma$ -photons on a  $^{57}\text{Fe}$  crystal on a narrow transition of this isotope at 14 keV (0.086 nm). The linewidth of this transition,  $\Gamma \approx (2\pi) 1$  MHz, is much narrower than the recoil-shift,  $\omega_{rec} \approx (2\pi) 500$  MHz  $\gg \Gamma$ , so that we should expect the scattered light to be considerably recoil-shifted and Doppler-broadened. In fact, the recoil-shift should be so large, that scattered photons cannot be reabsorbed by other atoms on this transition being at rest. This is *not* what Mößbauer observed in his experiments. He found that scattered photons can be reused for subsequent scattering, which means that the scattering must be elastic.

The explanation for this unexpected observation is that, if the nucleus is embedded in a crystal, the vibrational frequencies, which are even higher than the photonic recoil

frequency,  $\omega_{trp} \approx 2\pi \cdot 3$  THz, are unreachable. That is to say, we are in the *resolved sidebands Lamb-Dicke regime*,  $\omega_{trp} \gg \omega_{rec} \gg \Gamma$ . Here, the phonons corresponding to the vibrations cannot be excited, so that the recoil momentum must be absorbed by the whole lattice, whose entire mass is so large, that the photon frequency is not recoil-shifted by the scattering process. Hence, the first-order *Doppler effect* is avoided and the measured width of the transition is just the natural linewidth. Furthermore, the atom remains in the same vibrational state of their localizing potential. This is the *Möbbauser effect*.

	$\gamma$ for $^{57}\text{Fe}$	optical for $^{172}\text{Yb}^+$
photon energy	$\approx 14$ keV $\approx 4 \times 10^{18}$ Hz	$\approx 3$ eV $\approx 640$ THz
recoil	$\approx 2$ meV $\approx 500$ MHz $\approx 10^{-10}$	$\approx 20$ peV $\approx 5$ kHz $\approx 10^{-11}$
linewidth	$\approx 5$ neV $\approx 1$ MHz $\approx 2 \times 10^{-13}$	$\approx 5$ feV $\approx 1$ Hz $\approx 2 \times 10^{-15}$
lattice vibrations	$\approx 10$ meV $\approx 3$ THz	$\approx 3$ neV $\approx 1$ MHz

Table 18.1: Comparison of  $\gamma$ -radiation and the optical regime.

A similar effect can be observed with trapped atoms driven on very narrow transitions, as we will discuss in the following.

#### 18.3.3.4 Coupling of internal and external motion by photonic recoil, tracing over the internal excitation

When discussing the transfer of momentum to a harmonic oscillator in 3.6.2, we did not say how the momentum shift could be realized in practice. As we have seen in the example of the Möbbauser effect, a possible way is via the photonic recoil received on a light scattering process. The coupling of the relevant degrees of freedom of the system induced by the absorption of a photon by an atom is accounted for by an additional interaction term  $\hat{H}_{int}$  in the Hamiltonian. The relevant degrees of freedom are the electronic orbital  $|i\rangle$ , the vibrational state  $|n\rangle$ , and the number of photons  $|N\rangle$  in the light mode, assumed to be a plane wave  $\vec{\mathcal{E}}(\mathbf{r}, t) = E_0 \hat{\mathbf{e}}_y e^{ik_z z - i\omega t}$ . Neglecting the quantum nature of the light, we will disregard this degree of freedom in the following. Assuming that the trapping potential is the same for all electronic orbitals, as in (18.45), the total state can be expressed as a product state,  $|n, i\rangle \equiv |i\rangle \otimes |n\rangle$ . The interaction Hamiltonian,

$$\hat{H}_{int} = \frac{\hbar\Omega}{2} (e^{ik_z \hat{z}} \hat{a} |e\rangle \langle g| + e^{-ik_z \hat{z}} \hat{a}^\dagger |g\rangle \langle e|) - |e\rangle \hbar\omega \langle e|, \quad (18.46)$$

couple the dynamics on the internal transition, given by the Rabi frequency  $\hbar\Omega \equiv \langle e | d_y | g \rangle \mathcal{E}_0$ , with the absorption (or stimulated emission) of a photon  $\hat{a}$ , and the transfer of a recoil momentum. The last term comes from the transformation into the

interaction picture <sup>9</sup>. With this our total Hamiltonian (18.45) becomes,

$$\boxed{\hat{H} = \hbar\omega_{trp}(\hat{b}^\dagger\hat{b} + \frac{1}{2}) + |e\rangle\hbar(\omega_0 - \omega)\langle e| + \frac{\hbar\Omega}{2}(e^{ik\hat{z}}|e\rangle\langle g| + e^{-ik\hat{z}}|g\rangle\langle e|)} . \quad (18.47)$$

So, vibrational states are only coupled via electronic transitions,

$$\langle n, g|\hat{H}_{int}|0, g\rangle = 0 \quad \text{and} \quad \langle n, e|\hat{H}_{int}|0, g\rangle = \frac{1}{2}\hbar\Omega\langle n, e|e^{ik\hat{z}}|0, g\rangle . \quad (18.48)$$

Hence, we have to span the complete Hilbert space of all operators like  $\hat{\sigma}^\dagger = \sum_n |n\rangle\langle n| \otimes |e\rangle\langle g|$ .

We can expand the system's state into,

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} (c_{n,g}|n, g\rangle + c_{n,e}|n, e\rangle) , \quad (18.49)$$

and insert it together with the Hamiltonian (18.47) into the Schrödinger equation. Projecting onto the states  $\langle n, g|$  and  $\langle n, e|$ , we easily derive the following equations of motion,

$$\boxed{\begin{aligned} \frac{dc_{n,g}}{dt} &= -\omega_{trp}(n + \frac{1}{2})c_{n,g} - \frac{i\Omega}{2} \sum_{m=0}^{\infty} c_{m,e} \langle n|e^{-ik\hat{z}}|m\rangle \\ \frac{dc_{n,e}}{dt} &= -\omega_{trp}(n + \frac{1}{2})c_{n,e} - i(\omega_0 - \omega)c_{n,e} - \frac{i\Omega}{2} \sum_{m=0}^{\infty} c_{m,g} \langle n|e^{ik\hat{z}}|m\rangle \end{aligned}} . \quad (18.50)$$

The fact that only terms proportional to  $\langle n|e^{ik\hat{z}}|m\rangle$  contribute can be understood in terms of the *Frack-Condon overlap* between the vibrational states to be coupled. And the fact that the energy of the harmonic oscillator, and thus the effective detuning  $\Delta_n \equiv \omega - \omega_0 - \omega_{trp}(n + \frac{1}{2})$ , depend on the vibrational state couples the internal and the external dynamics.

Nevertheless, the off-diagonal coupling elements only contain the degrees of freedom of the harmonic oscillator.

### 18.3.3.5 Momentum kick by photonic recoil

We said earlier that a momentum kick can drive an atom from the vibrational ground state  $|0\rangle$  into a coherent superposition of states  $|\alpha\rangle$ , except when the Lamb-Dicke parameter is very small. When the kick is realized via photonic recoil, e.g. when an electronically excited atom decays to the ground state, the frequency of the emitted photon depends on the final vibrational state of the atom. That is we expect a coherent superposition of light frequencies, which in the limit  $\eta > 1$  generates a *Doppler broadening* and in the limit  $\eta < 1$  stays unshifted as for *elastic scattering*.

<sup>9</sup>Note, that this Hamiltonian cannot be used to describe spontaneous emission. To do so, we need to allow for 3D systems and decay modes,

$$\hat{H} = \hbar\omega_{trp}(|\mathbf{n}\rangle\langle \mathbf{n}| + \frac{1}{2}) + \hbar(\omega_0 - \omega)|e\rangle\langle e| + \frac{\hbar\Omega}{2}(e^{-i\mathbf{k}_i \cdot \hat{\mathbf{r}}} \hat{\sigma}^\dagger \hat{a}_{\mathbf{k}_i} + c.c.) + \hbar g \sum_{\mathbf{k}_f} (e^{i\mathbf{k}_f \cdot \hat{\mathbf{r}}} \hat{\sigma} \hat{a}_{\mathbf{k}_f}^\dagger + c.c.) .$$



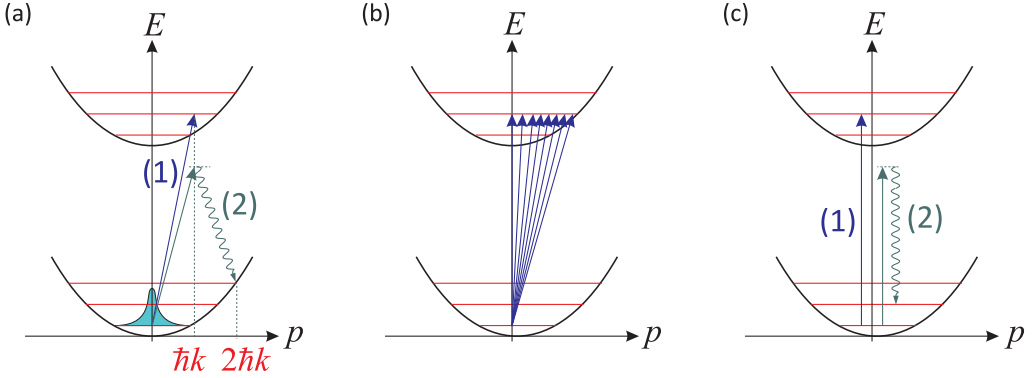


Figure 18.8: (a) Absorption (1) and Rayleigh scattering (2) in a weakly confining trap, where the momentum must stay conserved. (b) Illustration of the regime  $\omega_{rec} > \Gamma$ , where the atom moves during the absorption process. (c) Absorption and Rayleigh scattering in a strongly confining trap.

Let us now consider a single confined atom and address the question of the absorption probability. In first-order perturbation, using the Hamiltonian (18.47), the transition rate for absorption of a photon incident in  $z$ -direction is given by Fermi's Golden Rule,

$$\begin{aligned} \frac{1}{\tau} &= \frac{d}{dt} |\langle n, e | e^{i\hat{H}t/\hbar} | 0, g \rangle|^2 \simeq \frac{2\pi}{\hbar^2} |\langle n, e | \hat{H} | 0, g \rangle|^2 \\ &= \frac{2\pi}{\hbar^2} |\langle n, e | \frac{\hbar\Omega}{2} (e^{ik\hat{z}} \hat{\sigma}^\dagger + e^{-ik\hat{z}} \hat{\sigma}) | 0, g \rangle|^2 = \frac{\pi\Omega^2}{2} |\langle n, e | e^{ik\hat{z}} | 0, e \rangle|^2. \end{aligned} \quad (18.51)$$

Obviously, it is thus sufficient to calculate  $\langle n | e^{ik\hat{z}} | 0 \rangle$ , i.e. we can trace over the internal degrees of freedom. Using our previous results (3.130), we find with  $\alpha = -ika_{trp}/\sqrt{2}$ ,

$$\boxed{\frac{1}{\tau} = \frac{\pi\Omega^2}{2} |\langle n | \alpha \rangle|^2 = \frac{\pi\Omega^2}{2} e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!}}. \quad (18.52)$$

The interpretation of this result is that the absorption of a photon by an atom in state  $|0, g\rangle$  transfers recoil by *leaving the vibrational state of the atom in a coherent superposition state*. Inversely, for the emission process from state  $|0, e\rangle$  within the Lamb-Dicke regime, most of the time we will encounter the emitted photon at the resonance frequency  $\omega_0$ , and rarely at  $\omega_0 - \omega_{trp}$ . In any case, energy conservation is satisfied, since,

$$\begin{aligned} \sum_n n \hbar \omega_{trp} \langle n | \alpha \rangle \langle \alpha | n \rangle &= \sum_n n \hbar \omega_{trp} e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!} = \hbar \omega_{trp} |\alpha|^2 \sum_n n e^{-|\alpha|^2} \frac{|\alpha|^{2n-2}}{(n-1)!} \\ &= \frac{\hbar^2 k^2}{2m} \langle \alpha | \alpha \rangle = \hbar \omega_{rec}. \end{aligned} \quad (18.53)$$

Thus energy and momentum conservation are automatically satisfied by the way the kick is implemented.

### 18.3.3.6 A single anisotropically trapped atom in first-order perturbation

Let us now consider a single atom (e.g. a trapped ion) confined in an 3-dimensional anisotropic trap (e.g. strong confinement in one and weak confinement in the other direction) and address the question, whether the scattering will be anisotropic, as well. We generalize the problem to three dimensions by allowing for quantized vibrational states in three dimensions,  $\hat{\sigma}^\dagger = \sum_{\mathbf{n}} |\mathbf{n}\rangle \langle \mathbf{n}| \otimes |e\rangle \langle g|$  with  $|\mathbf{n}\rangle = |n_x, n_y, n_z\rangle$ .

In first-order perturbation, using the Hamiltonian (18.47), the transition rate for absorption or emission is given by Fermi's Golden Rule,

$$\begin{aligned} \frac{1}{\tau} &= \frac{d}{dt} |\langle \mathbf{n}, e | e^{i\hat{H}t/\hbar} | \mathbf{0}, g \rangle|^2 \simeq \frac{2\pi}{\hbar^2} |\langle \mathbf{n}, e | \frac{\hbar\Omega}{2} (e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} \hat{\sigma}^\dagger + e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}} \hat{\sigma}) | \mathbf{0}, g \rangle|^2 \\ &= \frac{\pi\Omega^2}{2} |\langle n_x, e | e^{ik\hat{x}} | 0, e \rangle \langle n_y, e | e^{ik\hat{y}} | 0, e \rangle \langle n_z, e | e^{ik\hat{z}} | 0, e \rangle|^2. \end{aligned} \quad (18.54)$$

Obviously, it is thus sufficient to calculate  $\langle n_j | e^{ik\hat{z}} | 0 \rangle$ , i.e. we can trace over the internal degrees of freedom. Using our previous results (3.130), we find with  $\alpha_j = -ik_j a_{trp,j} / \sqrt{2}$ ,

$$\boxed{\frac{1}{\tau} = \frac{\pi\Omega^2}{2} |\langle n_x | \alpha_x \rangle \langle n_y | \alpha_y \rangle \langle n_z | \alpha_z \rangle|^2 = \frac{\pi\Omega^2}{2} e^{-|\alpha_x|^2 - |\alpha_y|^2 - |\alpha_z|^2} \frac{|\alpha_x^{n_x} \alpha_y^{n_y} \alpha_z^{n_z}|^2}{n_x! n_y! n_z!}}.$$

In Exc. 18.3.4.1 we calculate and illustrate the transition matrix elements  $\langle \mathbf{0} | e^{ik\hat{z}} | 0 \rangle$  and  $\langle \mathbf{n} | e^{ik\hat{z}} | 0 \rangle$ .

### 18.3.3.7 A single anisotropically trapped atom in second-order perturbation

To understand Rayleigh scattering, we need to go to second perturbation order summing over all intermediate vibrational states according to the Kramers-Heisenberg formula,

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{d}{dt} |\langle \mathbf{n}, g, \mathbf{k}_f | e^{i\hat{H}t/\hbar} | \mathbf{0}, g, \mathbf{k}_i \rangle|^2 \simeq \frac{2\pi}{\hbar^2} |\langle \mathbf{n}, g, \mathbf{k}_f | \sum_{\mathbf{m}} \frac{\hat{H}^{(1)} | \mathbf{m}, e \rangle \langle \mathbf{m}, e | \hat{H}^{(1)} | \mathbf{0}, g, \mathbf{k}_i \rangle}{\omega_i - \omega_m} | \mathbf{0}, g, \mathbf{k}_i \rangle|^2 \\ &= \frac{\pi\hbar^2\Omega^4}{8} \left| \sum_{\mathbf{m}} \frac{\langle \mathbf{n}, \mathbf{k}_f | e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}} | \mathbf{m} \rangle \langle \mathbf{m} | e^{i\mathbf{q}\cdot\hat{\mathbf{r}}} | \mathbf{0}, \mathbf{k}_i \rangle}{E_i/\hbar + (0\omega_x + 0\omega_y + 0\omega_z + \frac{3}{2}) - E_m/\hbar - (m_x\omega_x + m_y\omega_y + m_z\omega_z + \frac{3}{2})} \right|^2 \\ &= \frac{\pi\hbar^2\Omega^4}{8} \left| \sum_{m_x, m_y, m_z} \frac{\langle n_x, n_y, n_z | e^{-i\mathbf{k}_f \cdot \hat{\mathbf{r}}} | m_x, m_y, m_z \rangle \langle m_x, m_y, m_z | e^{i\mathbf{k}_i \cdot \hat{\mathbf{r}}} | 0, 0, 0 \rangle}{(E_i - E_m)/\hbar - m_x\omega_x - m_y\omega_y - m_z\omega_z} \right|^2 \\ &= \frac{\pi\hbar^2\Omega^4}{8} \left| \sum_{m_x, m_y, m_z} \prod_{j=x,y,z} \frac{\langle n_j | e^{-ik_j r_j} | m_j \rangle \langle m_j | e^{ik_j r_j} | 0 \rangle}{(E_i - E_m)/\hbar - m_x\omega_{m_x} - m_y\omega_{m_y} - m_z\omega_{m_z}} \right|^2. \end{aligned} \quad (18.55)$$

The transition matrix elements can be calculated via (3.135). This expression represents (in the same time) the *dynamic structure factor* of the single trapped atom.

**Example 79 (Axial incidence):** Let us consider the particular case of Rayleigh scattering from the ground state of light incident in the direction  $\mathbf{k}_i \equiv k_{iz}\hat{\mathbf{e}}_z$ . We can then simplify,

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{\pi\hbar^2\Omega^4}{8} \left| \sum_{m_z} \frac{\langle 0|e^{-ik_x f \hat{x}}|0\rangle\langle 0|e^{-ik_y f \hat{y}}|0\rangle\langle 0|e^{-ik_z f \hat{z}}|m_z\rangle\langle m_z|e^{ik_z i \hat{z}}|0\rangle}{-m_z\omega_{trp}} \right|^2 \\ &= \frac{\pi\hbar^2\Omega^4}{8} e^{-|\alpha_{fx}|^2-|\alpha_{fy}|^2-|\alpha_{fz}|^2-|\alpha_{iz}|^2} \left| \sum_{m_z} \frac{1}{(E_m - E_i)/\hbar - m_z\omega_{trp,z}} \frac{\alpha_{fz}^{m_z}\alpha_{iz}^{m_z}}{m_z!} \right|^2 \\ &= \frac{\pi\hbar^2\Omega^4}{8} e^{-(\mathbf{k}_f \cdot \mathbf{a}_{trp})^2/2 - (\mathbf{k}_i \cdot \mathbf{a}_{trp})^2/2} \left| \sum_{m_z} \frac{1}{(E_m - E_i)/\hbar - m_z\omega_{trp,z}} \frac{(-\frac{1}{2}k_{fz}k_{iz}a_{trp,z}^2)^{m_z}}{m_z!} \right|^2, \end{aligned}$$

where  $\mathbf{a}_{trp} \equiv (a_{trp,x} \ a_{trp,y} \ a_{trp,z})$ . Looking into scattering into transverse direction,  $\mathbf{k}_{f,z} = 0$ , we get,

$$\left( \frac{d\sigma}{d\Omega} \right)_{\perp} = \frac{\pi\hbar^4\Omega^4}{8|E_m - E_i|^2} e^{-\mathbf{k}_{fx}^2 a_{trp,x}^2/2 - \mathbf{k}_{fy}^2 a_{trp,y}^2/2 - \mathbf{k}_{iz}^2 a_{trp,z}^2/2}.$$

Looking into backscattering,  $\mathbf{k}_{f,z} = -\mathbf{k}_{i,z}$ ,

$$\left( \frac{d\sigma}{d\Omega} \right)_{\parallel} = \frac{\pi\hbar^2\Omega^4}{8} e^{-\mathbf{k}_i a_{trp,z}^2} \left| \sum_{m_z} \frac{1}{(E_m - E_i)/\hbar - m_z\omega_{trp,z}} \frac{(-\frac{1}{2}k_{iz}^2 a_{trp,z}^2)^{m_z}}{m_z!} \right|^2.$$

we expect a spectrum with vibrational resonances.

## 18.3.4 Exercises

### 18.3.4.1 Ex: Transition elements in anisotropic harmonic traps

- Calculate and illustrate  $\langle \mathbf{0}|e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}|0\rangle$  for an anisotropic trap with cylindrical symmetry.
- Calculate  $\langle \mathbf{n}|e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}|0\rangle$  and  $\sum_{n_x, n_y, n_z} \langle \mathbf{n}|e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}|0\rangle$ .

### 18.3.4.2 Ex: Periodicity of a lattice

Calculate  $e^{i\alpha\hat{p}}e^{2i\hat{k}\hat{z}}e^{-i\alpha\hat{p}}$ .

### 18.3.4.3 Ex: Energy commutators

Calculate the commutator between the kinetic and the potential energy for (a) a harmonic oscillator and (b) a standing wave dipolar potential.

## 18.4 Further reading

H.J. Metcalf, P. van der Straten, Graduate Texts in Contemporary Physics, Springer (1999), *Laser Cooling and Trapping* [[http](#)]

Ch.J. Foot, (Oxford Master Series in Atomic, Optical and Laser Physics, 2005), *Atomic physics* [[http](#)]

G. Vandegrift, *The Moessbauer effect explained* [[DOI](#)]

## Part IV

# Collective Scattering of Light



# Chapter 19

## Cooperativity in light scattering

In Chp. 14.6.1 we discussed the interaction of light with individual atoms. In the practice of spectroscopy, however, we often work with ensembles of scatterers. Depending on their *spatial distribution* (e.g. disordered, quasi-continuous, periodic), their *motion* (hot gas or cold cloud), the possible existence of *correlations* between them, the presence of *boundary conditions* (e.g., free space, cavities, or photon bands), and finally, in case of degenerate quantum gases, of a possible *bosonic stimulation* of the scattering process, we expect new collective effects. In this chapter we will discuss several examples, in particular, localization effects induced by disorder, super- and subradiance, Bragg scattering, and the formation of forbidden photonic bands in periodic lattices. Phenomena leading to self-organization, such as the collective atomic recoil laser, will be discussed in Chp. 22.6.1.

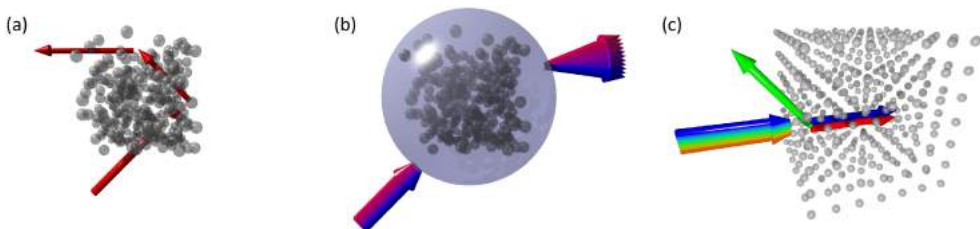


Figure 19.1: (a) Artist's view of multiple scattering of a photon through a dilute cloud. (b) Atomic cloud as a bulk object characterized by a refraction index  $n(\mathbf{r})$ . (c) Illustration of a photonic band in an optical lattice.

This chapter starts with introducing as the main theoretical tools the *structure factor* and the *coupled dipoles model*. In Sec. 19.1 we will derive the formalism and learn, how to employ it to calculate, e.g. the spatial distribution of light scattered by an atomic cloud and the radiation pressure force on the atoms focusing on situations, where interatomic interactions induced by the incident light can be neglected. In Sec. 19.2 we will, disregarding the atomic's cloud graininess and disorder, introduce the *smooth density approximation* and compare it to macroscopic Mie scattering. In Sec. 19.3 we will focus on cooperative effects inducing collective lineshifts and broadenings, such as the Lorentz-Lorenz and the Lamb shift. We will also discuss disorder-induced localization effects, super- and subradiance. In Sec. 19.2 we investi-

gate Bragg scattering, i.e. scattering from periodically ordered atoms, and finally in Sec. ?? we study scattering from correlated atoms.

## 19.1 Theoretical tools and models

As mentioned above, the process of light scattering by an atomic cloud depends on several factors, many of which can be summarized by a quantity called the *structure factor*. This structure factor, obtained in perturbation theory, describes the probability for the light to be scattered into a particular direction as a function of the properties of the atomic cloud (spatial distribution, motion, etc.). The quantity is well suited for dealing with stationary situations.

On the other hand we have at our disposal a microscopic theory called the *coupled dipole model*. In this model we treat every individual atom as a dipole, which interacts with all other atoms by rescattering the incident light. The resolution of the Schrödinger equation allows, several approximations having been made, to calculate the dynamics of the system.

### 19.1.1 The structure factor and definition of cooperativity

One way of characterizing the scattering process is by structure factor. The *static structure factor* is the normalized response of a system to a perturbation with the wave vector  $\mathbf{q}$ . It can be understood as the final density of states for the atom after the scattering process. In contrast, the *dynamic structure factor* also considers the final density of states for the emitted or scattered photon. That is, on one hand, the frequency and momentum of the photon must satisfy the Bragg condition. On the other hand, the density of available states can also be structured, for example, when the scattering process takes place inside a cavity.

In lowest-order perturbation theory (Fermi's Golden Rule) we get the general expressions [391],

$$\boxed{\frac{d\sigma}{d\Omega_s d\omega} = \left( \frac{d\sigma}{d\Omega_s} \right)_1 S(\mathbf{q}, \omega)}, \quad (19.1)$$

that is, the effective scattering cross section is reduced to the effective Rayleigh scattering cross section by an isolated atom times a geometric term called *dynamic structure factor*,

$$\boxed{S(\mathbf{q}, \omega) \equiv \frac{1}{2\pi} \int dt e^{i\omega t} \langle \hat{\rho}(\mathbf{q}, t) \hat{\rho}^\dagger(\mathbf{q}, 0) \rangle}, \quad (19.2)$$

where,

$$\hat{\rho}(\mathbf{q}, t) = \int_V \hat{n}(\mathbf{r}, t) e^{i\mathbf{q}\cdot\mathbf{r}} d^3r \quad (19.3)$$

is Fourier transform of the atomic density. Thus,  $S(\mathbf{q}, \omega)$  is the Fourier transform of the density-density correlation function. On the other hand,  $\int e^{i\omega t} d\omega = 2\pi\delta(t)$ , and we calculate the *static structure factor*,

$$\boxed{S(\mathbf{q}) \equiv \int S(\mathbf{q}, \omega) d\omega = \langle \hat{\rho}(\mathbf{q}, 0) \hat{\rho}^\dagger(\mathbf{q}, 0) \rangle}. \quad (19.4)$$

In the equations (19.2) and (19.3) we have written the quantities  $\hat{\rho}(\mathbf{q}, t)$  and  $\hat{n}(\mathbf{r}, t)$  as operators, in order to allow for the possibility, that the atomic ensemble is a quantum gas, i.e. a Bose-Einstein condensate characterized by a single wavefunction  $\hat{\psi}(\mathbf{r}, t)$  normalized to the density distribution,  $\hat{\rho}(\mathbf{r}, t) = \hat{\psi}^\dagger(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t)$ . We shall return to this subject in Sec. 28.1.1. In the following, we will restrict ourselves to atoms localized in space with well-defined velocities and calculate the structure factor (i) for disordered clouds of atoms excited by the passage of a photon in Sec. 19.1.6 and (ii) for Bragg scattering by optical lattices in Sec. 19.4. In these cases, we find in the literature often another definition of the structure factor as the expectation value of the Fourier transform of the atomic density,

$$F(\mathbf{q}) = \langle \hat{\rho}(\mathbf{q}) \rangle, \quad (19.5)$$

Thus, it describes the amplitude of the electric field of the scattered radiation. We study the structure factor for various atomic density distributions in Excs. 19.1.8.1 to 19.1.8.3.

**Example 80 (Structure factor of a discrete cloud):** In case of discrete clouds,  $n(\mathbf{r}, t) = \sum_j \delta^{(3)}(\mathbf{r} - \mathbf{r}_j)$ , we can disregard the quantum nature of the operators. The relationship (19.3) immediately gives,

$$\rho(\mathbf{q}, t) = \sum_j e^{i\mathbf{q} \cdot \mathbf{r}_j(t)} \quad (19.6)$$

and the relationship (19.2),

$$S(\mathbf{q}, \omega) = \frac{1}{2\pi} \int dt e^{i\omega t} \rho(\mathbf{q}, t) \rho^*(\mathbf{q}, 0) = \frac{1}{2\pi} \int dt e^{i\omega t} \sum_{j,k} e^{i\mathbf{q} \cdot [\mathbf{r}_j(t) - \mathbf{r}_k(0)]}. \quad (19.7)$$

Assuming atoms fixed in space,  $\mathbf{r}_j(t) = \mathbf{r}_j$ ,

$$S(\mathbf{q}, \omega) = \sum_{j,k} e^{i\mathbf{q} \cdot (\mathbf{r}_j - \mathbf{r}_k)} \delta(\omega). \quad (19.8)$$

That is, without recoil the light must be scattered elastically.

*Cooperativity* is defined as any **deviation of the structure factor from isotropy**. For example, Bragg scattering and optical cavities are highly cooperative, because they favor scattering in particular directions <sup>1</sup>.

### 19.1.2 The scalar coupled dipoles model

In the following, we develop the coupled dipoles model, within which we define the structure factor for light scattering by a cloud of scatterers making the following assumptions:

- The light is (mostly) treated as a scalar field. That is, we disregard effects due to the polarization of light and assume two-level atoms. Generalizations are shown in Sec. 19.5.4 [638, 465].

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<sup>1</sup>Note that cooperativity does not request the atoms to interact and exists in the single scattering regime. In the multiple scattering regime other forms of collective phenomena, such as collective Lamb shifts emerge, as we will see later on.



- Atoms are supposed to be fixed in space. That is, we disregard the Doppler shift of moving atoms and the photonic recoil. Therefore, it will suffice to consider the static structure factor.
- Atoms are initially uncorrelated and not degenerate. That means that we neglect effects such as bosonic stimulation or Fermi blocking <sup>2</sup>.

Be  $\omega_0$  the frequency of the incident light,  $\omega_a$  the frequency of the atomic resonance, and  $\omega$  the frequency of the scattered light. The Hamiltonian is nothing more than the generalization of (15.105) to several assumed atoms located at the positions  $r_j$ ,

$$\hat{H} = \sum_{j=1}^N \hbar g_{\mathbf{k}_0} (\hat{\sigma}_j e^{-i\omega_a t} + \hat{\sigma}_j^\dagger e^{i\omega_a t}) (\hat{a}_{\mathbf{k}_0}^\dagger e^{i\omega_0 t - i\mathbf{k}_0 \cdot \mathbf{r}_j} + \hat{a}_{\mathbf{k}_0} e^{-i\omega_0 t + i\mathbf{k}_0 \cdot \mathbf{r}_j}) + \sum_{\mathbf{k}} \sum_{j=1}^N \hbar g_{\mathbf{k}} (\hat{\sigma}_j e^{-i\omega_a t} + \hat{\sigma}_j^\dagger e^{i\omega_a t}) (\hat{a}_{\mathbf{k}}^\dagger e^{i\omega_k t - i\mathbf{k} \cdot \mathbf{r}_j} + \hat{a}_{\mathbf{k}} e^{-i\omega_k t + i\mathbf{k} \cdot \mathbf{r}_j}) \quad (19.9)$$

Here,  $\Omega_0 = 2g_{k_0} \sqrt{n_0}$  is the Rabi frequency of the interaction between an atom and the incident light (which is treated as a classical field with  $n_0$  photons),  $\hat{\sigma}_j$  is the deexcitation operator for the  $j$ -th atom,  $\hat{a}_{\mathbf{k}}$  is the photon annihilation operator, and  $g_k = d\sqrt{\omega/(\hbar\epsilon_0 V_{ph})}$  describes the coupling between the atom and the vacuum modes the volume of which is  $V_{ph}$ . The  $j$ -th atom has its lower and upper states denoted by  $|g_j\rangle$  and  $|e_j\rangle$ , respectively. That is, we treat the atoms as simple two-level systems. We also assume that all atoms are excited by the same unperturbed incident laser beam, thus neglecting their dephasing along the laser path or induced by near-field effects (which could arise for large spatial densities).

Within the *rotating wave approximation* RWA the Hamiltonian simplifies to,

$$\hat{H} = \hbar \sum_{j=1}^N [g_{k_0} \hat{\sigma}_j \hat{a}_{\mathbf{k}_0}^\dagger e^{i(\omega_0 - \omega_a)t - i\mathbf{k}_0 \cdot \mathbf{r}_j} + h.c.] + \hbar \sum_{j=1}^N \sum_{\mathbf{k}} [g_{\mathbf{k}} \hat{\sigma}_j \hat{a}_{\mathbf{k}}^\dagger e^{i(\omega_k - \omega_a)t - i\mathbf{k} \cdot \mathbf{r}_j} + h.c.] \quad (19.10)$$

The RWA only considers energy-conserving terms in single-photon processes. But this is an artifact from the field quantization. Energy conservation can be warranted by considering multi-photon virtual processes, which as a whole, conserve energy. These terms appear in the full Hamiltonian, but are neglected in the RWA. While the RWA often is a good assumption in single atom quantum optics, this is frequently not the case for collective scattering. Here, we adopt the RWA to simplify the subsequent solution of the Schrödinger equation, but we will need to generalize the results obtained a posteriori, as shown in the discussion of Sec. 19.1.4.

We call  $|0\rangle_a = |g_1, \dots, g_N\rangle$  the atomic ground state,  $|j\rangle_a = |g_1, \dots, e_j, \dots, g_N\rangle$  the state where only the atom  $j$  is excited, and we assume that the system is in a the

<sup>2</sup>Spontaneous emission by an atom in a Fermi gas of temperature  $T = 0$  can not occur if the photon wave vector is inside the Fermi lake,  $q < k_F$ .

superposition of states described by <sup>3</sup>,

$$|\Psi(t)\rangle = \alpha(t)|0\rangle_a |n_0\rangle_{\mathbf{k}_0} |0\rangle_{\mathbf{k}} + \sum_{j=1}^N \beta_j(t) |j\rangle_a |n_0 - 1\rangle_{\mathbf{k}_0} |0\rangle_{\mathbf{k}} \quad (19.11)$$

$$+ \sum_{\mathbf{k}} \gamma_{\mathbf{k}}(t) |0\rangle_a |n_0 - 1\rangle_{\mathbf{k}_0} |1\rangle_{\mathbf{k}} .$$

With this ansatz we imply that at every instant of time, there can be at most only one excitation in the atomic cloud. The temporal evolution of the amplitudes is obtained by inserting the Hamiltonian and the ansatz into the Schrödinger equation,  $i\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$ . Once the evolution of the amplitudes is calculated, we can determine the observables of the system, such as the radiative pressure force or the amplitudes of the scattered radiation fields or the fields inside the cloud.

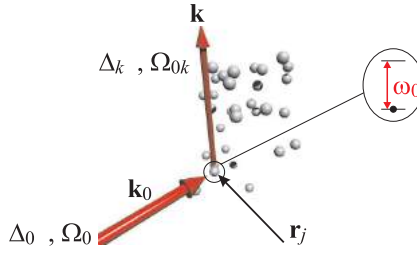


Figure 19.2: Scheme of the interaction of a light beam with a sample of atoms.

**Example 81 (Interaction Hamiltonian in the rotating frame):** The Hamiltonian in the rotating wave approximation is,

$$\hat{H} = \hbar g \left( \hat{\sigma} e^{-i\omega_a t} + \hat{\sigma}^\dagger e^{i\omega_a t} \right) \left( \hat{a}^\dagger e^{i\omega_0 t} + \hat{a} e^{-i\omega_0 t} \right) \simeq \hbar g \left( \hat{\sigma} \hat{a}^\dagger e^{i\Delta_0 t} + \hat{\sigma}^\dagger \hat{a} e^{-i\Delta_0 t} \right) .$$

For the Pauli matrices we have the following rules,

$$[\hat{\sigma}_z, \hat{\sigma}] = -\hat{\sigma} \quad \text{and} \quad [\hat{\sigma}_z, \hat{\sigma}^\dagger] = \hat{\sigma}^\dagger ,$$

such that,

$$\begin{aligned} [\hat{\sigma}_z, \hat{H}] &= \hbar g \left( -e^{i\Delta_0 t} \hat{a}^\dagger \hat{\sigma} + e^{-i\Delta_0 t} \hat{a} \hat{\sigma}^\dagger \right) \\ [\hat{\sigma}_z, [\hat{\sigma}_z, \hat{H}]] &= \hbar g \left( e^{i\Delta_0 t} \hat{a}^\dagger \hat{\sigma} + e^{-i\Delta_0 t} \hat{a} \hat{\sigma}^\dagger \right) = \hat{H} \\ [\hat{\sigma}_z, [\dots [\hat{\sigma}_z, \hat{H}]] \dots] &= \hbar g \left[ (-1)^n e^{i\Delta_0 t} \hat{a}^\dagger \hat{\sigma} + e^{-i\Delta_0 t} \hat{a} \hat{\sigma}^\dagger \right] . \end{aligned}$$

<sup>3</sup>This ansatz is well adapted to situations where the RWA holds. Otherwise, additional counter-rotating terms must be included [243].

Using the Baker-Hausdorff formula,

$$\begin{aligned}
 e^{i\omega_0 t \hat{\sigma}_z} \hat{H} e^{-i\omega_0 t \hat{\sigma}_z} &= \hat{H} + [\omega_0 t \hat{\sigma}_z, \hat{H}] + \frac{1}{2!} [\omega_0 t \hat{\sigma}_z, [\omega_0 t \hat{\sigma}_z, \hat{H}]] + \dots \\
 &= \hbar g \sum_{n=0}^{\infty} \frac{(i\omega_0 t)^n}{n!} \left[ (-1)^n e^{i\Delta_0 t} \hat{a}^\dagger \hat{\sigma} + e^{-i\Delta_0 t} \hat{a} \hat{\sigma}^\dagger \right] \\
 &= \hbar g e^{i\Delta_0 t} \hat{a}^\dagger \hat{\sigma} \sum_{n=0}^{\infty} \frac{(-i\omega_0 t)^n}{n!} + \hbar g e^{-i\Delta_0 t} \hat{a} \hat{\sigma}^\dagger \sum_{n=0}^{\infty} \frac{(i\omega_0 t)^n}{n!} \\
 &= \hbar g \left( e^{-i\omega_0 t} \hat{a}^\dagger \hat{\sigma} + e^{i\omega_0 t} \hat{a} \hat{\sigma}^\dagger \right) .
 \end{aligned}$$

### 19.1.2.1 Temporal evolution of the amplitudes

The time evolution of the amplitudes is obtained by inserting the Hamiltonian  $\hat{H}$  and the ansatz  $|\Psi(t)\rangle$  into the Schrödinger equation,

$$\frac{\partial}{\partial t} |\Psi(t)\rangle = -\frac{i}{\hbar} \hat{H} |\Psi(t)\rangle . \quad (19.12)$$

one obtains with  $\Omega_0 = 2g_{k_0} \sqrt{n_0}$ ,

$$\begin{aligned}
 \dot{\alpha}(t) &= -i \frac{\Omega_0}{2} e^{i\Delta_0 t} \sum_{j=1}^N \beta_j(t) e^{-i\mathbf{k}_0 \cdot \mathbf{r}_j} \\
 \dot{\beta}_j(t) &= -i \frac{\Omega_0}{2} \alpha(t) e^{-i\Delta_0 t + i\mathbf{k}_0 \cdot \mathbf{r}_j} - \sum_{\mathbf{k}} i g_{\mathbf{k}} \gamma_{\mathbf{k}}(t) e^{-i\Delta_{\mathbf{k}} t + i\mathbf{k} \cdot \mathbf{r}_j} \\
 \dot{\gamma}_{\mathbf{k}}(t) &= -i g_{\mathbf{k}} e^{i\Delta_{\mathbf{k}} t} \sum_{j=1}^N \beta_j(t) e^{-i\mathbf{k} \cdot \mathbf{r}_j} .
 \end{aligned} \quad (19.13)$$

We set the initial conditions,

$$\alpha(0) = 1 \quad , \quad \beta_j(0) = 0 \quad , \quad \gamma_{\mathbf{k}}(0) = 0 . \quad (19.14)$$

For low excitation rate, we can set  $\alpha(t) \simeq 1$ . Integrating the third equation,

$$\gamma_{\mathbf{k}}(t) = -i g_{\mathbf{k}} \sum_{j=1}^N e^{-i\mathbf{k} \cdot \mathbf{r}_j} \int_0^t e^{i\Delta_{\mathbf{k}} t'} \beta_j(t') dt' , \quad (19.15)$$

and substituting it into the second equation,

$$\dot{\beta}_j(t) = -i \frac{\Omega_0}{2} \alpha(t) e^{-i\Delta_0 t + i\mathbf{k}_0 \cdot \mathbf{r}_j} - \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \sum_{m=1}^N e^{i\mathbf{k} \cdot (\mathbf{r}_j - \mathbf{r}_m)} \int_0^t e^{i\Delta_{\mathbf{k}} (t' - t)} \beta_m(t') dt' . \quad (19.16)$$

### 19.1.3 The Markov approximation

For small systems,  $R < \lambda$ , we can make use of the Markov approximation, which holds when the collective decay time  $t_{decay} < R/c$ . Larger systems persist memory effects, which may lead to (Rabi) *collective Rabi oscillations*. In the Markov approximation given by  $\beta_j(t') \simeq \beta_j(t)$  the integro-differential equation (which is equivalent to a differential equation of arbitrarily high order) reduces to a simple first order differential equation. Defining <sup>4</sup>,

$$\beta_j \equiv \tilde{\beta}_j e^{-i\Delta_0 t + i\mathbf{k}_0 \cdot \mathbf{r}_j} , \quad (19.17)$$

we obtain,

$$\begin{aligned} \frac{d}{dt} \alpha(t) &= -i \frac{\Omega_0}{2} \sum_{j=1}^N \tilde{\beta}_j(t) \\ \frac{d}{dt} \tilde{\beta}_j(t) &= i\Delta_0 \tilde{\beta}_j(t) - \frac{\Omega_0^2}{4} \sum_{m=1}^N \int_0^t \tilde{\beta}_m(t') dt' \\ &\quad - \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \sum_{m=1}^N e^{i(\mathbf{k}-\mathbf{k}_0) \cdot (\mathbf{r}_j - \mathbf{r}_m)} \int_0^t e^{-i(\omega_{\mathbf{k}} - \omega_0)t''} \tilde{\beta}_m(t-t'') dt'' , \end{aligned} \quad (19.18)$$

where we substituted  $t'' \equiv t - t'$  in the last integral. Now, using the Markov approximation  $\tilde{\beta}_m(t-t'') \simeq \tilde{\beta}_m(t)$ , with  $\lim_{t \rightarrow \infty} \int_0^t e^{-i(\omega_{\mathbf{k}} - \omega_0)t'} dt' = \pi \delta(\omega_{\mathbf{k}} - \omega_0)$ , and with the rate of spontaneous emission,

$$\Gamma \equiv \frac{V_{ph}}{\pi c} k_0^2 g_{k_0}^2 , \quad (19.19)$$

the third term becomes for the case  $m = j$ ,

$$\begin{aligned} \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \int_0^t e^{-i(\omega_{\mathbf{k}} - \omega_0)t''} \tilde{\beta}_j(t-t'') dt'' &\simeq \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \tilde{\beta}_j(t) \pi \delta(\omega_{\mathbf{k}} - \omega_0) \\ &= \frac{V_{ph}}{(2\pi)^3} \tilde{\beta}_j(t) \int g_{\mathbf{k}}^2 \pi \delta(\omega_{\mathbf{k}} - \omega_0) d^3 k = \frac{V_{ph}}{(2\pi)^3} \tilde{\beta}_j(t) 4\pi g_{k_0}^2 \pi k_0^2 \frac{1}{c} = \frac{\Gamma}{2} \tilde{\beta}_j(t) . \end{aligned} \quad (19.20)$$

The third term becomes for the case  $m \neq j$ , evaluating the sum over the wavevectors by  $\sum_{\mathbf{k}} \rightarrow \frac{V_{ph}}{(2\pi)^3} \int d^3 k$ ,

$$\begin{aligned} \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \sum_{m \neq j}^N e^{i(\mathbf{k}-\mathbf{k}_0) \cdot (\mathbf{r}_j - \mathbf{r}_m)} \int_0^t e^{-i(\omega_{\mathbf{k}} - \omega_0)t''} \tilde{\beta}_m(t-t'') dt'' \\ \simeq \sum_{\mathbf{k}} g_{\mathbf{k}}^2 \sum_{m \neq j}^N e^{i(\mathbf{k}-\mathbf{k}_0) \cdot (\mathbf{r}_j - \mathbf{r}_m)} \tilde{\beta}_m(t) \pi \delta(\omega_{\mathbf{k}} - \omega_0) \\ = \frac{V_{ph}}{(2\pi)^3} \sum_{m \neq j}^N \tilde{\beta}_m(t) \int g_{\mathbf{k}}^2 e^{i(\mathbf{k}-\mathbf{k}_0) \cdot (\mathbf{r}_j - \mathbf{r}_m)} \pi \delta(\omega_{\mathbf{k}} - \omega_0) d^3 k = \frac{\Gamma}{2} \sum_{m \neq j}^N \gamma_{jm} \tilde{\beta}_m(t) , \end{aligned} \quad (19.21)$$

<sup>4</sup>Later on we will be particularly interested in so-called *timed Dicke states* characterized by  $\tilde{\beta}_j = \tilde{\beta}$  independent on  $j$ .

with

$$\gamma_{jm} \equiv \frac{2}{\Gamma} \frac{V_{ph}}{(2\pi)^3} \int_0^\infty \int_0^\pi \int_0^{2\pi} g_k^2 e^{i(\mathbf{k}-\mathbf{k}_0)\cdot(\mathbf{r}_j-\mathbf{r}_m)} \frac{\pi}{c} \delta(k-k_0) k^2 \sin\theta dk d\theta d\phi. \quad (19.22)$$

Finally,

$$\frac{d}{dt} \tilde{\beta}_j(t) = i\Delta_0 \tilde{\beta}_j(t) - \frac{\Omega_0^2}{4} \sum_{m=1}^N \int_0^t \tilde{\beta}_m(t') dt' - \frac{\Gamma}{2} \sum_{m=1}^N \gamma_{jm} \tilde{\beta}_m(t), \quad (19.23)$$

or

$$\frac{d}{dt} \alpha(t) = -i \frac{\Omega_0}{2} \sum_{j=1}^N \tilde{\beta}_j(t) \quad (19.24)$$

$$\frac{d}{dt} \tilde{\beta}_j(t) = i\Delta_0 \tilde{\beta}_j(t) - i \frac{\Omega_0}{2} \alpha(t) - \frac{\Gamma}{2} \sum_{m=1}^N \gamma_{jm} \tilde{\beta}_m(t).$$

This means that the problem is reduced to finding the  $\gamma_{jm}$ . Continuing the evaluation of Eq. (19.22),

$$\begin{aligned} \gamma_{jm} &= \frac{1}{\Gamma} g_k^2 \frac{V_{ph}}{4\pi^2 c} e^{-i\mathbf{k}_0\cdot(\mathbf{r}_j-\mathbf{r}_m)} \int_0^\infty \int_0^{2\pi} \int_{-1}^1 e^{ik|\mathbf{r}_j-\mathbf{r}_m|\cos\theta} d\cos\theta d\phi \delta(k-k_0) k^2 dk \\ &= \frac{1}{\Gamma} g_k^2 \frac{V_{ph}}{\pi c} e^{-i\mathbf{k}_0\cdot(\mathbf{r}_j-\mathbf{r}_m)} \int_0^\infty \frac{\sin k|\mathbf{r}_j-\mathbf{r}_m|}{k|\mathbf{r}_j-\mathbf{r}_m|} \delta(k-k_0) k^2 dk \\ &= e^{-i\mathbf{k}_0\cdot(\mathbf{r}_j-\mathbf{r}_m)} \frac{\sin k_0|\mathbf{r}_j-\mathbf{r}_m|}{k_0|\mathbf{r}_j-\mathbf{r}_m|}. \end{aligned}$$

Isolating the self-decaying term and assuming low saturation,  $\alpha(t) = 1$ , we get,

$$\boxed{\dot{\tilde{\beta}}_j = \left( i\Delta_0 - \frac{\Gamma}{2} \right) \tilde{\beta}_j - \frac{i\Omega_0}{2} - \frac{\Gamma}{2} \sum_{m \neq j}^N \gamma_{jm} \tilde{\beta}_m}. \quad (19.25)$$

In Exc. 19.1.8.4 we will analyze the validity of the Markov approximation for typical cold atoms experiments.

### 19.1.4 General solution with exponential kernel, validity of the RWA

The RWA is valid for  $\max(\Omega, \Gamma_n) \ll \omega$ ,

$$\int_0^t dt \cdot e^{-i(\omega_k - \omega_0)t} \simeq \mathcal{P} \left( \frac{1}{\omega_k + \omega_0} \right) - i\mathcal{P} \left( \frac{1}{\omega_k - \omega_0} \right) + \pi\delta(\omega_k - \omega_0). \quad (19.26)$$

The whole expression leads to the exponential kernel, the first two terms are the cosine part, the third term is the sine part. The rotating wave approximation consists in neglecting the first term, i.e. it only concerns the cosine part of the kernel.

Within the RWA we got <sup>5,6</sup>,

$$\gamma_{jm} = e^{-i\mathbf{k}_0(\mathbf{r}_j - \mathbf{r}_m)} \frac{i \sin(k_0 |\mathbf{r}_j - \mathbf{r}_m|)}{i k_0 |\mathbf{r}_j - \mathbf{r}_m|} . \quad (19.27)$$

Without the RWA we would have found [627, 622, 623, 674],

$$\gamma_{jm} = e^{-i\mathbf{k}_0(\mathbf{r}_j - \mathbf{r}_m)} \frac{e^{i k_0 |\mathbf{r}_j - \mathbf{r}_m|}}{i k_0 |\mathbf{r}_j - \mathbf{r}_m|} . \quad (19.28)$$

There has been a controversy between Friedberg and Scully about the role of virtual photons (or *collective Lamb-shift*) [249, 673, 250, 624]. These terms result from counterrotating terms in the rotating wave approximation. Scully assumes timed Dicke states in *infinitely large* clouds and finds the contributions weak. Friedberg does a mode expansion of the cloud and finds that different modes decay at different velocities. This yields time-dependent radiation patterns, which can be temporarily larger in backward direction.

Normally, the RWA is a good approximation, when  $\Omega \ll \omega$ . Deviations from this approximations lead e.g. to the Bloch-Siegert shift and important corrections for very far-detuned (quasi-electrostatic) optical trapping. The above requirement is not well satisfied for our experiment, since  $\Omega_N = \sqrt{N}\Omega \simeq 1..10$  THz.

Be  $|b_1 b_2 \dots a_j \dots b_N\rangle$  the state with all atoms in the ground state except atom  $j$  being in the excited state. Hence, the cloud's state is simply expressed by the wavefunction,

$$\Psi_{atom}(t) = \sum_{j=1}^N \beta_j(t) |b_1 b_2 \dots a_j \dots b_N\rangle . \quad (19.29)$$

For large  $\sigma$  the radiation pressure is independent on the choice of the kernel. In fact we may even set the kernel to 0. For small  $\sigma$  there appears a considerable deviation. Interestingly, the imaginary part of the kernel gets important for higher densities, even when the optical density is maintained, e.g. by compressing the cloud in  $z$ -direction. This means that the collective Lamb shift becomes more apparent in small compressed clouds. But we postpone a more thorough discussion to Sec. 19.3.

The analytic expansion into eigenmodes assumes the RWA. Hence, the numerics deviate from the analytics for small  $\sigma$  and large  $N$ . Is it possible to generalize the expansion to the exponential kernel (see [674])? The authors also suggest that the scattered radiation be frequency-shifted due to the imaginary part of the kernel. This might be an interesting observable for experiments.

#### 19.1.4.1 Low collective saturation

Note that for low *saturation*,  $\alpha(t) = 1$ , the first term simply becomes  $-\frac{i}{2}\Omega_0$ . Even though the single atom excitation rate may be small in case of large detuning, the *collective* Rabi frequency  $\sqrt{N}\Omega$  can be large. The presence of many excitations in

<sup>5</sup>Note that dipole-dipole interactions are mediated by the exchange of virtual photons. Hence, they are included in the Hamiltonian when the RWA is NOT applied.

<sup>6</sup>Note that Maxwell's equations contain non-RWA terms.

the cloud means, that higher Dicke states are populated. Then we may expect a complicated many-body dynamics, if decay into other states than the timed Dicke state is possible.

Even though the single atom excitation rate may be small in case of large detuning, the *collective* Rabi frequency  $\sqrt{N}\Omega$  can be large. The presence of many excitations in the cloud means, that higher Dicke states are populated. Then we may expect a complicated many-body dynamics, if decay into other states than the timed Dicke state is possible.

The model we use (ground state + first excited state in the times Dicke basis) does not allow more than 1 photon for  $N$  atoms. For such a model, neglecting saturation means 'much' less than 1 atom in the excited state, i.e. the probability of having the any atom in the excited state is less than 1. But having  $N$  atoms, this means that each atoms should have a excited state population of much less than  $1/N$ . Including the saturation in the naive way, means that when this term  $N\Omega_0^2$  is not negligible, than we will have less atoms in the first excited state of the timed Dicke basis, than if when we would neglect saturation. This is precisely why we call this saturation, we cannot take more atoms away from the ground state, because the system cannot absorb more than one photon. But when this term is not longer negligible, then in a cloud of  $N$  atoms, this does not prevent us from taking atoms away from the ground state (we have  $N$  atoms which each can take one photon). Either the term is negligible (and we could drop it) or we will try to keep its contribution (even at first order in  $N\Omega_0^2$ ), but then we cannot neglect the possibility of having 2 atoms excited.

#### 19.1.4.2 Steady-state solution

In steady-state the equations of the coupled dipoles model can be solved numerically for an arbitrary (ordered or disordered) cloud of immobile atoms located at positions  $\mathbf{r}_j$  illuminated by an electric field.

Assuming scalar light and the validity of the Markov approximation, and furthermore defining  $\bar{\beta}_j \equiv \tilde{\beta}_j e^{i\mathbf{k}_0 \cdot \mathbf{r}_j}$  and  $\bar{\Omega}_0(\mathbf{r}_j) \equiv \Omega_0(\mathbf{r}_j) e^{i\mathbf{k}_0 \cdot \mathbf{r}_j}$ , and using the exponential kernel,

$$\bar{\gamma}_{jm} = \frac{e^{i\mathbf{k}_0 \cdot |\mathbf{r}_j - \mathbf{r}_m|}}{ik_0 |\mathbf{r}_j - \mathbf{r}_m|}, \quad (19.30)$$

the Eq. (19.25) for the atomic states reads,

$$\frac{d}{dt} \bar{\beta}_j = \left( i\Delta_0 - \frac{\Gamma}{2} \right) \bar{\beta}_j - \frac{i\bar{\Omega}_0(\mathbf{r}_j)}{2} - \frac{\Gamma}{2} \sum_{m \neq j} \bar{\gamma}_{jm} \bar{\beta}_m. \quad (19.31)$$

Defining the matrix,

$$M_{jm} \equiv \left( i\Delta_0 - \frac{\Gamma}{2} \right) \delta_{jm} - \frac{\Gamma}{2} (1 - \delta_{jm}) \bar{\gamma}_{jm} = \begin{pmatrix} i\Delta_0 - \frac{\Gamma}{2} & i\gamma_{12} \frac{\Gamma}{2} & \cdots \\ i\gamma_{21} \frac{\Gamma}{2} & i\Delta_0 - \frac{\Gamma}{2} & \\ \vdots & & \ddots \end{pmatrix}, \quad (19.32)$$

we can rewrite Eq. (19.31) as,

$$\boxed{\frac{d}{dt} \bar{\beta}_j = \sum_m M_{jm} \bar{\beta}_m - \frac{i}{2} \bar{\Omega}_0(\mathbf{r}_j)}. \quad (19.33)$$

The steady-state solution of is simply obtained by  $\dot{\tilde{\beta}}_j = 0$  [153, 119],

$$M_{jm}\tilde{\beta}_m(\infty) = \frac{i}{2}\tilde{\Omega}_0(\mathbf{r}_j) . \quad (19.34)$$

This equation can now be solved by the dipole moment amplitudes,

$$\tilde{\beta}_m(\infty) = (M_{jm})^{-1} \frac{i}{2}\tilde{\Omega}_0(\mathbf{r}_j) , \quad (19.35)$$

where we use the exponential kernel,

$$\gamma_{jm} = \frac{e^{ik_0(|\mathbf{r}_j - \mathbf{r}_m| + \delta_{jm})}}{ik_0(|\mathbf{r}_j - \mathbf{r}_m| + \delta_{jm})} , \quad (19.36)$$

where the trick with the  $\delta_{jm}$ -symbol helps to remove divergences for equal atom positions.

In this form the solution is immediately suitable for numerical implementation of the coupled dipoles model, although in practice the number of atoms is limited to  $N < 10000$  for ordinary PCs.

#### 19.1.4.3 Limit of dilute clouds

Dilute clouds are characterized by a large interatomic distance  $k_0|\mathbf{r}_j - \mathbf{r}_m| \gg 1$ . In this case, the non-diagonal elements of the kernel (19.32) quickly vanish, and the equations of motion (19.33) decouple to,

$$\frac{d}{dt}\tilde{\beta}_j = \left( i\Delta_0 - \frac{\Gamma}{2} \right) \tilde{\beta}_j - \frac{i}{2}\tilde{\Omega}_0(\mathbf{r}_j) . \quad (19.37)$$

#### 19.1.4.4 Characterization of the atomic cloud in steady-state

Plot the spacial dependence of the phases of the atomic dipoles,  $\phi(\mathbf{r}_j) = \text{Im}(\ln \tilde{\beta}_j)$ .

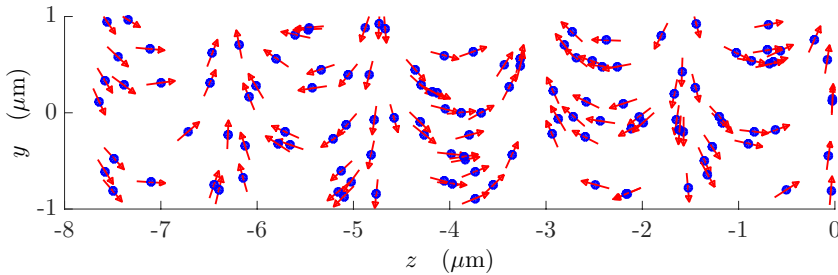


Figure 19.3: Phase delay in the excitation of the atomic dipoles (a) without rescattering ( $\gamma_{jm} = 0$ ) and (b) with rescattering.

#### 19.1.4.5 Time-dependence

In order to calculate the time-dependence, we reconsider the equation (19.33) for the excitation amplitudes. Its solution is formally given by the sum of the general solution



of the homogeneous equation and a particular (e.g. the asymptotic) solution of the inhomogeneous equation,

$$\bar{\beta}_j(t) = e^{M_{jm}t} \bar{\beta}_m(0) + (\mathbb{I} - e^{M_{jm}t}) \bar{\beta}_m(\infty). \quad (19.38)$$

Inserting the steady-state solution we finally get,

$$\boxed{\bar{\beta}_j(t) = e^{M_{jm}t} \bar{\beta}_m(0) + (\mathbb{I} - e^{M_{jm}t}) M_{mn}^{-1} \frac{i}{2} \bar{\Omega}_0(\mathbf{r}_m)}. \quad (19.39)$$

### 19.1.5 Calculation of light scattering in steady-state

To calculate the distribution of scattered light, we start from the Heisenberg equation for the field operator [243],

$$\frac{d\hat{a}_{\mathbf{k}}}{dt} = \frac{1}{i\hbar} [\hat{a}_{\mathbf{k}}, \hat{H}] = -ig_{\mathbf{k}} e^{i(\omega_{\mathbf{k}} - \omega_a)t} \sum_{j=1}^N \hat{\sigma}_j e^{-i\mathbf{k} \cdot \mathbf{r}_j}. \quad (19.40)$$

where the fast oscillating term proportional to  $e^{i(\omega_{\mathbf{k}} + \omega_a)t}$  has been neglected. Now,

$$\hat{\mathcal{E}}_{sct}(\mathbf{r}, t) = \sum_{\mathbf{k}} \mathcal{E}_k \hat{a}_{\mathbf{k}}(t) e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_k t)}, \quad (19.41)$$

where  $\mathcal{E}_k = \sqrt{\hbar\omega_k/2\varepsilon_0 V_{ph}}$ . Integrating Eq. (19.40) with  $\hat{a}_{\mathbf{k}}(0) = 0$ , inserting it in Eq. (19.41), and approximating the sum over the modes  $\mathbf{k}$  by an integral, we obtain,

$$\hat{\mathcal{E}}_{sct}(\mathbf{r}, t) = -i \frac{V_{ph}}{8\pi^3} \sum_{j=1}^N \int_0^t dt' \hat{\sigma}_j(t-t') e^{i\omega_a t'} \int d^3k \mathcal{E}_k g_k e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_j) - i\omega_k t'}. \quad (19.42)$$

Introducing spherical coordinates,  $d^3k = dk k^2 d\phi d\theta \sin\theta$ , and integrating the angular part Eq. (19.42) becomes,

$$\begin{aligned} \hat{\mathcal{E}}_{sct}(\mathbf{r}, t) = & -i \frac{V_{ph}}{4\pi^2} \sum_{j=1}^N \frac{1}{|\mathbf{r} - \mathbf{r}_j|} \int_0^t dt' \hat{\sigma}_j(t-t') e^{i\omega_a t'} \times \\ & \times \int dk k \mathcal{E}_k g_k [e^{-i\omega_k(t' - |\mathbf{r} - \mathbf{r}_j|/c)} - e^{-i\omega_k(t' + |\mathbf{r} - \mathbf{r}_j|/c)}]. \end{aligned} \quad (19.43)$$

Assuming the radiation spectrum centered around  $k \simeq k_0$ , we approximate  $k\mathcal{E}_k g_k \simeq k_0 \mathcal{E}_{k_0} g_{k_0}$ . Then, extending the lower limit of integration of  $k$  to  $-\infty$ , we obtain for  $t < |\mathbf{r} - \mathbf{r}_j|/c$  [556, 440],

$$\hat{\mathcal{E}}_{sct}(\mathbf{r}, t) \simeq -\frac{dk_0^2}{4\pi\varepsilon_0} \sum_{j=1}^N \frac{e^{ik_0|\mathbf{r} - \mathbf{r}_j|}}{|\mathbf{r} - \mathbf{r}_j|} \hat{\sigma}_j(t - |\mathbf{r} - \mathbf{r}_j|/c). \quad (19.44)$$

where we may neglect the radiation retardation in the limit  $t \gg \sigma_R/c$ . Using (19.19) and expressing the coupling strength,

$$\hbar g_k = d\mathcal{E}_k \quad \text{with} \quad \mathcal{E}_k = \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V_{ph}}}, \quad (19.45)$$

we get,

$$\hat{\mathcal{E}}_{sct}(\mathbf{r}, t) \simeq -\frac{i\hbar\Gamma}{2d} \sum_{j=1}^N \gamma_{oj}(\mathbf{r}) \hat{\sigma}_j(t), \quad (19.46)$$

where we defined the abbreviation,

$$\gamma_{oj}(\mathbf{r}) \equiv \frac{e^{ik_0|\mathbf{r}-\mathbf{r}_j|}}{ik_0|\mathbf{r}-\mathbf{r}_j|}. \quad (19.47)$$

When applied on the state of Eq. (19.11), neglecting virtual transitions, it yields  $\hat{\mathcal{E}}_{sct}|\Psi\rangle = \mathcal{E}_{sct}|g_1, \dots, g_N\rangle$ , where  $\mathcal{E}_{sct}$  is the electric field radiated by the excited atoms. Once the excitation amplitudes  $\beta_j(\infty)$  are known, the scattered light field and the total field can easily be calculated via [600],

$$\mathcal{E}_{sct}(\mathbf{r}) = \langle \hat{\mathcal{E}}_{sct}(\mathbf{r}) \rangle = -\frac{i\hbar\Gamma}{2d} \sum_{j=1}^N \gamma_{oj}(\mathbf{r}) \beta_j(\infty) \quad \text{and} \quad \mathcal{E}_{tot} = \mathcal{E}_{las} + \mathcal{E}_{sct}, \quad (19.48)$$

**Example 82 (Light scattering from a Gaussian beam):** Fig. 19.4 shows an example of light scattering from an incident light field parametrized as a Gaussian beam,

$$\mathcal{E}_{las}(\mathbf{r}) = \hat{\epsilon} \mathcal{E}_0 \frac{w_0}{w(z)} e^{-r^2/w(z)^2 + ikz + zikr^2/2R(z) - i\varphi(z)} = \hat{\epsilon} \frac{\hbar}{|\mathbf{d}|} \Omega_0(\mathbf{r}) e^{i\mathbf{k}_0 \cdot \mathbf{r}}. \quad (19.49)$$

Note that, for the chosen parameters, the result does not depend on the interaction terms. I.e. we can as well set the kernel to 0.

Note, that the phase factor  $e^{i\mathbf{k}_0 \cdot \mathbf{r}}$  can either be attributed to the atomic dipole moments or to the field. Here,  $N = 125$  atoms are periodically arranged in a three-dimensional cubic lattice.

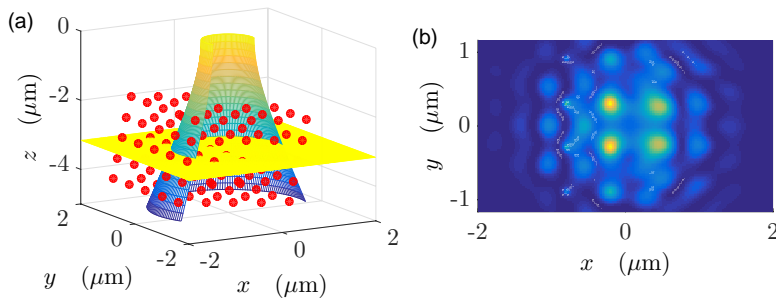


Figure 19.4: (code) (a) Geometry of light scattering from a cubic lattice with lattice constant  $d = 100$  nm. The light is irradiated from below and is partially reflected. (b) Intensity distribution of scattered light along the yellow plane.

### 19.1.6 Calculation of the steady-state radiation pressure force

Let us now calculate the radiative pressure force exerted by an incident beam of light  $\mathbf{k}_0$  on an atom  $j$  located at position  $\mathbf{r}_j$  inside an atomic cloud, as illustrated in Fig. 19.2,

$$\frac{d\hat{\mathbf{p}}_j}{dt} = \hat{\mathbf{F}}_j = -\nabla_{\mathbf{r}_j} \hat{H} . \quad (19.50)$$

Inserting the Hamiltonian in the RWA (19.10),

$$\begin{aligned} \hat{\mathbf{F}}_j = & i\hbar\mathbf{k}_0g_{k_0} \left[ \hat{\sigma}_j \hat{a}_{\mathbf{k}_0}^\dagger e^{i(\omega_0 - \omega_a)t - i\mathbf{k}_0 \cdot \mathbf{r}_j} - h.c. \right] \\ & + \sum_{\mathbf{k}} i\hbar\mathbf{k}g_k \left[ \hat{\sigma}_j \hat{a}_{\mathbf{k}}^\dagger e^{i(\omega_k - \omega_a)t - i\mathbf{k} \cdot \mathbf{r}_j} - h.c. \right] . \end{aligned} \quad (19.51)$$

Introducing  $\Delta_0 = \omega_0 - \omega_a$ , the expectation value of the force separates in two contribution,

$$\begin{aligned} \langle \hat{\mathbf{F}}_j \rangle \equiv \mathbf{F}_{aj} + \mathbf{F}_{ej} = & i\hbar\mathbf{k}_0g_{k_0} \left[ \alpha^*(t)\beta_j(t)e^{i\Delta_0 t - i\mathbf{k}_0 \cdot \mathbf{r}_j} - c.c. \right] \\ & + \sum_{\mathbf{k}} i\hbar\mathbf{k}g_k \left[ \beta_j(t)\gamma_{\mathbf{k}}^*(t)e^{i(\omega_k - \omega_a)t - i\mathbf{k} \cdot \mathbf{r}_j} - c.c. \right] \\ = & i\hbar\mathbf{k}_0g_{k_0} [\alpha^*(t)\tilde{\beta}_j(t) - c.c.] \\ & + \sum_{\mathbf{k}} i\hbar\mathbf{k}g_k \left[ \tilde{\beta}_j(t)e^{-i(\omega_0 - \omega_k)t + i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{r}_j} \gamma_{\mathbf{k}}^*(t) - c.c. \right] , \end{aligned} \quad (19.52)$$

where we reintroduced the abbreviation (19.17). In particular, the term  $m = j$  in the sum of  $\mathbf{F}_{ej}$  vanishes since  $\sum_{\mathbf{k}} \mathbf{k} = 0$ . Substituting  $\gamma_{\mathbf{k}}$  with equation (19.16),

$$\begin{aligned} \mathbf{F}_{aj} + \mathbf{F}_{ej} = & i\hbar\mathbf{k}_0g_{k_0} [\alpha^*(t)\tilde{\beta}_j(t) - c.c.] \\ & - \sum_{\mathbf{k}} \hbar\mathbf{k}g_k^2 \left[ \tilde{\beta}_j(t)e^{-i(\omega_0 - \omega_k)t + i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{r}_j} \sum_{m=1}^N e^{i\mathbf{k} \cdot \mathbf{r}_m} \int_0^t e^{-i(\omega_k - \omega_a)t'} \tilde{\beta}_m^*(t') dt' - c.c. \right] \\ = & -2\hbar\mathbf{k}_0g_{k_0} \text{Im} [\alpha^*(t)\tilde{\beta}_j(t)] \\ & - \sum_{\mathbf{k}} \hbar\mathbf{k}g_k^2 \sum_{m=1}^N \left[ \tilde{\beta}_j(t)e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot (\mathbf{r}_j - \mathbf{r}_m)} \int_0^t e^{i(\omega_0 - \omega_k)(t' - t)} \tilde{\beta}_m^*(t') dt' - c.c. \right] , \end{aligned} \quad (19.53)$$

and applying the Markov approximation (19.20),

$$\begin{aligned} \mathbf{F}_{aj} + \mathbf{F}_{ej} = & -2\hbar\mathbf{k}_0g_{k_0} \text{Im} [\alpha^*(t)\tilde{\beta}_j(t)] \\ & - \sum_{\mathbf{k}} \hbar\mathbf{k}g_k^2 \sum_{m=1}^N \left[ e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot (\mathbf{r}_j - \mathbf{r}_m)} \frac{\pi}{c} \delta(k - k_0) \tilde{\beta}_j(t) \tilde{\beta}_m^*(t) - c.c. \right] . \end{aligned} \quad (19.54)$$

This is the expression for the force acting on an atom at the position  $\mathbf{r}_j$ . Knowing the stationary excitation amplitudes  $\beta_j(\infty)$  and assuming  $\alpha(\infty) \simeq 1$ , the radiation pressure force can numerically be calculated. Remembering  $\Omega_0 = 2g_{k_0}$  we get for the absorption force acting on atom  $j$ ,

$$\mathbf{F}_{aj} = -2\hbar\mathbf{k}_0g_{k_0} \text{Im} \tilde{\beta}_j(\infty) . \quad (19.55)$$

To evaluate the emission force acting on atom  $j$ , for every atom  $m$  of the sum, we need to average over all possible scattering angles. To do so, we choose a reference frame in which the  $z$ -component of  $\mathbf{k}$  is directed along  $\hat{\mathbf{r}}_{jm} = \frac{\mathbf{r}_j - \mathbf{r}_m}{|\mathbf{r}_j - \mathbf{r}_m|}$ , that is,

$$\mathbf{k} = \hat{\mathbf{e}}_{x,jm} k \sin \theta_{jm} \cos \phi_{jm} + \hat{\mathbf{e}}_{y,jm} k \sin \theta_{jm} \sin \phi_{jm} + \hat{\mathbf{r}}_{jm} k \cos \theta_{jm} , \quad (19.56)$$

and evaluate the sum over the wavevectors by  $\sum_{\mathbf{k}} \rightarrow \frac{V_{ph}}{(2\pi)^3} \int d^3 k$ ,

$$\begin{aligned} \mathbf{F}_{ej} &= - \sum_{m=1}^N \tilde{\beta}_j(\infty) \tilde{\beta}_m^*(\infty) \frac{V_{ph}}{(2\pi)^3} \frac{\pi}{c} \int_{\mathbb{R}^3} d\theta_{jm} d\phi_{jm} dk \hbar k \begin{pmatrix} \sin \theta_{jm} \cos \phi_{jm} \\ \sin \theta_{jm} \sin \phi_{jm} \\ \cos \theta_{jm} \end{pmatrix} \times \\ &\quad \times g_k^2 [e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot (\mathbf{r}_j - \mathbf{r}_m)} \delta(k - k_0) k^2 \sin \theta_{jm} - c.c. \\ &= -\hbar k_0 \frac{\Gamma}{8\pi} \sum_{m=1}^N e^{i\mathbf{k}_0 \cdot (\mathbf{r}_j - \mathbf{r}_m)} \tilde{\beta}_j(\infty) \tilde{\beta}_m^*(\infty) \int_0^\pi \int_0^{2\pi} d\theta_{jm} d\phi_{jm} \begin{pmatrix} \sin \theta_{jm} \cos \phi_{jm} \\ \sin \theta_{jm} \sin \phi_{jm} \\ \cos \theta_{jm} \end{pmatrix} \times \\ &\quad \times e^{-ik|\mathbf{r}_j - \mathbf{r}_m| \cos \theta_{jm}} \sin \theta_{jm} - c.c. . \end{aligned} \quad (19.57)$$

remembering  $\Gamma = \frac{V_{ph}}{\pi c} k_0^2 g_{k_0}^2$  from Eq. (19.19). The integrals over  $\phi_{jm}$  vanishes whereas the integral over  $\theta_{jm}$  becomes, using,

$$\int_0^\pi d\theta \sin \theta \cos \theta e^{-i\alpha \cos \theta} = 2i \frac{\alpha \cos \alpha - \sin \alpha}{\alpha^2} = -2i j_1(\alpha) , \quad (19.58)$$

we find,

$$\begin{aligned} \mathbf{F}_{ej} &= -\hbar k_0 \frac{\Gamma}{4} \sum_{m=1}^N e^{i\mathbf{k}_0 \cdot (\mathbf{r}_j - \mathbf{r}_m)} \tilde{\beta}_j(\infty) \tilde{\beta}_m^*(\infty) \hat{\mathbf{r}}_{jm} \times \\ &\quad \times \int_0^\pi \cos \theta_{jm} \sin \theta_{jm} e^{-ik|\mathbf{r}_j - \mathbf{r}_m| \cos \theta_{jm}} d\theta_{jm} - c.c. \\ &= i\hbar k_0 \frac{\Gamma}{2} \sum_{m=1}^N e^{i\mathbf{k}_0 \cdot (\mathbf{r}_j - \mathbf{r}_m)} \tilde{\beta}_j(\infty) \tilde{\beta}_m^*(\infty) \hat{\mathbf{r}}_{jm} j_1(k|\mathbf{r}_j - \mathbf{r}_m|) - c.c. \\ &= -i\hbar k_0 \frac{\Gamma}{2} \sum_{m=1}^N \mathbf{f}_{jm} \tilde{\beta}_j(\infty) \tilde{\beta}_m^*(\infty) - c.c. , \end{aligned} \quad (19.59)$$

where we defined <sup>7</sup>,

$$\mathbf{f}_{jm} = -j_1(k|\mathbf{r}_j - \mathbf{r}_m|) e^{i\mathbf{k}_0 \cdot (\mathbf{r}_j - \mathbf{r}_m)} \hat{\mathbf{r}}_{jm} . \quad (19.60)$$

In summary we got,

$$\boxed{\begin{aligned} \mathbf{F}_{aj} &= -i\hbar k_0 \Omega_0 \text{Im} \tilde{\beta}_j(\infty) \\ \mathbf{F}_{ej} &= -i\hbar k_0 \Gamma \sum_{m=1}^N \mathbf{f}_{jm} \text{Im} [\tilde{\beta}_j(\infty) \tilde{\beta}_m^*(\infty)] \end{aligned}} . \quad (19.61)$$

<sup>7</sup>For exploitation in MATLAB we may express the spherical Bessel function by a Bessel function of the first kind:  $j_n(x) = \sqrt{\pi/2x} J_{n+1/2}(x)$ .

The steady state absorption and the emission part of the radiation pressure force on the *center of mass* of the atomic cloud follow from,

$$\mathbf{F}_a = \frac{1}{N} \sum_j \langle \hat{\mathbf{F}}_{aj} \rangle \quad \text{and} \quad \mathbf{F}_e = \frac{1}{N} \sum_j \langle \hat{\mathbf{F}}_{ej} \rangle . \quad (19.62)$$

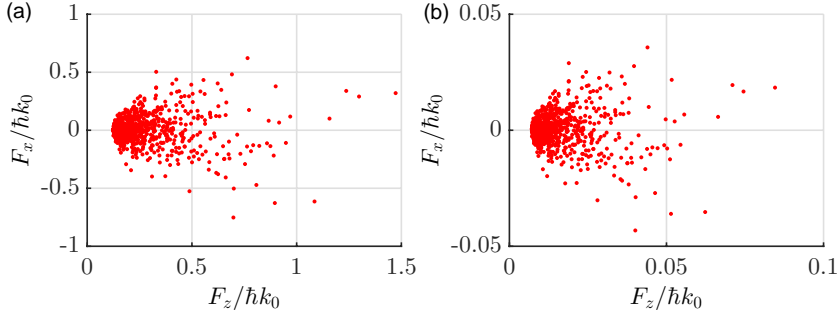


Figure 19.5: (code) Force distribution upon scattering of a photon by an atom of a spherical Gaussian cloud (a) without and (b) with rescattering according to Eqs. (19.62).

As long as the RWA and the Markov approximation are valid and only the lowest Dicke state is considered (no collective saturation), this simulation is supposed to be exact and contains all the physics including, e.g. multiple scattering. Fig. 19.5 shows a comparison of the cases when the off-diagonal components of the kernel (19.36) are present or not. Apparently, the presence of rescattering dramatically spoils the radiation pressure force, a phenomenon that we will extensively study in Secs. 19.1.7 and 19.2 [243, 32, 33, 549, 69, 34].

### 19.1.7 The structure factor of the 'timed' Dicke state

When a beam of light passes through an atomic cloud, its phase fronts will excite the atomic dipole moments as it traverses the cloud. That is, understanding the beam as a plane wave  $e^{i(\mathbf{k}_0 \cdot \mathbf{r} - \omega t)}$ , the dipoles start to oscillate with relative phase delays  $e^{i\mathbf{k}_0 \cdot (\mathbf{r}_j - \mathbf{r}_m)}$  depending on their position along the optical axis  $\mathbf{k}_0$ . The resulting collective state has been termed *timed Dicke state* [625]. Assuming that this phase delay is the only parameter distinguishing two atoms, we may write with Eq. (19.17),

$$\tilde{\beta}_j(t) = \beta_j(t) e^{i(\Delta_0 t - \mathbf{k}_0 \cdot \mathbf{r}_j)} \equiv \frac{1}{\sqrt{N}} \beta(t) , \quad (19.63)$$

where  $\beta$  is the macroscopic dipole moment. Note, that the fact that  $\beta(t)$  does not depend on the atomic position does not imply a continuous density distribution. The atoms are still sitting at their positions  $\mathbf{r}_j$ ; only are their dipole moments synchronized to the incident light wave.

The assumption of a timed Dicke state for the atomic cloud is, nevertheless, an approximation which is not always good [243]. For example, it neglects dispersive phase shifts of the excitation of the atomic dipole moments by the pump laser beam

being delayed on its propagation due to its interaction with the atoms. If such phase shifts (and absorption as well) are radially inhomogeneous, this can lead to deformation of the pump laser beam's phase front and thus to lensing. We will discuss this in Exc. 19.1.8.5 and in Sec. 19.2.

### 19.1.7.1 Structure factor for 'timed' Dicke states

We start again with the Eqs. (19.24) inserting the ansatz of *timed Dicke* states,

$$\begin{aligned}\dot{\beta}(t) &= \frac{1}{N} \sum_{j=1}^N \dot{\beta}(t) = \frac{1}{\sqrt{N}} \sum_{j=1}^N \frac{d}{dt} \tilde{\beta}_j(t) \\ &= \frac{1}{\sqrt{N}} \sum_{j=1}^N \left( i\Delta_0 \tilde{\beta}_j(t) - i\frac{\Omega_0}{2} \alpha(t) - \frac{\Gamma}{2} \sum_{m=1}^N \gamma_{jm} \tilde{\beta}_m(t) \right) \\ &= \left( i\Delta_0 - \frac{\Gamma}{2} N s_N \right) \beta(t) - i\frac{\sqrt{N}\Omega_0}{2} \alpha(t),\end{aligned}\tag{19.64}$$

where we introduced the abbreviation,

$$s_N \equiv \frac{1}{N} \frac{1}{N} \sum_{j,m=1}^N \gamma_{jm}.\tag{19.65}$$

Taking the kernel from (??), we get,

$$\begin{aligned}s_N &= \frac{1}{N} \frac{2}{\Gamma} \frac{V_{ph}}{(2\pi)^3} \int_{\mathbb{R}^3} g_k^2 \frac{1}{N} \sum_{j,m=1}^N e^{i(\mathbf{k}-\mathbf{k}_0)\cdot(\mathbf{r}_j-\mathbf{r}_m)} \frac{\pi}{c} \delta(k-k_0) k^2 \sin\theta dk d\theta d\phi \\ &= \frac{1}{N} \frac{2}{\Gamma} \frac{V_{ph}}{(2\pi)^3} \int_0^\infty \int_0^\pi \int_0^{2\pi} g_k^2 N |S_N(k, \theta, \phi)|^2 \frac{\pi}{c} \delta(k-k_0) k^2 \sin\theta dk d\theta d\phi \\ &= \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} |S_N(k_0, \theta, \phi)|^2 \sin\theta d\theta d\phi,\end{aligned}\tag{19.66}$$

introducing the normalized *static structure factor*,

$$S_N(\mathbf{k}) \equiv \rho(\mathbf{q}) = \frac{1}{N} \sum_{j=1}^N e^{i(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{r}_j},\tag{19.67}$$

where  $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$  and  $\rho(\mathbf{q})$  is the static structure factor defined in (19.3).

In steady state,  $\dot{\beta}(t) = 0$ , and disregarding saturation,  $\alpha(t) \simeq 1$ , the solution of (19.64) reads,

$$\beta(\infty) = \frac{\sqrt{N}\Omega_0}{2\Delta_0 + i\Gamma N s_N},\tag{19.68}$$

such that,

$$\begin{aligned}|\beta(\infty)|^2 &= \frac{N\Omega_0^2}{4\Delta_0^2 + N^2\Gamma^2 s_N^2} \\ \text{Im} [\alpha(\infty)\beta^*(\infty)] &= \frac{N^{3/2}\Gamma\Omega_0 s_N}{4\Delta_0^2 + N^2\Gamma^2 s_N^2}.\end{aligned}\tag{19.69}$$

The time-dependent solution is easily obtained as,

$$\beta(t) = \beta(0)e^{(\nu\Delta_0 - \Gamma N s_n/2)t} + \beta(\infty) . \quad (19.70)$$

The evolution of the cloud very much depends on the initial conditions, e.g.  $\beta_j(0) = 1$  for the uniformly excited *symmetric state*  $\beta_j(0) = e^{i\mathbf{k}_0 \cdot \mathbf{r}_j}$  for timed Dicke states.

In cylindrical coordinates the structure factor can be written,

$$S(k, \theta, \phi) = \frac{1}{N} \sum_{j=1}^N e^{i(kx_j \sin \theta \cos \phi + ky_j \sin \theta \cos \phi + (k \cos \theta - k_0)z_j)} . \quad (19.71)$$

It basically tells the angular distribution of the scattered light. Fig. 19.6 shows numerical calculations and analytical approximations of the structure factor for various shapes and sizes of the atomic cloud. Obviously, the radiation pattern very much depends on the size of the spherical cloud. For  $R < \lambda$  it is isotropic, for  $R > \lambda$  scattering mainly occurs in forward direction. Furthermore, if the cloud is ellipsoidal the radiation pattern is shifted into forward direction.

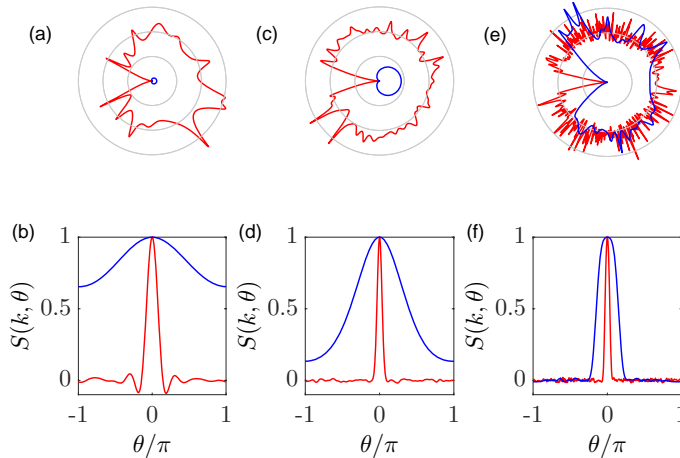


Figure 19.6: (code) Numerical calculation of  $S(k, \theta)$  according to (19.67) for  $10^4$  atomic positions  $r_j$  chosen by a random number generator. For the graphs (a-b) the cloud is *homogeneous and spherical* and has the sizes  $R = \lambda$  (red) and  $R = 10\lambda$  (blue). For the graphs (c-d) the cloud is *Gaussian and spherical* and has the same sizes as (a-b). For the graphs (d-e) the cloud is *homogeneous and ellipsoidal with aspect ratio  $R_z/R_\rho = 3$*  and has the same radial sizes as in (a-b).

### 19.1.7.2 Time evolution of radiation modes

We are interested in the power emitted into the solid angle  $\Omega_{\mathbf{k}}$ ,  $P(t) \propto |\dot{\gamma}_{\mathbf{k}}(t)|^2$ . For timed Dicke state (19.63) we get immediately from the equations of motion,

$$\begin{aligned} \dot{\gamma}_{\mathbf{k}}(t) &= -ig_k e^{i\Delta_k t} \sum_{j=1}^N \beta_j(t) e^{-i\mathbf{k}\cdot\mathbf{r}_j} \\ &= -ig_k e^{i(\Delta_k - \Delta_0)t} \frac{1}{\sqrt{N}} \beta(t) \sum_{j=1}^N e^{i(\mathbf{k}_0 - \mathbf{k})\cdot\mathbf{r}_j} = -ig_k e^{i(\Delta_k - \Delta_0)t} \sqrt{N} S_N(\mathbf{k}) . \end{aligned} \quad (19.72)$$

We see that the time-dependence factorizes from the structure factor, which is the only component containing an angular dependence. The same holds for *symmetric Dicke states* defined by  $|\beta_j| = |\beta_m|$ .

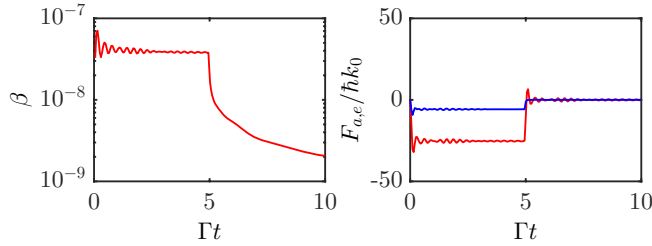


Figure 19.7: (code) Time-dependent of (a) the dipole amplitudes and (b) the forces for  $\sigma = 1$ ,  $\Delta_0 = 20\Gamma$ ,  $\Omega_0 = 0.01\Gamma$ , and  $\eta = 1$ .

### 19.1.7.3 Light scattering in the 'timed Dicke state'

The scalar electric field scattered by an arbitrary distribution of atoms has been calculated in (19.48). Substituting the stationary timed Dicke state (19.68), we get,

$$\mathcal{E}_{sct}(\mathbf{r}) = -\frac{i\hbar\Gamma}{2d} \frac{\sqrt{N}\Omega_0}{2\Delta_0 + i\Gamma N S_N} \sum_{j=1}^N \frac{e^{i k_0 |\mathbf{r} - \mathbf{r}_j|}}{i k_0 |\mathbf{r} - \mathbf{r}_j|} . \quad (19.73)$$

Note that the 'timed Dicke' state starts from the assumption of an infinitely extended plane wave incident light field. This excludes situations where the incident beam size is smaller than the cloud's size.



### 19.1.7.4 Force in the 'timed Dicke state' on a particular atom in a cloud

The time-dependent expressions (19.55) for the forces in the coupled dipoles model can be further evaluated for timed Dicke states (19.63),

$$\begin{aligned}
 \mathbf{F}_{aj} + \mathbf{F}_{ej} & \quad (19.74) \\
 &= -\frac{2\hbar\mathbf{k}_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(t) - \sum_{\mathbf{k}} \frac{\hbar\mathbf{k} g_k^2}{N} \sum_{m=1}^N \left[ e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot (\mathbf{r}_j - \mathbf{r}_m)} \frac{\pi}{c} \delta(k - k_0) |\beta(t)|^2 - c.c. \right] \\
 &= -\frac{2\hbar\mathbf{k}_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(t) - \sum_{\mathbf{k}} \hbar\mathbf{k} g_k^2 \left[ S_N(\mathbf{k}) e^{-i(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{r}_j} \frac{\pi}{c} \delta(k - k_0) |\beta(t)|^2 - c.c. \right].
 \end{aligned}$$

Evaluating the sum over the wavevectors by  $\sum_{\mathbf{k}} \rightarrow \frac{V_{ph}}{(2\pi)^3} \int d^3k$ ,

$$\begin{aligned}
 \mathbf{F}_{aj} + \mathbf{F}_{ej} &= \frac{-2\hbar\mathbf{k}_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(t) \quad (19.75) \\
 &- |\beta(t)|^2 \frac{V_{ph}}{(2\pi)^3} \int_0^\infty \int_0^\pi \int_0^{2\pi} \hbar\mathbf{k} g_k^2 \left[ S_N(k, \theta, \phi) e^{-i(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{r}_j} \frac{\pi}{c} \delta(k - k_0) - c.c. \right] k^2 \sin \theta d\theta d\phi dk.
 \end{aligned}$$

Let us consider an atom sitting on axis,  $\mathbf{r}_j = 0$ , and use cylindrical coordinates,  $\mathbf{k}_0 = k_0 \hat{\mathbf{e}}_z$  and  $\mathbf{k} = \hat{\mathbf{e}}_x k \sin \theta \cos \phi + \hat{\mathbf{e}}_y k \sin \theta \sin \phi + \hat{\mathbf{e}}_z k \cos \theta$ , and using the definition (19.19) of  $\Gamma$ ,

$$\begin{aligned}
 \mathbf{F}_{aj} + \mathbf{F}_{ej} &= \frac{-2\hbar k_0 g_{k_0}}{\sqrt{N}} \hat{\mathbf{e}}_z \text{Im } \beta(t) \quad (19.76) \\
 &- |\beta(t)|^2 \frac{\Gamma}{8\pi} \hbar k_0 \int_0^\pi \int_0^{2\pi} (\hat{\mathbf{e}}_x \sin \theta \cos \phi + \hat{\mathbf{e}}_y \sin \theta \sin \phi + \hat{\mathbf{e}}_z \cos \theta) [S_N(k, \theta, \phi) - c.c.] \sin \theta d\theta d\phi.
 \end{aligned}$$

Using the abbreviation,

$$\tilde{f}_N \equiv \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} \text{Re } S_N(k_0, \theta, \phi) \sin \theta \cos \theta d\theta d\phi, \quad (19.77)$$

the  $z$ -component becomes,

$$F_{zaj} + F_{zej} = -\frac{2\hbar k_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(t) - |\beta(t)|^2 \Gamma \hbar k_0 \tilde{f}_N. \quad (19.78)$$

In steady state and normalizing to the standard radiation pressure,

$$F_{z1j} = \Gamma \hbar k_0 \frac{\Omega_0^2}{4\Delta_0^2 + \Gamma^2} = \hbar k_0 \sigma(\Delta) \frac{I}{\hbar\omega}, \quad (19.79)$$

where  $\sigma(\Delta_0)$  is the optical cross section and  $I$  the intensity of the incident light, we can write,

$$\frac{F_{zaj} + F_{zej}}{F_{z1j}} = \left( -\frac{2\hbar k_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(\infty) - |\beta(\infty)|^2 \Gamma \hbar k_0 \tilde{f}_N \right) \frac{4\Delta_0^2 + \Gamma^2}{\Gamma \hbar k_0 \Omega_0^2}. \quad (19.80)$$

Finally, inserting the the expression (19.68) for the dipole moment, we obtain for the timed Dicke state,

$$\boxed{\frac{F_{zaj} + F_{zej}}{F_{z1j}} = \frac{(2\Delta_0/\Gamma)^2 + 1}{(2\Delta_0/\Gamma)^2 + N^2 s_N^2} N(s_N - \tilde{f}_N)}, \quad (19.81)$$

using  $\Omega_0 = 2g_{k_0}$ .

The factors  $s_N$  and  $f_N$  can be calculated exactly, as will be done in Exc. 19.1.8.6,

$$s_N = \frac{1}{N^2} \sum_{j,m=1}^N \frac{\sin(k_0|\mathbf{r}_j - \mathbf{r}_m|)}{k_0|\mathbf{r}_j - \mathbf{r}_m|} \cos[k_0(z_j - z_m)] \quad (19.82)$$

$$f_N = \sqrt{\frac{\pi}{2}} \frac{1}{N^2} \sum_{j,m=1}^N \frac{J_{3/2}(k_0|\mathbf{r}_j - \mathbf{r}_m|)}{(k_0|\mathbf{r}_j - \mathbf{r}_m|)^{3/2}} k_0(z_j - z_m) \sin[k_0(z_j - z_m)] .$$

However, this is only practicable for atom numbers small enough for numerical simulations. For larger atom number we may use the analytic expressions including the disorder term [70].

### 19.1.7.5 Force on the center of mass of the cloud

The force acting on the center of mass of the atomic cloud is given by the average of the forces (19.75) sensed by particular atoms,

$$\begin{aligned} \mathbf{F}_a + \mathbf{F}_e &= \frac{1}{N} \sum_{j=1}^N (\mathbf{F}_{aj} + \mathbf{F}_{ej}) \quad (19.83) \\ &= -\frac{2\hbar\mathbf{k}_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(t) \\ &\quad - |\beta(t)|^2 \frac{V_{ph}}{(2\pi)^3} \int_{\mathbb{R}^3} \hbar\mathbf{k} g_k^2 \left[ S_N(k, \theta, \phi) \frac{1}{N} \sum_{j=1}^N e^{-i(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{r}_j} \frac{\pi}{c} \delta(k - k_0) - c.c. \right] k^2 \sin\theta d\theta d\phi dk \\ &= \frac{-2\hbar\mathbf{k}_0}{\sqrt{N}} g_{k_0} \text{Im } \beta(t) - |\beta(t)|^2 \frac{V_{ph}}{(2\pi)^3} \int_{\mathbb{R}^3} \hbar\mathbf{k} g_k^2 |S_N(k, \theta, \phi)|^2 \frac{\pi}{c} \delta(k - k_0) k^2 \sin\theta d\theta d\phi dk . \end{aligned}$$

Using cylindrical coordinates,  $\mathbf{k}_0 = k_0 \hat{\mathbf{e}}_z$  and  $\mathbf{k} = \hat{\mathbf{e}}_x k \sin\theta \cos\phi + \hat{\mathbf{e}}_y k \sin\theta \sin\phi + \hat{\mathbf{e}}_z k \cos\theta$ , and the definition of  $\Gamma$ ,

$$\begin{aligned} \mathbf{F}_a + \mathbf{F}_e &= \frac{-2\hbar k_0}{\sqrt{N}} \hat{\mathbf{e}}_z g_{k_0} \text{Im } \beta(t) \quad (19.84) \\ &\quad - |\beta(t)|^2 \frac{\Gamma}{8\pi} \hbar k_0 \int_0^\pi \int_0^{2\pi} (\hat{\mathbf{e}}_x \sin\theta \cos\phi + \hat{\mathbf{e}}_y \sin\theta \sin\phi + \hat{\mathbf{e}}_z \cos\theta) 2|S_N(k, \theta, \phi)|^2 \sin\theta d\theta d\phi . \end{aligned}$$

Using the abbreviation,

$$f_N \equiv \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} |S_N(k_0, \theta, \phi)|^2 \sin\theta \cos\theta d\theta d\phi , \quad (19.85)$$

we get for the  $z$ -component an analogous formula to (19.78),

$$\begin{aligned} F_{za} + F_{ze} &= \frac{-2\hbar k_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(t) - |\beta(t)|^2 \frac{\Gamma}{8\pi} \hbar k_0 \int_0^\pi \int_0^{2\pi} 2|S_N(k, \theta, \phi)|^2 \sin\theta \cos\theta d\theta d\phi \\ &= \frac{-2\hbar k_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(t) - |\beta(t)|^2 \Gamma \hbar k_0 f_N . \quad (19.86) \end{aligned}$$

In steady state and normalizing again to the standard radiation pressure (19.79),

$$\frac{F_{za} + F_{ze}}{F_{z1}} = \left( -\frac{2\hbar k_0 g_{k_0}}{\sqrt{N}} \text{Im } \beta(\infty) - |\beta(\infty)|^2 \Gamma \hbar k_0 f_N \right) \frac{4\Delta_0^2 + \Gamma^2}{\Gamma \hbar k_0 \Omega_0^2} . \quad (19.87)$$

Finally, inserting the the expression (19.68) for the dipole moment, we obtain for the timed Dicke state,

$$\boxed{\frac{F_{za} + F_{ze}}{F_{z1}} = \frac{(2\Delta_0/\Gamma)^2 + 1}{(2\Delta_0/\Gamma)^2 + N^2 s_N^2} N(s_N - f_N)}, \quad (19.88)$$

using  $\Omega_0 = 2g_{k_0}$ . Inserting the expressions (19.66) for  $s_N$  and (19.85) for  $f_N$ , we may also write,

$$\frac{F_{0a} + F_{0e}}{F_{z1}} = \frac{(2\Delta_0/\Gamma)^2 + 1}{(2\Delta_0/\Gamma)^2 + N^2 s_N^2} N \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} |S_N(k, \theta, \phi)|^2 (1 - \cos \theta) \sin \theta d\theta d\phi. \quad (19.89)$$

Let us assume in the following that the scattering of every single photon can be treated independently [623]. In particular, the density distribution may change between two scattering events. The force is something like the first moment of the structure factor. This makes it so adapted to measure fluctuation-induced deviations from the structure factor <sup>8</sup>.

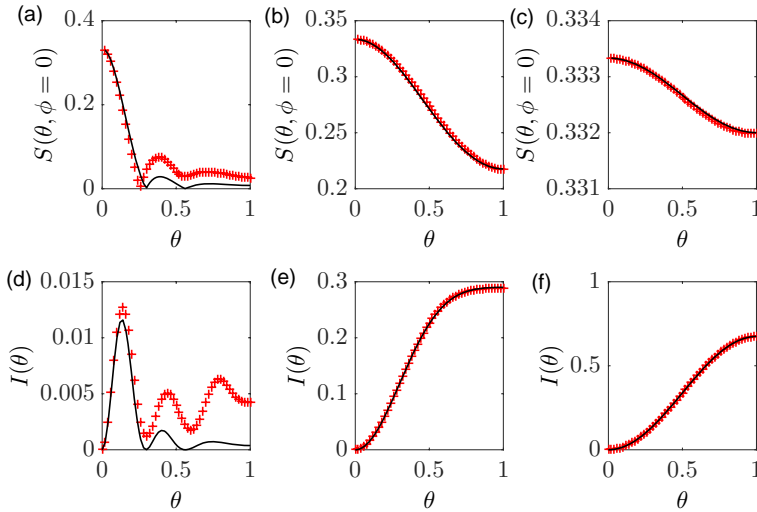


Figure 19.8: (code) (a-c) Calculation of the structure factor  $|S(k = k_0, \theta, \phi = 0)|^2$  for an isotropic homogeneous density distribution. (d-f) Calculation of the force  $I(\theta) = \int_0^{2\pi} |S(k = k_0, \theta, \phi)|^2 (1 - \cos \theta) d\phi$ . The red curves show numerical calculations based on (19.67), the green curves show analytical calculations according to (19.97). (a,d)  $k_0 R = 1$  and  $N = 100$ . (b,e)  $k_0 R = 5$  and  $N = 100$ . (c,f)  $k_0 R = 5$  and  $N = 1000$ .

We want to compare this force to the force acting on a cloud of  $N$  uncorrelated scatterers, i.e. atoms receiving recoil from the pump photons but reemitting isotrop-

<sup>8</sup>Insert a clarifying discussion of what we said in the EPDJ and what we did not: We said there is a collective effect coming from the structure factor of the cloud. We did NOT say that interatomic interactions are essential...!

ically,

$$\langle F_{unc,z} \rangle = \frac{V_{ph}}{(2\pi)^3} \sigma(\Delta) \frac{I}{\hbar\omega} \hbar k_0 \int_0^\infty \int_0^\pi \int_0^{2\pi} |S_N(k, \theta, \phi)|^2 k^2 \sin \theta d\theta d\phi dk. \quad (19.90)$$

For such a cloud the structure factor is  $S_N = N^{-1/2}$ . Note that this is unlike  $N$  atoms in the Dicke limit, where  $S_N = 1$ .

A dense homogeneous cloud with  $S_N(\mathbf{k}) \propto \delta^3(\mathbf{k}_0 - \mathbf{k})$  does not scatter light and experiences no force,  $\langle F_{hom} \rangle = 0$ . This is however not true any more in the limit of small extended clouds, where fluctuations introduce disorder. This can be shown by simulating a random atomic distribution  $\mathbf{r}_j$  and integrating the resulting force over all possible  $\mathbf{k}$ . For simplicity we assume a very sharp momentum distribution,  $|\mathbf{k}| = |\mathbf{k}_0|$  or  $\frac{V_{ph}}{2\pi^2} \int_0^\infty k^2 dk = 1$ ,

$$\langle F_z \rangle = \sigma(\Delta) \frac{I}{\hbar\omega} k_0 (s_N - f_N). \quad (19.91)$$

Finally to compare with experiment we evaluate the ratio,

$$\frac{\langle F_z \rangle}{\langle F_{unc,z} \rangle} = 1 - \frac{f_N}{s_N}. \quad (19.92)$$

We describe the cloud as being made of two fractions: An isotropically scattering fraction of  $N_0 = \sqrt{N}$  disordered atoms, whose structure factor is  $S_{iso}(\mathbf{k}) = 1$ , and a forward scattering homogeneous cloud with structure factor  $S_{hom}(\mathbf{k}) = \delta_{\mathbf{k}_0, \mathbf{k}}$ . The surface integration of the total structure factor,

$$S_N(\mathbf{k}) = \frac{N_0}{N} S_{iso}(\mathbf{k}) + \frac{N - N_0}{N} S_{hom}(\mathbf{k}) = \frac{N_0}{N} + \frac{N - N_0}{N} \delta_{\mathbf{k}_0, \mathbf{k}} \simeq \frac{N_0}{N} \quad (19.93)$$

yields the same  $N$ -dependence of the force,

$$\frac{\langle F_z \rangle}{\langle F_{iso,z} \rangle} = \frac{1}{4\pi N^2} \int_0^\pi \int_0^{2\pi} |\sqrt{N}|^2 (1 - \cos \theta) \sin \theta d\theta d\phi = \frac{1}{N}. \quad (19.94)$$

The interpretation is the following. In the experimentally realized situation, we are very far in the large cloud limit completely dominated by forward scattering, which means that *if the cloud were homogeneous no radiation pressure force should be expected* at all. However diffuse scattering from disordered atoms (or fluctuations) disturbs the forward scattering. It is this scattering which gives rise to radiation pressure.

There is an interesting analogy: Diffuse scattering not only inhibits forward scattering in homogeneous clouds, but also coherent backscattering from ordered structures. E.g. in optical lattices [642] it disturbs the detection of photonic band gaps. In an optical lattice the atoms are in the Dicke limit and do not absorb photonic recoil. Hence, no displacement due to radiation pressure is expected. However, diffuse scattering is observed as absorptive features in the spectra [72, 642].

The Bragg scattering is expressed by a periodic structure factor. A widely used approach to describe the impact of disordered atoms in lattices is to divide the cloud into a perfectly ordered part with density  $n f_{DW}$  and isotropically scattering part with density  $n(1 - f_{DW})$  [642]. The factor  $f_{DW}$  is known as Debye-Waller factor. In Exc. 19.1.8.7 we try an alternative treatment of radiation pressure based on a Monte-Carlo simulation.

### 19.1.7.6 Cooperative scattering and single photon superradiance

A non-isotropic structure factor scattering light into a specific direction of space (e.g. the Bragg angle) at a rate scaling like  $N^\alpha$  with  $\alpha > 1$  needs several 'cooperating' particles. In this sense cooperation only means, that the particles be arranged in space in a particular way, i.e. in a lattice or in a particular bulk shape like a homogeneous sphere or a Gaussian cigar-shaped density distribution. It also immediately becomes clear that disorder ought to play a major role. However, cooperation goes further, since cooperative scattering can be observed in spontaneous emission of an atomic cloud being excited by just a single photon. Single-photon superradiance is the topic of the following sections.

For now let us state that a non-isotropic structure factor results in collective scattering. The density distribution (which is the Fourier transform of the structure factor) can adopt two extremes: A periodic lattice results in backscattering into specific directions, a homogeneous clouds shows nothing but forward scattering. Both situations are never perfectly realized, but are subject to density fluctuations (Debye-Waller factor in a lattice, radiation pressure in a homogeneous cloud).

A single photon on its trip through an atomic cloud successively excites the atomic dipole moment thus establishing a phase relation between potential radiators [217, 675, 624, 676]. One could think that the scattering process localizes atom and photon, i.e. only one atom scatters. However, we don't know which atom scatters, and this introduces a correlation of the dipole moments along the propagation direction of the light beam.

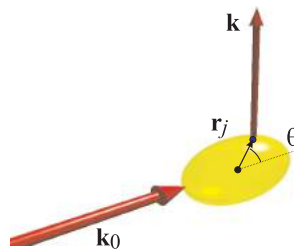


Figure 19.9: Scattering of a photon by an atom of an ellipsoidal cloud.

While normally the radiation rate of a dilute cloud is  $\propto N$ , in the presence of coherent interactions it scales as  $\propto N^2$ . Coherent interactions are not conditioned to overlapping space functions of the atoms, i.e. it is not compulsory that the density be  $n^{-1/3} > \lambda$ . For example, scattering from ordered structures also scales as  $\propto N^2$  [378]. However, the scattering will be dramatically different if  $n^{-1/3} < \lambda$ .

Spontaneous emission radiation pattern from uncorrelated scatterers only depend on the relative orientation of  $\hat{\sigma}$  and  $\vec{B}$ , but not on the  $\mathbf{k}$ -vector of the incident light. This also holds for Dicke superradiance in the small cloud limit, but not for large clouds. Here forward scattering dominates.

We have seen in this section that, despite its simplicity, the coupled dipoles model has a large range of applications. It allows for a deeper understanding of known classical phenomena and, as we will study in Excs. 21.2.5.2 to 21.2.5.4 and in forthcoming sections, it allows to unravel new effects.

### 19.1.8 Exercises

#### 19.1.8.1 Ex: Structure factor of a linear array

- Based on the definition (19.1) compute the structure factor of a linear array of point-like scatterers.
- Based on the definition (19.2) compute the structure factor of a linear array of 10 Gaussian density distributions.

#### 19.1.8.2 Ex: Structure factor of a cloud

Based on the definition (19.1) compute the structure factor of (i) a slit, (ii) a pinhole, and (iii) a homogeneous spherical cloud.

#### 19.1.8.3 Ex: Structure factor and Snell's law

Calculate the structure factor for a light beam passing through a plane interface between two dielectrics.

#### 19.1.8.4 Ex: Validity of Markov approximation

- Calculate the single-atom scattering rate for a rubidium cloud of  $N = 10^6$  atoms driven with  $P = 100$  mW laser power focused into a waist of  $w_0 = 100 \mu\text{m}$  and detuned by  $\Delta = (2\pi) 100$  GHz from the  $D_2$ -line at 780 nm [119].
- Assume for the cloud a homogeneous spherical density distribution with radius  $R = 250/k_0$ . Based on Ref. [675] estimate whether the Markov approximation is valid.

#### 19.1.8.5 Ex: Lensing by a dense atomic cloud with the coupled dipoles model

Simulate the pump laser phase shift and lensing by a small dense cloud by the coupled dipoles model for red and blue detuning. Discuss the influence of rescattering by removing artificially the off-diagonal terms from the scattering kernel. Discuss whether lensing is observed within the timed Dicke approximation.

#### 19.1.8.6 Ex: Exact calculation of projected structure factors

Calculate the integrals (19.65), (19.77), and (19.85).

#### 19.1.8.7 Ex: Monte-Carlo simulation of cooperative radiation pressure

In a regime of negligible interatomic interaction single photons are scattered by individual atoms, which thereby receive the entire photonic recoil. That is, the acceleration occurs in quantized steps, which can be easily resolved in experiments [352, 640] with Bose-Einstein condensates. In the absence of collective effects, we generally observe halo-shaped momentum distributions. Because of the recoil received upon absorption, the halos are centered at  $\hbar k$ , and since the emission is generally isotropic, they have a radius of  $\hbar k$ . On the other hand, as we have seen earlier, cooperative effects can suppress radiation pressure. In the following we try a different approach

based on a Monte-Carlo simulation with a Langevin force.

This approach starts from the idea that it is possible to simulate the radiation pressure without explicit calculation of the force by treating the scattering process as a Langevin force. The simulation describes the scattering of single photons by individual atoms. Cooperativity is included 1. in the scattering rate, which is *influenced by collective effects*, 2. by weighing the probability for the direction  $(\theta, \phi)$  into which the photons are scattered with the structure factor. The enhancement of the collective scattering rate corresponds to the rate of absorption part of the radiation pressure, <sup>9,10</sup>

$$\gamma_c = \gamma_R \frac{F_{c,abs}}{F_{1,abs}} = \sigma_{opt}(\Delta_0) \frac{I}{\hbar\omega} \cdot \frac{4\Delta_0^2 + \Gamma^2}{4\Delta_0^2 + N^2\Gamma^2 s_N^2} N,$$

where  $s_N = N^{-1} + (2\sigma)^{-2}$ . The structure factor is numerically calculated for a randomly distributed cloud.

### 19.1.8.8 Ex: Super- and subradiance with two atoms

Super- and subradiance have been observed in two ion crystals [555, 195]. In this exercise, we study this system in the framework of the coupled dipoles model.

- Calculate the structure factor of this system.
- Write down the equations of motion (19.25) and solve them in steady-state.

### 19.1.8.9 Ex: Signatures of subradiance

Super- and subradiance are contained in the coupled dipoles model. Try to identify the presence of subradiant states via a reduced decay rate of  $\beta(t)$  starting from the timed Dicke state.

### 19.1.8.10 Ex: Other applications of the coupled dipoles model

Discuss whether the coupled dipoles model can be extended to provide a microscopic description of gaseous metamaterials (negative refractive index) and the Goos-Hänchen, Imbert-Fedorov, Spin-Hall, and *Ewald-Oseen effects*, and interference with a LO. Is it possible to check Ewald-Oseen's theorem in media with negative refractive index?

## 19.2 Continuous density distributions and Mie scattering

In the last sections we developed the coupled dipoles model describing light scattering from ensembles of individual microscopic particles by a set of equations of motion, in the simplest case, one for every atomic dipole. This limits the number of atoms

<sup>9</sup>Note that in reality the scattering of a photon converts the scattering atom into a coherent superposition of directions into which the atom might have scattered. This is of course not described by the simulation.

<sup>10</sup>Although the atomic motion is frozen, it is not correct to say that the external degree of freedom is not involved in the collective dynamics, since the spatial atomic distribution shapes the structure factor.

that can be considered in numerical simulations to a few 1000. On the other hand, most cold atom experiments nowadays are performed with  $10^5$  to  $10^9$  atoms. The following section is devoted to introducing concepts and approximations allowing us to understand light scattering from large atomic clouds.

The main step will consist in an approximation called smooth or *continuous density approximation*, where the discrete distribution of point-like scatterers is replaced by an inhomogeneous but smooth continuous density distribution characterized by a refraction index field  $n_{rfr}(\mathbf{r})$ . The interaction of this density distribution with light is then treated in the framework of Maxwell's equations, i.e. inhomogeneities are treated as macroscopic boundary conditions to the electromagnetic fields. In the following we will term this regime as *Mie scattering*.

At first sight Rayleigh scattering from point-like particles and Mie scattering from extended objects are quite different phenomena. Rayleigh scattering exhibits resonances due to the internal structure of the particles, e.g. an atom. Mie scattering shows resonances induced by the boundary conditions the scattering objects impose to the field. On the other hand, from a microscopic viewpoint, any extended object (e.g. a dielectric sphere) is nothing but an assembly of microscopic scattering particles. The question we need to study is then whether a description of the diffraction from this object as the sum of the radiation patterns scattered from the individual constituent particles is correct; or in how far the graininess of the cloud's density distribution and cooperative effects arising from the interaction *between* the individual particles play a role [119].

Interesting phenomena are expected in the transition regime between the limits of a dense bunch of individual scatterers and macroscopic dielectric objects. One of them is a strong modification of the radiation pressure force [153], which can conveniently be studied with atomic ensembles. The reason is that, in the smooth density approximation, the cloud can be understood as a macroscopic object characterized by a refraction index, which can be tuned over huge ranges by changing the cloud's density and volume, or by tuning the frequency of the incident light exploiting the existence of atomic resonances. We will see in the following that it is possible to study radiation pressure with cold atoms in the Rayleigh-Debye-Gans limit of small phase-shifts, as well as in the Mie limit of large phase shifts [32]. Despite the absence of sharp boundaries for the atomic cloud, we predict the occurrence of Mie resonances, which could be detected experimentally [33].

### 19.2.1 Continuous density approximation

In light scattering experiments, disorder (or granularity) plays a role when the number of atoms projected onto a cross section perpendicular to the incident beam is small enough so that a light mode focused down to the diffraction limit (that is  $\sim \lambda^2$ ) would be able to resolve and count the atoms. In other words, the stochastic fluctuations induced by the random positions of the atoms can be neglected when the total number of atoms  $N$  is larger than the number of modes  $\sim \sigma^2$  that fit into the cloud's cross section, i.e. when the optical density is  $b_0 = 3N/\sigma^2 \gg 1$ . Under this hypothesis, the differential equation (19.25) for  $\tilde{\beta}_j$  can be simplified by replacing the discrete sum



over atom positions by an integral over a density distribution  $\rho(\mathbf{r})$ ,

$$\left[ \sum_{j=1}^N \rightarrow \int \rho(\mathbf{r}') d^3 r' \quad \text{and} \quad \tilde{\beta}_j(t) \rightarrow \tilde{\beta}(\mathbf{r}', t) \right]. \quad (19.95)$$

For example, the smoothed structure factor reads,

$$S(\mathbf{k}) = \frac{1}{N} \sum_{j=1}^N e^{i(\mathbf{k}-\mathbf{k}_0)\mathbf{r}_j} = \frac{1}{N} \int d^3 r' \rho(\mathbf{r}') e^{i(\mathbf{k}-\mathbf{k}_0)\mathbf{r}'}. \quad (19.96)$$

In the Exc. 19.2.5.1 we calculate the structure factors for a homogeneous spherical cloud of radius  $R$  and for a Gaussian ellipsoidal cloud with the *rms*-width  $\sigma_{\rho,z}$ :

$$S_{\text{homog.sphere}}(\mathbf{k}) = \frac{3}{q^3 R^3} (\sin qR - qR \cos qR) \quad (19.97)$$

$$S_{\text{gauss.ellipse}}(\mathbf{k}) = e^{-\frac{1}{2}k^2 \sigma_\rho^2 \sin^2 \theta - \frac{1}{2} \sigma_z^2 (k \cos \theta - k_0)^2}.$$

The simulated structure factor (red curve in Figs. 19.10) agrees well with the analytical expression (green curve). Since small clouds have a larger fluctuations, the fact that the total force is a sum of intensities rather than amplitudes leads to a finite value at large scattering angles  $\theta$ .

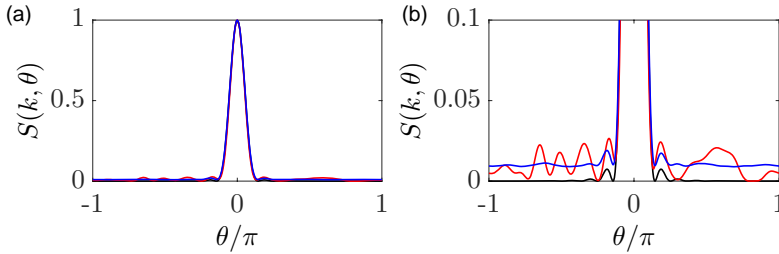


Figure 19.10: (code) (a) The red curve shows a calculation of the structure factor:  $|S(k = k_0, \theta, \phi = 0)|^2$  for 200 atoms randomly distributed in a homogeneous spherical cloud of size  $R = 10/k_0$ . The blue curve shows an average over 500 realizations of such a cloud according to  $\sum_{m=1}^{200} |S(k, \theta, \phi = 0)|^2$ . The black curve is an analytical calculation according to Eq. (19.97) [675]. (b) Same curves as in (a) but with a stretched *y*-axis.

In the continuous limit defined by (19.95) for the equations of motion (19.31)<sup>11</sup>,

$$\dot{\tilde{\beta}}(\mathbf{r}, t) = i \left( \Delta_0 + i \frac{\Gamma}{2} \right) \tilde{\beta}(\mathbf{r}, t) - \frac{i}{2} \Omega_0 - \frac{\Gamma}{2} \int d^3 r' \rho(\mathbf{r}') \frac{\sin(k_0 |\mathbf{r} - \mathbf{r}'|)}{k_0 |\mathbf{r} - \mathbf{r}'|} \tilde{\beta}(\mathbf{r}', t) e^{-i\mathbf{k}_0 \cdot (\mathbf{r} - \mathbf{r}')}. \quad (19.98)$$

Transforming back to  $\beta_j \equiv \tilde{\beta} e^{i\mathbf{k}_0 \cdot \mathbf{r}}$ , we obtain the fundamental equation for the dipolar excitation field,

$$\left[ \dot{\beta}(\mathbf{r}, t) = i \left( \Delta_0 + i \frac{\Gamma}{2} \right) \beta(\mathbf{r}, t) - \frac{i \Omega_0}{2} e^{i\mathbf{k}_0 \cdot \mathbf{r}} - \frac{\Gamma}{2} \int d^3 r' \rho(\mathbf{r}') \frac{\sin(k_0 |\mathbf{r} - \mathbf{r}'|)}{k_0 |\mathbf{r} - \mathbf{r}'|} \beta(\mathbf{r}', t) \right]. \quad (19.99)$$

<sup>11</sup>Note that the 'timed Dicke' assumption (19.63) has not been used here.

**Example 83 (Connection between coupled dipoles model and Helmholtz equation):** The steady-state solution of (19.99) can also be obtained from the *Helmholtz equation* of Maxwell's theory [243, 32, 33], as shown in <sup>12</sup>,

$$\boxed{[\nabla^2 + k_0^2 n_{rfr}^2(\mathbf{r})]\beta(\mathbf{r}) = 0 \quad \text{defining} \quad n_{rfr}^2(\mathbf{r}) \equiv 1 - \frac{4\pi\rho(\mathbf{r})}{k_0^3(2\Delta_0/\Gamma + \iota)}}. \quad (19.100)$$

## 19.2.2 Simulations of the time evolution

We start from the second equation (19.18),

$$\begin{aligned} \dot{\tilde{\beta}}_j(t) &= \iota\Delta_0\tilde{\beta}_j(t) - \frac{\Omega_0^2}{4} \sum_{m=1}^N \int_0^t \tilde{\beta}_m(t') dt' \\ &\quad - \sum_{\mathbf{k}} g_k^2 \sum_{m=1}^N e^{\iota(\mathbf{k}-\mathbf{k}_0)(\mathbf{r}_j-\mathbf{r}_m)} \int_0^t e^{-\iota(\omega_k-\omega_0)(t-t')} \tilde{\beta}_m(t') dt'. \end{aligned} \quad (19.101)$$

Substituting the timed Dicke state (19.63),

$$\begin{aligned} \dot{\beta}(t) &= \frac{1}{N} \sum_{j=1}^N \dot{\beta}_j(t) = \frac{1}{\sqrt{N}} \sum_{j=1}^N \dot{\tilde{\beta}}_j(t) \\ &= \iota\Delta_0\beta(t) - \frac{N\Omega_0^2}{4} \int_0^t \beta(t') dt' - \frac{V_{ph}}{(2\pi)^3} \int d^3k g_k^2 N^2 |S(\mathbf{k})|^2 \int_0^t e^{-\iota(\omega_k-\omega_0)(t-t')} \frac{\tilde{\beta}_m(t')}{\sqrt{N}} dt', \end{aligned} \quad (19.102)$$

where we used  $\sum_{m=1}^N e^{\iota(\mathbf{k}-\mathbf{k}_0)(\mathbf{r}_j-\mathbf{r}_m)} = N^2 |S(\mathbf{k})|^2$  from Eq. (19.66). Finally, at resonance and low saturation we may neglect the first two terms,

$$\begin{aligned} \dot{\beta}(t) &= -N \frac{V_{ph}}{(2\pi)^3} \int_{\mathbb{R}} d^3k \int_0^t dt' g_k^2 \beta(t') e^{\iota(\nu_k-\omega)(t-t')} |S(\mathbf{k})|^2 \\ &= -N \frac{V_{ph}}{(2\pi)^3} \int_0^t dt' \beta(t') \int_0^\infty \int_0^\pi g_k^2 e^{\iota(\nu_k-\omega)(t-t')} |S(k, \theta)|^2 2\pi k^2 \sin\theta d\theta dk \\ &= -N \frac{V_{ph}}{(2\pi)^3} g_k^2 \int_0^t dt' \beta(t') \int_0^\infty e^{\iota(\nu_k-\omega)(t-t')} k^2 I(k) dk = -\Omega_N^2 \int_0^t dt' \beta(t') G(t-t'), \end{aligned} \quad (19.103)$$

with the collective Rabi frequency  $\Omega_N = \sqrt{N}g_k$  and the surface integrated structure factor,

$$I(k) = \int_0^{2\pi} \int_0^\pi |S(k, \theta, \phi)|^2 \sin\theta d\theta d\phi, \quad (19.104)$$

and

$$G(\tau) = \frac{V_{ph}}{(2\pi)^3} e^{-\iota\omega\tau} \int_0^\infty e^{\iota ck\tau} k^2 I(k) dk, \quad (19.105)$$

<sup>12</sup>See script on *Electrodynamics* (2020)Sec. 21.3.2.

with  $\omega = ck_0$  and  $\nu_k = ck$ . The integral  $I(k)$  has been solved by Nicola for an ellipsoidal Gaussian density distribution. It is quite close to,

$$I(k) \simeq I(k_0) \simeq \sqrt{\frac{\pi}{2}} \frac{1}{k\sigma_z} e^{F^2/2} [1 - \operatorname{erf}(F/\sqrt{2})], \quad (19.106)$$

with the Fresnel number  $F = k\sigma_r^2/\sigma_z$ .

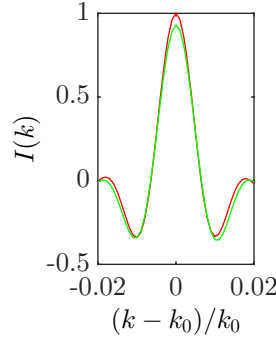


Figure 19.11: (code) Averaging of the structure factor over the whole  $k$ -space.

### 19.2.2.1 Analytical method

To evaluate the above integro-differential equation, we use the rule for differentiating integrals with variable boundaries,

$$\frac{\partial}{\partial t} \int_{\phi(t)}^{\psi(t)} f(x, t) dx = \int_{\phi(t)}^{\psi(t)} \frac{\partial f(x, t)}{\partial t} dx + f(\psi(t), t) \psi'(t) - f(\phi(t), t) \phi'(t), \quad (19.107)$$

it is easy to show,

$$\frac{\partial}{\partial t} \int_0^t f(t') G(t - t') dt' = f(t) G(0) + \int_0^t f(t') \dot{G}(t - t') dt' \quad (19.108)$$

and to thusly evaluate the integral until  $\frac{\partial^n}{\partial t^n} G(t - t')$  gets smooth enough to be neglected.

### 19.2.2.2 Numerical method

We can directly solve the integro-differential equation numerically using,

$$G(\tau) = \left[ 1 + \frac{3c}{4R} \tau - \frac{c^3}{16R^3} \tau^3 \right] \Theta(3R - c\tau), \quad (19.109)$$

for a homogeneous spherical cloud and,

$$G(\tau) = \frac{k\sigma_r^2}{k\sigma_r^2 + ic\tau} e^{-(c\tau/\sigma_z)^2/2}, \quad (19.110)$$

for an ellipsoidal Gaussian cloud. The iteration is done via,

$$\beta(t + dt) = \beta(t) - dt \Omega_N^2 \int_0^t \beta(t') G(t - t') dt' . \quad (19.111)$$

The discretization is done via,

$$\begin{aligned} t_{m+1} &= t_m + dt \\ \beta_{m+1} &= \beta_m - dt N g_k^2 \sum_{m'=1}^m \beta_{m'} G(t_m - t_{m'}) dt . \end{aligned} \quad (19.112)$$

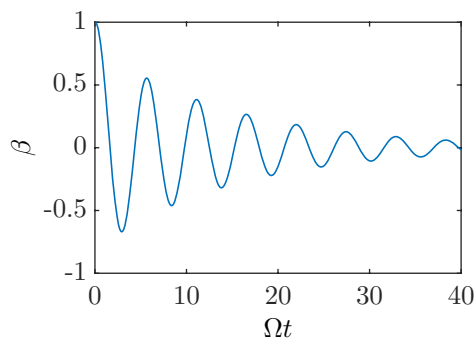


Figure 19.12: (code) Calculation of the time evolution of  $\beta$  for a homogeneous spherical cloud. The parameters are  $\lambda \simeq 780$  nm and  $c/\Omega \simeq 30$  cm with  $\Omega = \sqrt{N}g_k$  for typically  $g_k \simeq 1$  MHz and  $N \simeq 10^6$ .

With the solution of the integro-differential equation  $\beta(t)$ , we can calculate the probability that atoms are excited [675]<sup>13</sup>,

$$P(t) = |\beta(t)|^2 = \sum_j |\beta_j(t)|^2 = \int d^3r |\beta(t, \mathbf{r})|^2 . \quad (19.113)$$

**Example 84 (Solutions for a homogeneous spherical cloud):** For a homogeneous spherical cloud, we find three regimes characterized by the size of the cloud compared to the two length scales  $\lambda$  and  $c/\Omega$ :

$$\beta(t) = \beta(0) \begin{cases} e^{-N\Gamma t} & \text{for } R < \lambda \ll c/\Omega \\ e^{-27N\Gamma t/8(k_0 R)^2} & \text{for } \lambda < R \ll c/\Omega . \\ \cos \Omega t e^{-3ct/8R} & \text{for } \lambda \ll c/\Omega < R \end{cases}$$

<sup>13</sup>Compare to Jaynes-Cummings model in a CQED environment: A single photon is coherently exchanged between the cavity and the atomic excitation, we get Rabi oscillations. Here, the atomic cloud is the cavity.

We know that the Mollow triplet in the dressed states picture gives rise to an oscillating decay curve resembling that of Fig. 19.12. Does this curve also have an interpretation in terms of collective dressed states?

### 19.2.2.3 Complete numerical simulation

In order to be independent from initial conditions, we generate a random distribution  $\mathbf{r}_{j'}$  and solve the differential equation,

$$\dot{\beta}_j(t) = -Ng_k^2 \int_0^t dt' \frac{V_{ph}}{(2\pi)^3} \int d^3k \frac{1}{N} \sum_{j'=1}^N \beta_{j'}(t') e^{i(\nu_k - \omega)(t-t') + i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_{j'})} . \quad (19.114)$$

We propagate the amplitudes in time via,

$$\beta_j(t+dt) = \beta_j(t) - dt g_k^2 \frac{V_{ph}}{(2\pi)^3} \int_0^t dt' \sum_{j'=1}^N \beta_{j'}(t') \int_0^\infty k^2 e^{i(ck - \omega)(t-t')} I_{jj'}(k) dk , \quad (19.115)$$

where  $I_{jj'}(k) \equiv \int_0^\pi \int_0^{2\pi} e^{ik[(x_j - x_{j'}) \sin \theta \cos \phi + (y_j - y_{j'}) \sin \theta \sin \phi + (z_j - z_{j'}) \cos \theta]} \sin \theta d\theta d\phi$ , and discretize via,

$$t_{m+1} = t_m + dt \quad (19.116)$$

$$\beta_j(t_{m+1}) = \beta_j(t_m) - dt^2 g_k^2 \sum_{m'=1}^m \sum_{j'=1}^N \beta_{j'}(t_{m'}) G_{jj'}(t_m - t_{m'}) ,$$

with  $G_{jj'}(t_m - t_{m'}) = \frac{V_{ph}}{(2\pi)^3} \int_0^\infty k^2 e^{i(ck - \omega)(t_m - t_{m'})} I_{jj'}(k) dk$ .

### 19.2.3 Radiation pressure force in macro- and microscopic scattering

As mentioned at the beginning of this section, scattering of light by an extended object such as an atomic ensemble or a dielectric sphere is fundamentally different from scattering at a point-like scatterer such as a single atom. On one hand, the finite size of the object leads to Mie scattering. On the other hand, the spatial distribution of the scatterers rules the degree of cooperativity. Homogeneous and periodic distributions tend to scatter cooperatively, whereas disorder suppresses cooperativity. In an atomic cloud, the amount of disorder can be tuned via the optical density seen by the incident light, and its role can be studied via the radiation pressure exerted by the light on the atomic cloud. We present an analytic expression for the radiation pressure valid for any numbers of atoms and arbitrary density distributions, which interpolates between the regimes of dominating disorder and dominating cooperativity. Furthermore, we present first experimental signatures of radiation pressure reduction due to cooperative scattering.

The radiation pressure exerted by a plane wave laser beam with frequency  $\omega_0$  and wave vector  $\mathbf{k}_0 = k_0 \hat{\mathbf{e}}_z$  on a single two-level atom with resonance frequency  $\omega_a = \omega_0 - \Delta_0$  is correctly described by the standard formula (19.79). Generalization to scattering by atomic ensembles and extended objects is only possible, if a number of effects is explicitly taken into account. The most important ones are named in the following.

- Cooperativity* and
- disorder*: Cooperativity is the tendency of atoms located in the same area of space, forming regular structures or being forced by the mode structure of the environment (e.g. optical cavities) to scatter light synchronously into the same

direction, as in the case of Dicke superradiance. While homogeneously or periodically distributed atoms concentrate the scattered light in specific solid angles by forward or Bragg scattering, randomly distributed atoms do not cooperate and scatter light isotropically. In this respect, cooperativity and disorder are antagonists. *c. Mie scattering and refraction:* The finite volume and the shape of the cloud represent an inhomogeneity at which light is scattered in a global way. As long as the optical density is low, the pump mode depletion is mainly due to the fact, that the atomic cloud distorts the phase front of the incident light. For high optical density, scattering is predominantly absorptive. *d. Multiple scattering* and *e. resonance fluorescence:* Near resonance, multiple scattering leads to radiation trapping. Even off-resonance, inelastic scattering pumps resonant photons into the atomic cloud, which have a high probability to be reabsorbed. Taking account of all these effects, the real radiation pressure can differ by orders of magnitude from the naive prediction of the above formula.

For smooth density distributions  $F_c$  is only limited by Mie scattering at the inhomogeneity represented by the *finite extend* of the atomic cloud [153]. The radiation pressure depends on the number of atoms  $N$  in the volume, and the scaling  $F_c(N)$  depends on the pump laser detuning and the radial cross section of the cloud. But small scale inhomogeneity *within the cloud*, i.e. disorder, can play an eminent role for collective scattering. This is the case, when the number of atoms is beyond a critical value, which mainly depends on the volume and shape of the cloud. In the following we will derive an analytic expression for the radiation pressure as a function of atom number, which interpolates between the regimes of dominating disorder (single-atom Rayleigh scattering) and dominating cooperativity (pure Mie scattering).

On the other hand, we point out, that we do not consider multiple scattering in our treatment. This is a good assumption far from resonance, where the scattering is predominantly Rayleigh scattering and inelastic scattering can safely be disregarded. In contrast, our extensions of single to multi-atom scattering are not valid near resonance.

The radiation pressure provides sensitive signatures for the impact of cooperativity and disorder. We describe an experiment measuring the displacement of cold atoms confined in a far-off resonance dipole trap and interpret our observations in terms of collective scattering.

### 19.2.3.1 Radiation pressure for timed Dicke states

As a first approach we will calculate the radiation pressure for a timed Dicke state from Eq. (19.88) by explicit analytical integration of the surface-integrated structure factors  $s_\infty$  and  $f_\infty$  in the smooth density limit (19.95) for an ellipsoidal Gaussian smooth density distribution, as shown in Exc. 19.2.5.2. In the spherical case,

$$\rho(\mathbf{r}) = \rho_0 e^{-r^2/2\bar{r}^2} \quad \text{with} \quad \rho_0 = \frac{N}{(2\pi)^{3/2}\bar{r}^3}, \quad (19.117)$$

and introducing  $\sigma \equiv k\bar{r}$ , we get,

$$\begin{aligned} s_\infty &= \frac{1 - e^{-4\sigma^2}}{4\sigma^2} \xrightarrow{\sigma \gg 1} \frac{1}{4\sigma^2} \\ f_\infty &= \frac{1}{4\sigma^2} \left[ 1 - \frac{1}{2\sigma^2} + \left( 1 + \frac{1}{2\sigma^2} \right) e^{-4\sigma^2} \right] \xrightarrow{\sigma \gg 1} s_\infty - 2s_\infty^2 . \end{aligned} \quad (19.118)$$

Hence,

$$\boxed{\frac{F_{za} + F_{ze}}{F_{z1}} = \frac{(2\Delta_0/\Gamma)^2 + 1}{(2\Delta_0/\Gamma)^2 + N^2 s_\infty^2} N(s_\infty - f_\infty)} . \quad (19.119)$$

Note that the radiation pressure calculated from Eq. (19.119) also holds for elongated ellipsoidal Gaussian clouds characterized by an aspect ratio  $\eta > 1$ , even though the expressions for the surface-integrated structure factors become more complicated.

It is revealing to compare the smooth density expressions (19.119) with numerical simulations based on randomly generated atomic distributions from which the structure factor is directly from the sum (19.67). Interestingly, we find in certain parameter regimes (in particular at low atom numbers) considerable deviations between  $s_N, f_N$  and  $s_\infty, f_\infty$  and consequently between the numerical simulations and the analytic calculations of the radiation pressure. We attribute these deviations to disorder in the atomic cloud, which is not seen in the smooth density limit, but naturally incorporated in the numerical approach.

By comparison to numerical simulations [black solid lines and blue circles in Figs. 19.13(a)] we found that the surface-integrated structure factors in the presence of disorder are well described by [70],

$$s_N = \frac{1}{N} + s_\infty \quad \text{and} \quad f_N = f_\infty . \quad (19.120)$$

### 19.2.3.2 Cooperativity versus disorder

We expect disorder to play a dominant role, when the coarse graininess, which is related to the average distance between two atoms,  $|\mathbf{r}_i - \mathbf{r}_j|$ , can be resolved by the incident light. For the *absorption process*, this means that disorder gets important, when the number of spatial modes supported by the pump laser in a radial cross section of the atomic cloud,

$$N_{ca} = s_\infty^{-1} \simeq 4\sigma^2 , \quad (19.121)$$

(for voluminous clouds) surpasses the number of atoms,  $N < N_{ca}$ . This is just the case, when the mean resonant optical density (for a ray passing through the center of the cloud  $x = y = 0$ ) is larger than 1,

$$b_0 = \int_{-\infty}^{\infty} dz \rho(z) \sigma_{opt} = \frac{3N}{\sigma^2} = \frac{12N}{N_{ca}} > 1 , \quad (19.122)$$

where  $\sigma_{opt} = \frac{3\lambda^2}{2\pi}$  is the resonant optical cross section and  $\rho(\mathbf{r})$  the spherical Gaussian density distribution (19.117). For the *scattering process*, the number of modes available for the reemitted light also counts. Hence, the critical number of atoms that can be resolved by light scattering is larger than  $N_{ca}$ :

$$N_{ce} = (s_\infty - f_\infty)^{-1} \simeq \frac{1}{2}(2\sigma)^4 = \frac{1}{2}N_{ca} \cdot \sigma^2 . \quad (19.123)$$

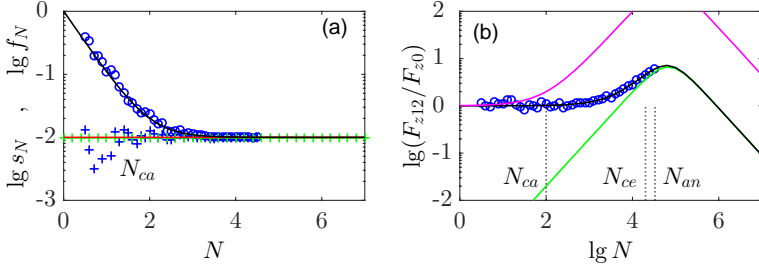


Figure 19.13: (code) (a) Numerical evaluation of  $s_N$  (blue circles) and  $f_N$  (blue crosses) [119]. Analytical calculation of  $s_N$  (black solid line) according to Eq. (19.120). Smooth density limit of  $s_\infty$  (red solid line) and  $f_\infty$  (green crosses). The cloud is assumed spherical,  $\eta = 1$ , and Gaussian with size  $\sigma = 5$ . (b) Numerical evaluation (blue circles) of the corresponding force ratio as a function of atom number  $N$  for  $\Delta_0 = (2\pi) 2$  GHz and small collective saturation,  $\sqrt{N}\Omega_0 \ll \Delta_0$ . Analytical calculation in the smooth density limit (green solid line) and according to Eq. (19.125) (black solid line). The magenta line traces the radiation pressure force resulting from pump photon absorption only.

In order to simplify the discussion, we neglect saturation,  $\Omega_0 \rightarrow 0$ . Using  $\Delta_0 \gg \Gamma$  and defining a third characteristic atom number,

$$N_{cr} = \frac{2\Delta_0}{\Gamma s_\infty}, \quad (19.124)$$

Eq. (19.119) can be written,

$$\frac{F_c}{F_1} \simeq \frac{1 + N/N_{ce}}{1 + (N/N_{cr})^2}. \quad (19.125)$$

In the limit of very large detunings,  $\Delta_0/\Gamma \gg \sigma^2 \gg 1$ , the three introduced characteristic atom numbers introduced in Eqs. (19.121), (19.123) and (19.124) satisfy  $N_{ca} < N_{ce} < N_{cr}$ , and we obtain the  $N$ -dependence of the radiation pressure depicted in Fig. 19.13.

In the regime  $N < N_{ca}$ , radiation pressure is dominated by the absorption process,  $s_N \gg f_N$ , because the emission is isotropic. The absorption radiation pressure exerted on a hypothetical smooth density distribution occupying the same volume as the atomic cloud [green line in Fig. 19.13] is dramatically reduced with respect to the single-atom radiation pressure (cyan dash-dotted line). However, disorder suppresses cooperativity and increases the radiation pressure up to the single-atom value. The novelty as compared to Ref. [623] is the fact that cooperativity and disorder not only influence the collective emission of a photon by an atomic cloud, but also the collective *absorption* of a photon from a pump laser beam.

Neglecting the photon reemission at higher atom numbers would result in an increase of radiation pressure in the regime  $N_{ca} < N < N_{ce}$  (magenta line). However, in this regime, the emission process becomes increasingly important,  $s_N \simeq f_N$ , because the emission changes its radiation pattern from isotropic to forward scattering.



Consequently, the radiation pressure is reduced with respect to its purely absorptive component. This regime is still ruled by disorder, so that the critical atom number for the impact of disorder on the absorption process,  $N_{ca}$ , has no impact. It does not even show up in the formula (19.125).

In the regime  $N_{ce} < N < N_{cr}$ , disorder steps back and cooperativity wins, so that the radiation pressure approaches the smooth density limit. Since in this regime, the smooth density radiation pressure depends on atom number like  $\propto N$ , as already shown in Ref. [153], we observe an increase of the radiation pressure beyond the single-atom value. This is only possible, because the collective enhancement of absorption (magenta line) rises as fast with  $N$ , as the collective enhancement of emission.

For even higher atom numbers,  $N_{cr} < N$ , the radiation pressure dramatically alters its  $N$ -dependency from  $\propto N$  to  $\propto N^{-1}$ . This change of behavior is *not* caused by the interplay of cooperativity and disorder, but can be understood within the framework of Mie scattering, as discussed in the next section.

### 19.2.3.3 Rayleigh-Debye-Gans versus Mie scattering

Radiation pressure is observed in many experiments, as it is the basis for optical cooling techniques (like magneto-optical traps) and limits the efficiency of resonant absorption imaging of cold atoms, because their acceleration leads to considerable Doppler-shifts. However, as stated before, the impact of disorder on radiation pressure can only be seen for large optical densities,  $b \gg 1$ , which may partially explain, why this effect has not been observed until two experiments explicitly searched for it [70, 59] (see Fig. 19.14).

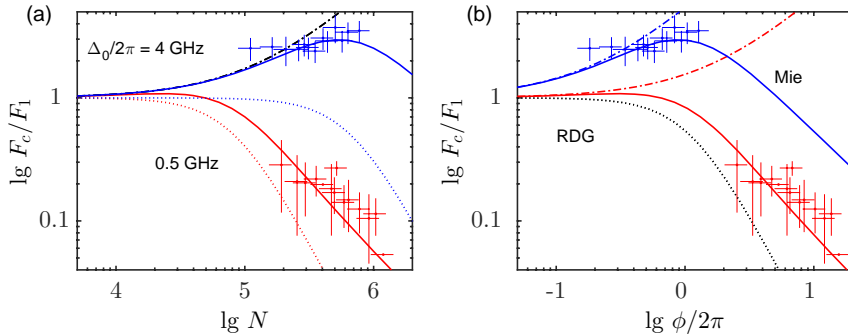


Figure 19.14: (code) (a) Double-logarithmic plot of the measured (symbols) and calculated (lines)  $N$  dependence of the radiation pressure force. The red symbols and lines correspond to the detuning  $\Delta_0 = (2\pi) 0.5$  GHz and the intensity  $I_0 = 95$  mW/cm<sup>2</sup>. For the blue symbols and lines,  $\Delta_0 = (2\pi)4$  GHz and  $I_0 = 730$  mW/cm<sup>2</sup>. The red (bottom) and blue (top) solid lines show calculations based on the full expression (19.119) without adjustable parameters. The red (bottom) and blue (top) dotted lines represent just the fraction of expression (19.119). The dash-dotted lines representing just the parentheses coincide for both values of  $\Delta_0$ . (b) Same data as (a), but plotted as a function of the push beam phase shift  $\varphi$ . In this diagram the dotted lines representing the fraction coincide for both values of  $\Delta_0$  [59].

Depending on the parameter regime chosen, the measurements exhibited in Fig. 19.14 present data for reduced or enhanced radiation pressure for larger  $N$ . As explained above, the reduction is understood as microscopic Rayleigh scattering at disordered atoms together with superradiant acceleration of the decay, while the enhancement is observed when the bulk cloud becomes so small and dense that it turns into an inhomogeneous dielectric sphere refracting and lensing incident light by macroscopic Mie scattering.

The question then remains why the radiation pressure, with increasing  $N$ , after an initial rise the drops again. To answer this question we must have a look at the phase shift induced in the pump light by the cloud's refraction index.. From calculations done in Secs. 1.2.7 and 24.6.1 we know that (below saturation) the optical density  $b$  and the phase shift  $\varphi$  are linked to the refraction index  $n_{rfr}$  and the optical scattering cross section  $\sigma_{opt}$  via,

$$\frac{ib}{2} + \varphi = \frac{\omega}{c} \int_{-\infty}^{\infty} [n_{rfr}(\mathbf{r}) - 1] dz = \left( \iota - \frac{2\Delta_0}{\Gamma} \right) \sigma_{opt}(\Delta_0) \int_{-\infty}^{\infty} \rho(\mathbf{r}) dz \quad (19.126)$$

where  $\sigma_{opt}(\Delta_0) = \frac{2\pi}{k^2} \frac{\Gamma^2}{4\Delta_0^2 + \Gamma^2}$  and  $n_{rfr}(\mathbf{r}) - 1 = -\frac{4\pi\rho(\mathbf{r})}{k_0^3(2\Delta_0/\Gamma + \iota)}$ ,

such that,

$$b = -\sigma_{opt}(\Delta_0) \int_{-\infty}^{\infty} \rho(\mathbf{r}) dz = b_0 \frac{\Gamma^2}{4\Delta_0^2 + \Gamma^2} \quad \text{and} \quad \varphi = \frac{2\Delta_0}{\Gamma} b . \quad (19.127)$$

Estimating coarsely  $k \int_{-\infty}^{\infty} [n_{rfr}(\mathbf{r}) - 1] dz \simeq \sigma [n_{rfr}(\mathbf{r}) - 1]$ , where  $\sigma \equiv k\bar{r}$ , we may simplify,

$$\frac{ib}{2} + \varphi = \sigma [n_{rfr}(\mathbf{r}) - 1] . \quad (19.128)$$

At high atom numbers (i.e. in the smooth density limit), the dependency of the radiation pressure on atom number (19.125) exhibits a maximum at  $N_{cr}$ . For an atomic cloud with density  $n$  and the resonant optical density  $b_0$ , the characteristic atom number can be expressed in terms of the phase shift  $\varphi$  experienced by the pump laser beam on its path across the cloud. Absorption losses for the pump beam (e.g. resonance fluorescence, whose differential cross section contributes  $\sigma_{opt}$  to the total scattering cross section [440]) is completely negligible at large detunings. Only elastic Rayleigh scattering occurs, which in the smooth density limit of Mie scattering becomes pure *diffraction* (real part of the refraction index). We can then understand the atomic cloud as a non-absorbing dielectric sphere with a Gaussian index of refraction.

Rewriting Eq. (19.125) in terms of the refraction index,

$$\frac{F_c}{F_1} \simeq \frac{N}{1 + (2\varphi)^2} \frac{2}{(2\sigma)^4} , \quad (19.129)$$

we see that, as long as  $\varphi < \frac{1}{2}$ , the force increases linearly like  $\propto N$ . The proportionality comes from the perfect (in the sense of not spoiled by disorder) cooperative enhancement of the scattering rate in the smooth density limit. The enhancement is only limited by the finite size  $\sigma$  of the cloud, which is accounted for in the second

fraction. This regime, characterized by <sup>14</sup>,

$$\sigma[n_{r,fr}(\mathbf{r}) - 1] \ll 1 \quad (19.130)$$

is termed the *Rayleigh-Debye-Gans regime*.

For larger phase shifts,  $\varphi > \frac{1}{2}$ , refraction more and more distorts the wavefront of the pump beam, which spoils the pump mode depletion and hence reduces radiation pressure. Consequently, the radiation pressure decreases again like  $N^{-1}$ . This is the *Mie regime* of scattering. The maximum is thus a pure diffraction effect, a so-called Mie resonance. It corresponds to the  $n_{r,fr}$ , where the Rayleigh-Debye-Gans scattering approximation loses its validity according to (19.130). In Excs. 19.2.5.3 and 19.2.5.4 we study Mie and Rayleigh-Debye-Gans scattering, and in 19.2.5.5 we discuss the question is whether recoil is imparted to individual atoms or to the center-of-mass of the whole cloud.

In the limit of the approximations made, our formula correctly describes the radiation pressure force on extended objects. These objects can either be ensembles of scatterers like homogeneous, ordered or disordered atomic clouds of arbitrary shapes and volumes, or macroscopic objects like dielectric spheres. The formula thus represents a bridge between microscopic Rayleigh scattering and macroscopic Mie scattering. At very low atom numbers, the atomic cloud basically represents a randomly distributed bunch of scatterers, whose intrinsic disorder spoils cooperativity. The radiation pressure is then well described by the single-atom value. At large atom numbers, the atomic cloud forms a smooth density distribution characterized by an almost perfect a cooperativity, which is only limited by Mie scattering.

#### 19.2.3.4 Light scattering in the continuous density approximation

The scalar electric field scattered by an arbitrary distribution of atoms has been calculated in (19.48). In the continuous density approximation (19.95), we get,

$$\vec{\mathcal{E}}_{sct}(\mathbf{r}) = -\frac{i\hbar\Gamma}{2d} \sum_{j=1}^N \frac{e^{ik_0|\mathbf{r}-\mathbf{r}_j|}}{ik_0|\mathbf{r}-\mathbf{r}_j|} \beta_j(\infty) \rightarrow -\frac{i\hbar\Gamma}{2d} \int d^3r' \rho(\mathbf{r}') \frac{e^{ik_0|\mathbf{r}-\mathbf{r}'|}}{ik_0|\mathbf{r}-\mathbf{r}'|} \beta(\mathbf{r}', \infty). \quad (19.131)$$

In particular, for a timed Dicke state,

$$\begin{aligned} \vec{\mathcal{E}}_{sct}(\mathbf{r}) &= -\frac{i\hbar\Gamma}{2d} \frac{\sqrt{N}\Omega_0}{2\Delta_0 + i\Gamma N s_N} \sum_{j=1}^N \frac{e^{ik_0|\mathbf{r}-\mathbf{r}_j|}}{ik_0|\mathbf{r}-\mathbf{r}_j|} \\ &\rightarrow -\frac{i\hbar\Gamma}{2d} \frac{\sqrt{N}\Omega_0}{2\Delta_0 + i\Gamma(1 + N s_\infty)} \int d^3r' \rho(\mathbf{r}') \frac{e^{ik_0|\mathbf{r}-\mathbf{r}'|}}{ik_0|\mathbf{r}-\mathbf{r}'|}. \end{aligned} \quad (19.132)$$

#### 19.2.4 Spherical harmonics expansion and generalized timed Dicke state

The results derived in (19.119) assumed the cloud to be in a timed Dicke state. As we have seen in Exc. 19.1.8.5, timed Dicke states do not account for pump laser phase

<sup>14</sup>Note the necessity of another condition  $[n_{r,fr}(\mathbf{r}) - 1] \ll 1$  termed Born approximation, which demands that the incident wave be not appreciably reflected.

shifts induced by the cloud's refraction index. The timed Dicke states might work well for homogeneous cylinders, but not for ellipsoidal clouds, which we assume in our analytical treatments. Therefore, a better approach consists in expanding the cloud into spherical harmonics. Under the assumption that the cloud is radially symmetric,  $\rho(\mathbf{r}) = \rho(r)$ , we get [243],

$$\beta(r, \theta, t) = \sum_{n=0}^{\infty} \sqrt{\frac{2n+1}{4\pi}} \alpha_n(t) j_n(k_0 r) P_n(\cos \theta) e^{-i k_0 r \cos \theta}, \quad (19.133)$$

where the coefficients  $\alpha_n$  are the solutions of,

$$\dot{\alpha}_n = \left[ i\Delta_0 - \frac{\Gamma}{2}(1 + \lambda_n) \right] [\alpha_n - \alpha_n(\infty)], \quad (19.134)$$

In steady state,

$$\alpha_n(\infty) = \frac{2i^n \sqrt{\pi(2n+1)} \Omega_0}{2\Delta_0 + i\Gamma(1 + \lambda_n)}, \quad (19.135)$$

where,

$$\lambda_n \equiv 4\pi \int_0^{\infty} dr \rho(r) j_n^2(k_0 r) \quad (19.136)$$

is the decay rate of eigenmode  $n$ .

Inserting this into the steady-state solution (19.99) and integrating over the volume,

$$\langle \beta_{\infty} \rangle \equiv \frac{2\pi}{N} \int_0^{2\pi} d\theta \sin \theta \int_0^{\infty} dr^2 \rho(r) \beta(r, \theta) = \frac{\Omega_0}{N} \sum_{n=0}^{\infty} \frac{(2n+1)\lambda_n}{2\Delta_0 + i\Gamma(1 + \lambda_n)} \quad (19.137)$$

$$\langle |\beta_{\infty}|^2 \rangle \equiv \frac{2\pi}{N} \int_0^{2\pi} d\theta \sin \theta \int_0^{\infty} dr^2 \rho(r) |\beta(r, \theta)|^2 = \frac{\Omega_0^2}{N} \sum_{n=0}^{\infty} \frac{(2n+1)\lambda_n}{4\Delta_0^2 + \Gamma^2(1 + \lambda_n)^2}.$$

**Example 85 (Spherical harmonics expansion for a Gaussian density distribution):** The density distribution determines the coefficients  $\lambda_n$ . For a Gaussian distribution  $n(r) = N/[(2\pi)^{3/2} \sigma_R^3] e^{-r^2/2\sigma_R^2}$  using the sine kernel,

$$\lambda_n = N \sqrt{\frac{\pi}{2}} \frac{e^{-\sigma^2}}{\sigma} I_{n+1/2}(\sigma^2).$$

For a homogeneous sphere,  $n(r) = n_0$ , of radius  $\sigma = k_0 R$ , using the sine kernel [[674], Eq. (18)],

$$\lambda_n = \frac{3N}{2} [j_n^2(\sigma) - j_{n-1}(\sigma)j_{n+1}(\sigma)].$$

#### 19.2.4.1 Expansion of the radiation pressure forces

This allows us to calculate the forces,

$$F_a = -\hbar k_0 \Omega_0 \Gamma \text{Im} \langle \beta_{\infty} \rangle \quad (19.138)$$

$$F_e = -\hbar k_0 \Omega_0^2 \Gamma \sum_{n=0}^{\infty} \frac{2(n+1)\lambda_n \lambda_{n+1} [4\Delta_0^2 + \Gamma^2(1 + \lambda_n)(1 + \lambda_{n+1})]}{[4\Delta_0^2 + \Gamma^2(1 + \lambda_n)(1 + \lambda_{n+1})]^2 + 4\Delta_0^2 \Gamma^2 (\lambda_{n+1} - \lambda_n)^2}.$$

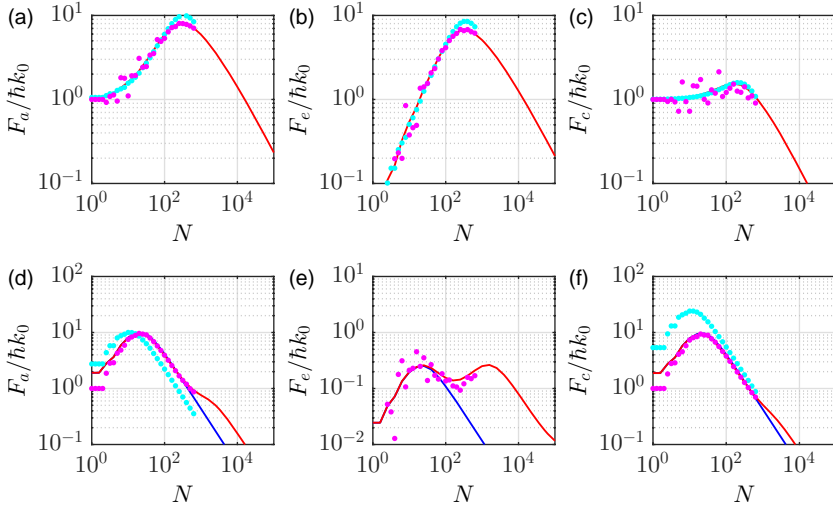


Figure 19.15: (code) (a) Absorption, (b) emission, and (c) total force for a Gaussian cloud with the following parameters:  $\sigma = 2$ ,  $\Delta_0 = 10\Gamma$ ,  $\Omega_0 = 0.001\Gamma$ , and  $\eta = 1$ . The magenta dots show a fully numerical calculation for a randomly generated cloud according to formula (19.62). The red lines show a calculation according to the complete formula (19.138). The cyan dots show a calculation assuming timed Dicke states according to (19.81) via numerical calculation of the structure factor according to (19.82) for the same randomly generated cloud as for the full simulation. The blue lines are obtained within the timed Dicke state approximation with structure factors estimated from formula (19.119). (d-f) Same as (a-c) but with  $\sigma = 0.2$ .

As seen in Fig. 19.15, the results obtained via the complete analytical formula (19.138) coincide with the fully numerical simulations according to formula (19.62). But both disagree with analytical and numerical results obtained within the timed Dicke state approximation.

It is possible to approximate the Bessel function  $I_{n+1/2}(\sigma^2)$  and to obtain analytical solutions. The new formula works for  $\sigma \gg 1$  and  $\eta = 1$  [243],

$$F_a = \frac{\Omega_0^2 \sigma^2}{\Gamma N} \ln \left( 1 + \frac{N^2 \Gamma^2 s_N}{\sigma^2 (4\Delta_0^2 + \Gamma^2)} \right) = \frac{\Omega_0^2}{4N\Gamma s_\infty} \ln \left( 1 + \frac{4N^2 \Gamma^2 s_\infty s_N}{4\Delta_0^2 + \Gamma^2} \right) \quad (19.139)$$

$$F_e = -F_a + \frac{\Omega_0^2 \sigma^2}{\Delta_0 N} \arctan \frac{\Delta \Gamma N}{\sigma^2 (4\Delta_0^2 + \Gamma^2 + \frac{\Gamma^2 N}{2\sigma^2})} = \frac{\Omega_0^2}{4N\Delta_0 s_\infty} \arctan \frac{4\Delta_0 \Gamma N s_\infty}{4\Delta_0^2 + \Gamma^2 + 2\Gamma^2 N s_\infty}$$

$$b_0 = \frac{3N}{\sigma^2}$$

$$s_N = \frac{1}{N} + s_\infty = \frac{1}{N} + \frac{1}{(2\sigma)^2} .$$

#### 19.2.4.2 Expansion of the scattered radiation intensity

The incident electric field is ...

The radiated electric field  $\hat{\mathcal{E}}^{(+)}(\mathbf{r}, t)|\psi\rangle$  where  $\hat{\mathcal{E}}^{(+)}(\mathbf{r}, t) = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t}$ ,

$$\begin{aligned} \hat{\mathcal{E}}^{(+)}(\mathbf{r}, t)|\psi\rangle &= \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \gamma_{\mathbf{k}}(t) e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t} |0\rangle|1\rangle_{\mathbf{k}} \\ &= -i \frac{V_{ph} g_{k_0} \varepsilon_{k_0} k_0}{4\pi c \sqrt{N}} e^{-i\omega_0 t} \sum_{j=1}^N \beta_j(t) e^{i\mathbf{k}_0 \cdot \mathbf{r}_j} \frac{e^{ik_0|\mathbf{r}-\mathbf{r}_j|} - e^{-ik_0|\mathbf{r}-\mathbf{r}_j|}}{|\mathbf{r}-\mathbf{r}_j|}. \end{aligned} \quad (19.140)$$

We neglect the second term, which describes an incoming wave and go to smooth densities. We expand into spherical harmonics and obtain,

$$\hat{\mathcal{E}}^{(+)}(\mathbf{r}, t)|\psi\rangle = e^{-i\omega_0 t} \sum_{n=0}^{\infty} \frac{V_{ph} g_{k_0} \varepsilon_{k_0}}{c \sqrt{N}} \frac{\lambda_n}{2\Delta_0 + i\Gamma(1 + \lambda_n)} \Omega_0(2n+1) i^n h_n^{(1)}(k_0 r) P_n(\cos \theta). \quad (19.141)$$

### 19.2.4.3 Mie resonances

It is an interesting question whether the maxima found in the curves of Fig. 19.15 can be associated with Mie resonances [86, 647, 62]. To show this we need to apply the formalism of Mie scattering to atomic clouds with the smooth density approximation, where it is described by a continuous refraction index, as studied in Ref. [32]. The Mie formalism had been developed for homogeneous spheres, which can be dielectric or absorptive. For more general refractive index distribution the formalism gets quickly cumbersome<sup>15</sup>. Also Mie resonances are generally thought of being conditioned to the existence of sharp boundaries.

The results of Ref. [32] surprisingly show that Mie resonances are expected for parabolic distributions of atoms, as is the case for example for Bose-Einstein condensates in the Thomas-Fermi limit. However, the spectra of Mie resonances exhibit much less structure. This is understood by the fact that 'whispering gallery' Mie resonances may live on the surface of a sphere whose refraction index drops quadratically to zero, while cavity type Mie resonances may not.

## 19.2.5 Exercises

### 19.2.5.1 Ex: Structure factor of a homogeneous spherical and of a Gaussian ellipsoidal cloud

- Calculate the structure factor of a homogeneous spherical cloud of radius  $R$ , and discuss the limits  $qR \ll 1$  and  $qR \gg 1$ . Plot the structure factor as a function of  $\theta$  for various radii  $R$ .
- Calculate the structure factor of an ellipsoidal Gaussian cloud having the *rms*-widths  $\sigma_z$  and  $\sigma_r$ , and discuss the limits  $qR \ll 1$  and  $qR \gg 1$ . Plot the structure factor as a function of  $\theta$  for various aspect ratios  $\sigma_z/\sigma_r$ .

<sup>15</sup>There is a treatment for parabolic radial variations [386].

### 19.2.5.2 Ex: Force coefficients of a homogeneous spherical and of a Gaussian ellipsoidal cloud

- Calculate the force coefficients  $s_N$ ,  $\tilde{f}_N$ , and  $f_N$  from the Eqs. (19.65), Eqs. (19.77), and Eqs. (19.85), respectively, for a homogeneous spherical cloud of radius  $R$ .
- Repeat the calculation of (a) for an ellipsoidal Gaussian cloud having the *rms*-widths  $\sigma_z$  and  $\sigma_r$ .

### 19.2.5.3 Ex: RDG and Mie

Estimate whether it is possible to distinguish Rayleigh-Debye-Gans scattering from Mie scattering in strontium spectra.

### 19.2.5.4 Ex: Mie scattering from absorbing spheres

Calculate the force on a homogeneous dielectric sphere as a function of the absorptive and dispersive part of the refraction index [386].

### 19.2.5.5 Ex: Momentum halos and heating, is the recoil cooperative?

Discuss the question is whether recoil is imparted to individual atoms or to the center-of-mass of the whole cloud.

## 19.3 Scattering from disordered and dense clouds

### 19.3.0.1 Vectorial light

The procedure can be generalized to the vectorial case [639, 638, 465], where we get a similar steady-state solution as in (19.36),

$$\boxed{\vec{\beta}_j = (M_{jm})^{-1} \hat{\epsilon} \frac{i}{2} \Omega_0(\mathbf{r}_m)}, \quad (19.142)$$

only that the dipole moment amplitudes and the incident light field are now considered as vectors. The expression for the matrix  $M_{jm}$  is the same as in (19.35). However, the vectorial kernel must be calculated in a different way. Using the abbreviations,

$$\mathbf{r}_{jm} = \mathbf{r}_j - \mathbf{r}_m \quad , \quad r_{jm} = |\mathbf{r}_j - \mathbf{r}_m| + \delta_{jm} \quad , \quad c_{jm} = \frac{i}{k_0 r_{jm}} - \frac{1}{(k_0 r_{jm})^2}, \quad (19.143)$$

the new vectorial kernel can be written,

$$\gamma_{jm}^{(3)} = \frac{3\gamma_{jm}}{2} \frac{(1 + c_{jm})r_{jm}^2 \delta_{mn} - (1 + 3c_{jm})\mathbf{r}_{jm}\mathbf{r}_{jm}^\top}{r_{jm}^2}. \quad (19.144)$$

The steady-state scattered light field and the total field are now,

$$\vec{\mathcal{E}}_{sct}(\mathbf{r}) = -\frac{i\Gamma}{2} \sum_{j=1}^N \frac{3\gamma_{oj}(\mathbf{r})}{2} \frac{(1 + c_{oj}(\mathbf{r}))k_0^2 |\mathbf{r} - \mathbf{r}_j|^2 \vec{\beta}_j - (1 + 3c_{oj}(\mathbf{r}))[(\mathbf{r} - \mathbf{r}_j) \cdot \vec{\beta}_j](\mathbf{r} - \mathbf{r}_j)}{|\mathbf{r} - \mathbf{r}_j|^2}. \quad (19.145)$$

A movie can be assisted at [\(watch movie\)](#).

### 19.3.0.2 Coherent backscattering

Shining coherent light on a homogeneous cloud, we expect no coherent scattering (exception made of multiple-atom scattering in backward direction, CBS and of fluctuations like speckle patterns). Like radiation trapping, *coherent backscattering* (CBS) is a manifestation of interference in multiple scattering. Just like photon echoes it is *not* due to interatomic correlations. While in radiation trapping this leads to an energy storage inside the atomic cloud connected to destructive interference of the radiation emitted to the cloud's outside, when the coherent beam is reflected at a diffuse scattered, one observes *speckle patterns*. This holds as well for laser light reflection as for atomic wave reflections at a rough surface. See also (watch talk).

The coherent backscattering is an effect of constructive interference between two light scattering paths having the exact time-reversed single scattering sequence,

$$I = \left| \sum_j \vec{\mathcal{E}}_j e^{i\varphi_j} \right|^2 = \sum_j \left| \vec{\mathcal{E}}_j \right|^2 + \sum_{j \neq k} \vec{\mathcal{E}}_j \vec{\mathcal{E}}_k^* e^{i(\varphi_j - \varphi_k)}. \quad (19.146)$$

Only the second term makes speckles. However, the atomic motion smoothes out the speckle pattern in all directions. Only in the presence of correlations in the atomic positions they do not. E.g. in crystals or in the backscattering directions. Therefore, the constructive interference depends strongly on the backscattering angle  $\vartheta$ . Fast atomic motion internal excitations can dynamically break the time-reversal symmetry of the scattering path, esp. when the laser is close to resonance and the phase delay per scattering process is long. Coherent backscattering is a weak form of *Anderson localization* (also strong localization) of light.

## 19.3.1 Exercises

### 19.3.1.1 Ex: The green flash

Discuss whether the 'green flash' at sunset could be due to *superradiant extinction*. It can last seconds because refraction sweeps the ray through the spectrum (see the movie *Le rayon vert* by Éric Rohmer).

### 19.3.1.2 Ex: Faraday effect with vectorial kernel in the coupled dipoles model

Try to simulate the pump laser phase shift and lensing by a small dense cloud by the coupled dipoles model for red and blue detuning. Discuss the influence of rescattering.

## 19.4 Scattering from periodic structures and photonic bands

Long-range spatial ordering can have a dramatic influence on the propagation of light and the cooperativity of scattering, as we have already pointed out in the introduction of the structure factor in Sec. 19.1.1. This is true for the scattering of electronic waves in crystals. But atomic gases can also be arranged in periodic luminous potentials



generated by dipolar forces (introduced in Sec. 18.2.2) exerted by counterpropagating laser beams. Such potentials, called *optical lattices*, can be realized with various geometries in 1, 2 or 3 dimensions. See also ([watch talk](#)).

Periodic structures are usually probed by Bragg scattering. This procedure can be applied to atoms ordered in optical lattices [72, 712, 641, 643]: A test beam with wavevector  $\mathbf{k}_{brg}$  and intensity  $I_{brg}$  is irradiated into the atomic cloud, and the power  $P_s$  of the first-order reflected beam by Bragg is detected under a solid angle  $\Omega_s$ . Bragg diffraction is an interference effect of radiation patterns emitted by Rayleigh scattering from periodically aligned point-like antennas, the interference being constructive in only specified directions.

For optically dilute lattices, where multiple reflections can be neglected, the imaginary part of the atomic response is sufficient to describe Bragg reflection. For optically dense lattices, multiple reflections between consecutive atomic layers lead to interference phenomena between reflected and transmitted light fields and cause the emergence of frequency bands, inside which the propagation of light waves through the cloud is prohibited. These bands are known as *forbidden photonic bands*.

Photonic bands in optical lattices are interesting for several reasons:

1. They may facilitate the study of the phenomenon of Anderson localization. In fact, Anderson location of light in atomic gases requires very high densities or very large optical cross sections. Now, it is expected that, if the disorder is realized within periodic structures near the Bragg condition, the high density requirement is dramatically relaxed.
2. They modify the local density of states in a way to suppress spontaneous emission.
3. In optical lattices, unlike other systems, the scattering is very weak except when the light is tuned close to atomic resonances. Consequently, the expected forbidden bands are very narrow. This bears the advantage that we can adjust the optical density and tune the photon energy and the Bragg angle (i.e. the quasi-momentum) independently, which facilitates the mapping of the dispersion relation.
4. Crystals are always hampered by defects in the periodicity [401]. In latest-generation photonic crystals, the typical distance over which coherent light turns diffuse is limited to less than  $20 \mu\text{m}$ . This limitation plays no role in optical lattices, where the delocalized photons rigorously guarantee perfect long-range order, even though the Debye-Waller factor may introduce local disorder.

Spectra of photonic bands in atomic clouds were detected experimentally [614] in one-dimensional structures. Most of the above mentioned effects require omnidirectional photonic bands, but this is technically very difficult, mainly because of the narrow linewidth of the atomic transitions. We will develop this point in the course of this section. We also mention the prediction of forbidden photon bands in Bose condensates [460].

A presentation on this subject is available here ([watch talk](#)).

### 19.4.1 Bragg scattering

We write the density in a periodic lattice as [158],

$$\boxed{n(\mathbf{r}) = [n_0(\mathbf{r}) \sum_{l,m,n} \delta(\mathbf{r} - l\mathbf{a} - m\mathbf{b} - n\mathbf{c})]s(\mathbf{r})}, \quad (19.147)$$

where  $s(\mathbf{r})$  is the density distribution in an elementary cell <sup>16</sup>. We define the reciprocal lattice by,

$$\mathbf{a}^* \equiv \frac{\mathbf{b} \times \mathbf{c}}{V}, \quad \mathbf{b}^* \equiv \frac{\mathbf{c} \times \mathbf{a}}{V}, \quad \mathbf{c}^* \equiv \frac{\mathbf{a} \times \mathbf{b}}{V}, \quad V \equiv \mathbf{a}(\mathbf{b} \times \mathbf{c}). \quad (19.148)$$

The Fourier transform of the density is,

$$\rho(\mathbf{u}) = \sum_{l,m,n} \rho_{hkl} \delta(\mathbf{u} - l\mathbf{a} - m\mathbf{b} - n\mathbf{c}) \star s(\mathbf{r}), \quad (19.149)$$

where the *structure factor* is,

$$\rho_{hkl} = \int_0^{a,b,c} n(x,y,z) e^{2\pi i(hx/a + ky/b + lz/c)} dx dy dz = V \iiint_0^1 n(\mathbf{r}) e^{2\pi i\mathbf{h}\cdot\mathbf{r}} d\mathbf{r}, \quad (19.150)$$

with  $\mathbf{h} \equiv (h, k, l)$  and  $\mathbf{r} \equiv (x/a, y/b, z/c)$ . The density is given by the inverse transformation,

$$n(\mathbf{r}) = V^{-1} \sum_{h,k,l} \rho_{hkl} e^{-2\pi i\mathbf{h}\cdot\mathbf{r}} s(\mathbf{r}). \quad (19.151)$$

We consider a wave being scattered from the direction  $\mathbf{k}_0$  towards the direction  $\mathbf{k}_s \equiv \mathbf{k}_0 + \Delta\mathbf{k}$ . The structure factor  $\rho$  describes the amplitude of the radiation field scattered by the lattice. If the density distribution is the same at all sites of the lattice,

$$n(\mathbf{r}) = n_1(\mathbf{r}) \star \sum_{\mathbf{R}} \delta^{(3)}(\mathbf{r} - \mathbf{R}), \quad (19.152)$$

the structure factor becomes,

$$\rho(\Delta\mathbf{k}) = \sum_m e^{im\Delta\mathbf{k}\cdot\mathbf{R}} \int_V n_1(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}} d^3r. \quad (19.153)$$

**Example 86 (Elementary cell with gaussian distribution):** With the ansatz  $n_1(\mathbf{r}) = n_0 e^{-r^2/2\bar{r}^2}$ , such that  $\int n_1(\mathbf{r}) d^3r = n_0(2\pi)^{3/2}\bar{r}^3 = N_1$ ,

$$\begin{aligned} \rho(\Delta\mathbf{k}) &= \sum_m e^{im\Delta\mathbf{k}\cdot\mathbf{R}} \int_V n_1(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}} d^3r \\ &= \frac{1 - e^{iN_s\Delta k R}}{1 - e^{i\Delta k R}} \times n_0 \int_V e^{-x^2/2\bar{r}^2} e^{-y^2/2\bar{r}^2} e^{-z^2/2\bar{r}^2} e^{i\Delta\mathbf{k}\cdot\mathbf{r}} d^3r \\ &\approx N_s \delta(\Delta k - 2\pi/R) n_0 (2\pi)^{3/2} \bar{r}^3 e^{-6\Delta k^2 \bar{r}^2} = N \delta(\Delta k - 2\pi/R) e^{-6\Delta k_x^2 \bar{r}^2}. \end{aligned} \quad (19.154)$$

<sup>16</sup>This is similar to the square of the Bloch function defined in Sec. 5.1

### 19.4.1.1 Impact of disorder in one-dimensional lattices

A wave be incident on a lattice in the direction  $\mathbf{k}_0$  and scattered into the direction  $\mathbf{k}_s \equiv \mathbf{k}_0 + \Delta\mathbf{k}$ . The structure factor  $F_{hkl}$  describes the amplitude of radiation field scattered by the lattice,

$$\rho_{hkl} = \int_V \rho(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r} . \quad (19.155)$$

Let the density distribution be,

$$n(\mathbf{r}) = \sum_j \rho_j(\mathbf{r}) \star \delta^{(3)}(\mathbf{r} - \mathbf{r}_j) = n_1(\mathbf{r}) \star \sum_j \delta(\mathbf{r} - j\hat{\mathbf{e}}_z \frac{\lambda_{dip}}{2}) , \quad (19.156)$$

that is, for perfect periodicity, introducing the density distribution of a unit cell and a 1D lattice.

The *Debye-Waller factor* describes the diffusion of the density over the sites of the lattice due to the thermal motion,

$$\begin{aligned} \overline{\rho_{hkl}} &= \int_V n_1(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}} d^3r \sum_j \overline{e^{i(j\hat{\mathbf{e}}_z \lambda_{dip}/2 + \mathbf{u})\Delta\mathbf{k}}} \\ &= f_i \sum_j \overline{e^{i(j\hat{\mathbf{e}}_z \lambda_{dip}/2 + \mathbf{u})\Delta\mathbf{k}}} = \rho_{hkl} \overline{e^{i\mathbf{u}\Delta\mathbf{k}}} , \end{aligned} \quad (19.157)$$

with

$$\overline{e^{i\mathbf{u}\Delta\mathbf{k}}} \approx e^{-|\mathbf{G}|^2 u^2 / 6} . \quad (19.158)$$

**Example 87 (Optical lattice):** The exponential distribution  $e^{-6\Delta k_x^2 \bar{r}^2}$  is called Debye-Waller factor and describes the smearing out of the population over the lattice due to the thermal motion of the atoms. The  $\delta$ -function sets the wavevector of emitted light. That is, the power of light is only emitted in particular directions given by the Bragg condition. Here, the solid angle  $\Delta\Omega_s$  does not depend on the thermal distribution (as long as the atoms are within the Lamb-Dicke regime), but on the lattice size, which determines the goodness of the approximation of the Airy function (the sum in the above equation) by a Dirac  $\delta$ -function. The width of the Airy function for a lattice of size  $w_0$  is approximately  $\Delta k = 2\sqrt{3}/w_0$ . With this the solid angle is,

$$\Delta\Omega_s = \frac{12}{k^2 w_0^2} . \quad (19.159)$$

We can also estimate the solid angle from the diameter  $d$  of the Gaussian beam at a distance  $x$  away from a scattering medium of size  $w_0$ ,

$$\begin{aligned} d &= w_0 \sqrt{1 + \left(\frac{\lambda x}{\pi w_0^2}\right)^2} \\ \Delta\Omega_s &= \frac{\pi d^2}{x^2} = \frac{\lambda^2}{\pi w_0^2} = \frac{4\pi}{k^2 w_0^2} . \end{aligned} \quad (19.160)$$

The power scattered into this solid angle is,

$$P_s = |A_s|^2 F^2 \Delta\Omega_s = |A_s|^2 e^{-2W} N^2 \Delta\Omega_s . \quad (19.161)$$

It depends quadratically on the number of atoms. Strictly speaking, the derivation only applies to perfectly ordered lattices, i.e. all the lattice sites are equally occupied. Defects lead to diffuse scattering, i.e. a background of isotropically distributed power at the expense of Bragg scattering. The sharpness of the Bragg radiation distribution remains intact.

We parametrize the density in an optical 1D lattice as follows:

$$n_l(\mathbf{r}) = n_0 e^{-(x^2-y^2)/2\sigma_r^2} e^{-z^2/2\sigma_z^2} \quad (19.162)$$

$$n_a(\mathbf{r}) = \sum_{m=1}^{N_s} \delta(\mathbf{r} - md\hat{\mathbf{e}}_z) \star n_l(\mathbf{r}) = \sum_{m=1}^{N_s} n_l(\mathbf{r} - md\hat{\mathbf{e}}_z) .$$

We will show in Exc. 19.4.4.1, that the structure factor is then,

$$S_{\mathbf{k}_0}(\mathbf{k}) = \frac{n_0}{N} \frac{1 - e^{iN_s dq_z}}{e^{-idq_z} - 1} e^{-q_x^2 \sigma_r^2 / 2} e^{-q_y^2 \sigma_r^2 / 2} e^{-q_z^2 \sigma_z^2 / 2} . \quad (19.163)$$

In Exc. 19.4.4.2 we derive the structure factor in spherical coordinates.

Some comments are needed:

1. The structure factor treatment assumes low optical density, which is not necessarily guaranteed when the laser is tuned close to a resonance [641].
2. As the structure factor is independent of the laser detuning, it will not reveal any spectral structure, such as a band-gap or dip due to diffuse scattering. Also, absorption is not incorporated into the model.

### 19.4.1.2 The structure factor and the Bragg condition

The reciprocal space, obtained by Fourier transformation of the periodic density distribution, also adopts the shape of a periodic lattice. The Bragg condition requires that the difference between the incident and emitted wavevectors,  $\Delta \mathbf{k} \equiv \mathbf{k}_s - \mathbf{k}_i$ , matches a vector of the reciprocal lattice,  $\mathbf{r}_j = j\mathbf{G}$ . The Bragg condition is thus automatically incorporated into the structure factor (19.199).

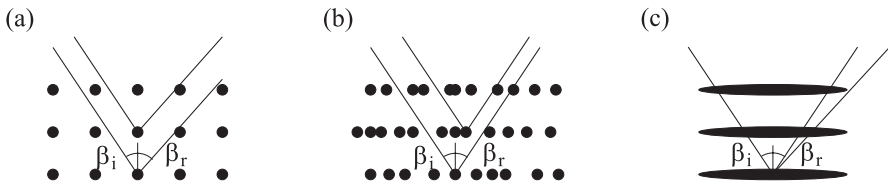


Figure 19.16: Several Bragg lattices.

With the lattice constant  $d = \frac{1}{2}\lambda_{dip}$  the interference is constructive when the difference of the paths of two beams reflected by different layers is a multiple of the wavelength,

$$\frac{1}{2}\lambda_{dip} \cos \beta_i + \frac{1}{2}\lambda_{dip} \cos \beta_s = \lambda . \quad (19.164)$$

This is illustrated in Fig. 19.16(a). If the transverse distribution can be considered as homogeneous, as shown in Fig. 19.16(b), we have as second condition,

$$\beta_i = -\beta_s . \quad (19.165)$$

That is, the angles of incidence and reflection must be the same, as if we were dealing with a dielectric mirror. In contrast, if the transverse extent of the atomic layers gets smaller (until converging to the limit of a one-dimensional chain of point-scatterers,  $\mathbf{G} \equiv 2k_{dip}\hat{e}_z$ ), we return to the condition (19.164). In intermediate situations, illustrated in Fig. 19.16(c), and for  $\lambda_{dip} \cos \beta_i \neq \lambda$  the reflection angle does not follow any of the relations (19.164) and (19.165).

### 19.4.1.3 Incoherent background

A finite size or defects in the periodic ordering of the atoms may lead to an isotropic background of Rayleigh-scattered light,

$$\frac{dP_s}{d\Omega_s} = |A_s|^2 [e^{-2W}|F|^2 + N_1N(1 - e^{-2W})] . \quad (19.166)$$

The amount of photons scattered into the *same solid angle* as the one of Bragg scattering is typically for 1D lattices,

$$\frac{(1 - e^{-2W})N_1N}{e^{-2W}|F|^2} = (e^{2W} - 1) \frac{N_1}{N} \approx 0.002 . \quad (19.167)$$

However, if we compare the total amount of coherently Bragg-scattered light, we obtain,

$$\frac{(1 - e^{-2W})N_1N}{e^{-2W}|F|^2} \frac{4\pi}{d\Omega_s} \approx 2500 . \quad (19.168)$$

## 19.4.2 Transfer matrices calculation 1D-lattices

For one-dimensional optical lattices, that is, when the atoms are trapped in a potential dipole generated by a stationary light wave, we may consider applying the transfer matrix formalism developed in Secs. 3.3. The premisses of this model are the homogeneity and the infinite extent of the cloud in a direction transverse to the optical axis.

We calculate the reflection coefficient  $\beta$  of a classical polarizable sample from the microscopic polarizability and the optical density (depth) of a thin layer,  $n\delta z\sigma_0$ , where  $\sigma_0$  is the resonant optical cross section,

$$\beta = n \frac{k_{brg}\delta z}{2} \frac{\alpha_{pol}}{\varepsilon_0} = \frac{n\delta z}{2} \frac{6\pi}{k_{brg}^2} \frac{-1}{\iota + 2\Delta_{brg}/\Gamma} = \frac{n\delta z\sigma_0}{2} \frac{-1}{\iota + 2\Delta_{brg}/\Gamma} . \quad (19.169)$$

We remember that the polarizability is linked to the macroscopic susceptibility  $\chi_e = n\alpha_{pol}/\varepsilon_0$ <sup>17</sup>. With the notation introduced in Fig. 19.17 we find the equations relating

<sup>17</sup>Note the analogy to the calculation (20.87) made for the reflection coefficient of an atom in a cavity in Sec. 20.2.2,

$$\beta = \frac{k}{\pi w^2} \frac{\alpha_{pol}}{\varepsilon_0} = \frac{6}{k^2 w^2} \frac{-1}{2\Delta/\Gamma + \iota} = \frac{\sigma_0}{\pi w^2} \frac{-1}{2\Delta/\Gamma + \iota} .$$

the incident electric fields with the transmitted and reflected ones,

$$\begin{aligned} E_z^+ &= (1 + i\beta)E_0^+ + i\beta E_z^- \\ E_0^- &= (1 + i\beta)E_z^- + i\beta E_0^+ , \end{aligned} \quad (19.170)$$

or in  $\mathcal{S}$ -matrix notation,

$$\begin{pmatrix} E_z^+ \\ E_0^- \end{pmatrix} = \mathcal{S}_\beta \begin{pmatrix} E_z^- \\ E_0^+ \end{pmatrix} , \quad (19.171)$$

where

$$\mathcal{S}_\beta = \begin{pmatrix} i\beta & 1 + i\beta \\ 1 + i\beta & i\beta \end{pmatrix} = \begin{pmatrix} r & t \\ t & r \end{pmatrix} , \quad (19.172)$$

and where we defined the coefficients

$$t = 1 + i\beta \quad \text{and} \quad r = i\beta , \quad (19.173)$$

which satisfy  $|t|^2 - |r|^2 = 1$ . Recasting the problem into the  $\mathcal{T}$ -matrix notation,

$$\begin{pmatrix} E_z^+ \\ E_z^- \end{pmatrix} = \mathcal{T}_\beta \begin{pmatrix} E_0^+ \\ E_0^- \end{pmatrix} , \quad (19.174)$$

where

$$\mathcal{T}_\beta = \frac{1}{1 + i\beta} \begin{pmatrix} 1 + 2i\beta & i\beta \\ -i\beta & 1 \end{pmatrix} = \frac{1}{t} \begin{pmatrix} t^2 - r^2 & r \\ -r & 1 \end{pmatrix} . \quad (19.175)$$

We have  $\det \mathcal{T}_\beta = 1$ . For weak reflection,  $\beta \ll 1$ ,

$$\mathcal{T}_\beta \simeq \begin{pmatrix} 1 + i\beta & i\beta \\ -i\beta & 1 - i\beta \end{pmatrix} . \quad (19.176)$$

We note that the employed model is classical, since we describe the gas by a sequence

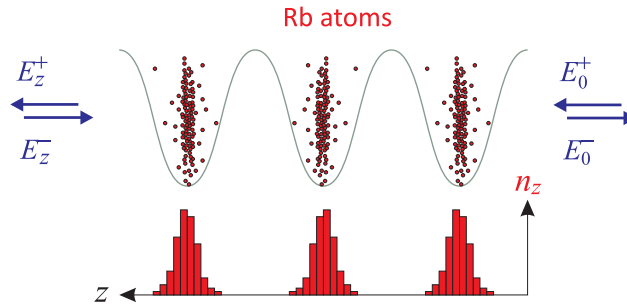


Figure 19.17: Illustration of the transfer matrix model.

of layers, each characterized by a refractive index. Applying the transfer matrix model, we calculate how the incident and reflected light fields transform from one layer to another. The intrinsically 1D model allows to calculate the reflection, transmission, and absorption by the atomic lattice as a function of the incident laser frequency.

We still need to multiply with the transfer matrix describing the propagation of the incident beam through the layer,

$$\mathcal{T}_d = \begin{pmatrix} e^{i\mathbf{k}\cdot\mathbf{d}} & 0 \\ 0 & e^{-i\mathbf{k}\cdot\mathbf{d}} \end{pmatrix}, \quad (19.177)$$

such that the transfer matrix for passing the beam through an atomic layer is,

$$\mathcal{T} = \mathcal{T}_\beta \mathcal{T}_d. \quad (19.178)$$

For  $N_s$  layers we must obviously concatenate the matrices  $\mathcal{M}^{N_s}$ . The reflection coefficient is now simply,

$$r_{N_s} = \frac{(\mathcal{T}^{N_s})_{12}}{(\mathcal{T}^{N_s})_{22}}, \quad (19.179)$$

and can be evaluated numerically or analytically [193]. If the incident beam hits the cloud under an angle,  $\mathbf{k} \cdot \mathbf{d} = kd \cos \theta = k_z d$ , and furthermore, as shown in [194] Eq. (A10), the theory must be generalized by replacing,

$$\beta \rightarrow \frac{\beta}{2} (\cos^{-1} \theta + \cos \theta). \quad (19.180)$$

However, for  $\theta < 60^\circ$  the correction is small.

#### 19.4.2.1 Limit of optically dilute clouds

For optically dilute clouds,  $r \ll 1$ , we expect standard Bragg scattering as described by equation (19.176),

$$\mathcal{T} = \mathcal{T}_\beta \mathcal{T}_d \simeq \begin{pmatrix} e^{ik_z d} & i\beta e^{-ik_z d} \\ -i\beta e^{ik_z d} & e^{-ik_z d} \end{pmatrix}, \quad (19.181)$$

with  $\mathbf{k} \cdot \mathbf{d} = kd \cos \theta = k_z d$ . Near the Bragg angle we have  $\cos \theta \simeq \cos \theta_{brg} = \lambda_{sp}/\lambda_{dip}$  and near resonance we have  $2\pi/k = \lambda \simeq \lambda_{sp}$ , so that, with  $d = \lambda_{dip}/2$ , we obtain  $k_z d \simeq \pi$  and,

$$\mathcal{T}^{N_s} \simeq \begin{pmatrix} e^{i\pi} & i\beta e^{-i\pi} \\ -i\beta e^{i\pi} & e^{-i\pi} \end{pmatrix}^{N_s} = \begin{pmatrix} -1 & -i\beta \\ i\beta & -1 \end{pmatrix}^{N_s} = (-1)^{N_s} \begin{pmatrix} 1 & N_s i\beta \\ -N_s i\beta & 1 \end{pmatrix}, \quad (19.182)$$

which we will verify in Exc. 19.4.4.3. The total reflectivity being  $r_{N_s} \simeq N_s i\beta$ , we get the reflection,

$$|r_{N_s}|^2 \simeq \frac{N_s^2 \beta^2 \Gamma_{sp}^2}{4\Delta^2 + \Gamma_{sp}^2}. \quad (19.183)$$

Thus, the profile of the reflection curve is Lorentzian.

### 19.4.2.2 Limit of optically dense clouds

In order to obtain analytical expressions in the regime of dense clouds, we write the transfer matrix for a single layer, using the expressions (19.175) and (19.177), as follows [194],

$$\mathcal{T} = \mathcal{T}_\beta \mathcal{T}_d = \begin{pmatrix} (1 + \imath\beta)e^{\imath\mathbf{k}\cdot\mathbf{d}} & \imath\beta e^{-\imath\mathbf{k}\cdot\mathbf{d}} \\ -\imath\beta e^{\imath\mathbf{k}\cdot\mathbf{d}} & (1 - \imath\beta)e^{-\imath\mathbf{k}\cdot\mathbf{d}} \end{pmatrix}. \quad (19.184)$$

Given that  $\det \mathcal{T} = 1$ , the matrix represents a unitary transformation and the eigenvalues can be cast into the form  $e^{\pm\imath\phi}$ . Letting,

$$\cos \Theta \equiv \frac{1}{2} \text{Tr } \mathcal{T} = \cos k_z d - \beta \sin k_z d, \quad (19.185)$$

we can write the matrix,

$$\mathcal{T} = \mathbb{I} \cos \Theta + \imath A \sin \Theta = e^{\imath\Theta A} \quad (19.186)$$

with

$$A = \frac{1}{\sin \Theta} \begin{pmatrix} \beta \cos k_z d + \sin k_z d & \beta e^{-\imath k_z d} \\ -\beta e^{\imath k_z d} & -\beta \cos k_z d - \sin k_z d \end{pmatrix} \quad (19.187)$$

The eigenvectors of  $\mathcal{T}$ , and therefore of each power of  $\mathcal{T}$ , are *Bloch states of the periodic lattice*. We verify in Exc. 19.4.4.4, that the following relationships are satisfied,

$$\text{Tr } A = 0, \quad A^2 = 1, \quad \det A = 1. \quad (19.188)$$

The eigenvalues of  $A \sin \Theta$  are  $\lambda_A \pm 1$ . The eigenvalues of the transfer matrix are,

$$\begin{aligned} \lambda &= \cos k_z d - \beta \sin k_z d \pm \imath \sqrt{1 - (\cos k_z d - \beta \sin k_z d)^2} = \cos \Theta \pm \imath \sin \Theta \\ &= e^{\pm\imath \arccos(\cos k_z d - \beta \sin k_z d)} = e^{\pm\imath\theta}. \end{aligned} \quad (19.189)$$

This decomposition allows us to calculate the transfer matrix for a succession of  $\mu$  layers. We get,

$$\begin{aligned} \mathcal{T}^\mu &= e^{\imath\mu\theta A} = \mathbb{I} \cos(\mu\theta) + \imath A \sin(\mu\theta) \\ &= \mathbb{I} \cos[\mu \arccos(\cos k_z d - \beta \sin k_z d)] + \imath A \sin[\mu \arccos(\cos k_z d - \beta \sin k_z d)], \end{aligned} \quad (19.190)$$

which gives us the reflection coefficient,

$$\begin{aligned} r_\mu &= \frac{(\mathcal{T}^\mu)_{12}}{(\mathcal{T}^\mu)_{22}} = \frac{\imath \sin(\mu\theta) \mathcal{T}_{12}}{\cos(\mu\theta) + \imath \sin(\mu\theta) \mathcal{T}_{22}} \\ &= \frac{-\imath\beta e^{\imath k_z d}}{\sin \theta \cot(\mu\theta) - \imath \sin k_z d - \imath\beta \cos k_z d}. \end{aligned} \quad (19.191)$$

This is the final result. Near the Bragg angle,  $\cos \theta \simeq 1$ , we have,

$$\begin{aligned} r_{N_s} &= \frac{\imath\beta}{\sin \theta \cot(N_s \theta) - \imath\beta} \simeq \frac{\imath N_s \zeta}{1 - \imath N_s \beta} \\ |r_{N_s}|^2 &\simeq \frac{N_s^2 \beta_{sp}^2 \Gamma_{sp}^2}{4\Delta^2 + (1 + n\beta_{sp}^2) \Gamma_{sp}^2}. \end{aligned} \quad (19.192)$$

The intensity reflection profile, therefore, is a Lorentzian also in the limit of thick clouds. The additional condition for the occurrence of prohibited photonic bands is a large number of atomic layers,  $N_s \gg 1$ . We note that the model is an extension of the *Kronig-Penney model* introduced in Sec. 5.3.



### 19.4.2.3 Application of transfer matrices to real 1D optical lattices

The analytical treatment shown in the previous sections does not take account of possible lattice imperfections, since the atomic layers are assumed to be identical, infinitely thin, immobile and located at fixed periodic distances. Realistic optical lattices are different for several reasons:

1. Atomic clouds are not perfectly localized in ultra-thin layers, but distributed in a Gaussian way as a function of the cloud's temperature. The Debye-Waller factor (19.157) describes the impact of this distribution on the Bragg model.
2. The atoms are in thermal motion causing an inhomogeneous Doppler shift and are affected by the photonic recoil received in each scattering process. This causes a broadening of the reflection profiles and decreases the interference capability.
3. The number of atoms per layer may vary. Also, the global extent of the cloud is not infinite, that is, we have  $N_s$  layers filled with atoms with a gradual decrease at the confines of the cloud.
4. The atoms trapped in the optical potential are subjected to a dynamic Stark shift <sup>18</sup> causing an inhomogeneous broadening of the atomic transition as well.
5. The periodicity of the lattice is slightly modified because the refractive index experienced by the laser beams creating the dipole potential locally depends on the atomic density concentrated in the lattice's anti-nodes. The consequence is a local decrease of the lattice constant  $d$  <sup>19</sup>.

All of the aforementioned imperfections may be included in a numerical treatment of the transfer matrices. For this we subdivide the atomic cloud into sufficiently thin sublayers, as shown in Fig. 19.17. Each sublayer, being characterized by its own 2D atomic density and its own shift from resonance, is described by an individual transfer matrix. The matrices are concatenated, and the reflection profile is computed, as shown in the expression (19.179) [642]. Fig. 19.18 shows a numerical calculation of a photonic band in a rubidium optical lattice. The experimental variables are the incidence angle  $\theta$  of the probe laser and its tuning  $\Delta$  from a transition  $\lambda_{sp}$ .  $\Delta$  determines  $\sigma$  and  $\beta$  via the polarizability (19.169) <sup>20</sup> and thus governs the propagation of light inside the layers.  $\theta$  determines  $k_z d$  and thus probes the periodicity *between* the layers.

Depending on the atomic density we can identify different behaviors <sup>21</sup>:

<sup>18</sup>Or 'light-shift', see Exc. 14.3.5.14.

<sup>19</sup>More correctly: If between  $\lambda_{dip}$  and  $\lambda_{D1}$  a photonic band were created for the laser beams that produce the optical lattice [194, 711], these beams would be reflected without being able to penetrate the lattice. In fact, the periodicity changes in such a way, that the frequency of the beams is at the edge of the band gap. Deutsch *et al.* [194] showed that a self-consistent solution gives the modified lattice constant,

$$d' = \frac{\lambda_{dip}}{2} \left[ 1 + \frac{\phi_{dip}}{\pi} (1 - \text{sign} \Delta_{dip}) \right],$$

where  $\phi_{dip} = \arctan \left( -\frac{\Delta_{dip}}{\Gamma} n d \sigma_{D1}(\Delta_{dip}) \right)$ .

<sup>20</sup> $\Delta$  also enters  $k_z d$ , but so weakly, that we can dispense this dependence.

<sup>21</sup>The densities are assumed to be sufficiently low to eliminate collective effects such as, for example, superradiance.

1. At the limit of thin lattices, we do not expect multiple scattering. The absorptive (imaginary) part of polarizability dominates,  $\beta \approx \text{Im } \beta$ . Thus, the reflection coefficient is almost real,  $re^{i\phi} \approx |r|$ , the phase shifts are negligible, the profile of the reflection spectrum is symmetric. In this scheme, the interference of the radiation patterns of individual atoms is destructive in all directions, except under the Bragg angle. There are losses caused by scattering in non-paraxial modes. They are also due to elastic Rayleigh scattering but, because of the finite Debye-Waller factor, the radiation becomes diffuse and incoherent.
2. At the limit of thick lattices, we have multiple scattering. The (real) dispersive part of the polarizability is  $\beta \approx \text{Re } \beta$ . Thus, absorption is suppressed, we observe large phase shifts and the reflection spectrum profile is asymmetric. Multiple beam interference gives rise to global scattering.

Physically, the set parameters consistent of the quasi-momentum and the energy of the Bloch wave,  $(\Theta, \Delta)$ , is more relevant because it allows analyzing the *dispersion relation*<sup>22</sup>. We observe the existence of energies  $\Delta$ , where the real part of the quasi-momentum vanishes (modulo  $\pi$ ). The 3D representation in Fig. 19.18(e) illustrates the occurrence of an *avoided crossing* due to the band gap at the edge of the Brillouin zone.

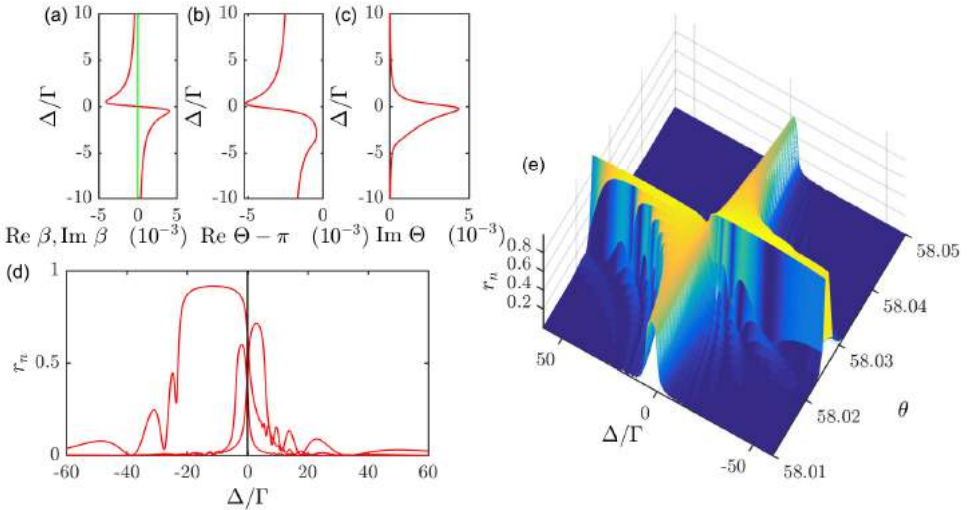


Figure 19.18: (code) Numerical calculation of a photonic band in a 1D optical lattice (wavelength  $\Lambda_{dip} = 797$  nm) far-tuned from the rubidium D1 transition ( $\lambda_{D1} = 795$  nm). The probe laser exciting the Bragg resonance is tuned close to the rubidium resonance at  $\lambda_{sp} = 422$  nm. We assume atomic densities of  $n = 4 \cdot 10^{11} \text{ cm}^{-3}$  and  $N_s = 40000$  atomic layers. (a) Real and imaginary parts of the reflection index ( $\propto$  polarizability) as a function of detuning  $\Delta$ . (b,c) Real and imaginary parts of the quasi-momentum ( $x$ -axis) as a function of the detuning  $\Delta$ . (d,e) 2D and 3D representation of the reflection coefficient.

<sup>22</sup>We note, that  $\Theta$  via the relation (19.185) of the angle of incidence  $\theta$ , but only weakly of the energy  $\Delta$ .

In fact, Bragg resonances can be understood in reciprocal space as reflections at the edges of the Brillouin zone. Through the angle of incidence of the injected light beam, we adjust the quasi-momentum. The frequency of the light beam determines the energy. The forbidden photonic bands are caused by the formation of an energetic gap in the dispersion relation induced by the interaction of the atoms with the optical lattice.

#### 19.4.2.4 Intensity distribution and LDOS within a lattice

The density matrix formalism (19.175) not only allows to calculate the overall reflectivity of the 1D optical lattice, but also the local intensity  $I \propto |E_a^+ + E_a^-|^2$  at a point  $z = a$  inside the lattice[642].

To calculate this intensity we assume that the network is located between the points  $z = 0$  and  $z = b$  of the optical axis with  $0 < a < b$ . The transfer through the entire structure is given by,

$$\begin{pmatrix} E_b^+ \\ E_b^- \end{pmatrix} = \mathcal{T} \begin{pmatrix} E_0^+ \\ E_0^- \end{pmatrix} . \quad (19.193)$$

We use the boundary condition that,  $E_0^+$  being preset, there is no reflection of light behind the last layer, i.e.,  $E_b^- = 0$ . We obtain,

$$E_0^- = -\frac{\mathcal{T}_{21}}{\mathcal{T}_{22}} E_0^+ \quad \text{and} \quad E_b^+ = \left( \mathcal{T}_{11} - \frac{\mathcal{T}_{12}\mathcal{T}_{21}}{\mathcal{T}_{22}} \right) E_0^+ . \quad (19.194)$$

Now we separate the entire structure into two parts  $\mathcal{T} = \mathcal{T}^{(b)}\mathcal{T}^{(a)}$ , such that the field between the two parts is,

$$\begin{pmatrix} E_1^+ \\ E_1^- \end{pmatrix} = \mathcal{T}^{(a)} \begin{pmatrix} 1 \\ -\mathcal{T}_{21}/\mathcal{T}_{22} \end{pmatrix} E_0^+ . \quad (19.195)$$

The sum gives,

$$\boxed{E_1^+ + E_1^- = \left( \mathcal{T}_{11}^{(a)} + \mathcal{T}_{21}^{(a)} - \frac{\mathcal{T}_{21}}{\mathcal{T}_{22}} (\mathcal{T}_{12}^{(a)} + \mathcal{T}_{22}^{(a)}) \right) E_0^+} . \quad (19.196)$$

The *local density of states* (LDOS) in a photonic band can be evaluated from [693, 265],

$$N(\omega) = 2\omega \sum_{\mathbf{k}} \delta(\omega^2 - \omega_{\mathbf{k}}^2) . \quad (19.197)$$

William found out:

$$k_{eff} = \frac{d\phi}{dz} , \quad (19.198)$$

with  $\phi = \arctan(\text{Im } E/\text{Re } E)$ . The  $E$ -field between two layers can be calculated using transfer matrices. The density of the states is given as the derivative of the inverse function of the dispersion relation:

$$N(\omega) = \frac{dk_{eff}(\omega)}{d\omega} . \quad (19.199)$$

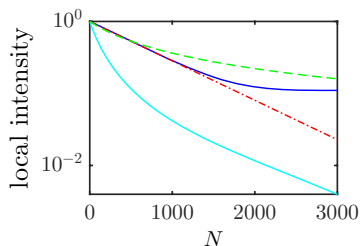


Figure 19.19: (code) The intensity decreases exponentially over a infinite lattice. For a finite lattice (here  $N_s = 3000$ ), the intensity approaches a constant value at the end of the lattice. The graph shows in blue the intensity along the lattice, in red the exponential decay due to absorption in a homogeneous cloud (Lambert-Beer law), in green the hyperbolic decay following Ohm's law and in cyan the transmission assuming a lattice of  $N$  layers.

#### 19.4.2.5 Suppression of spontaneous emission in forbidden photonic bands

The decrease in the LDOS is equivalent to the suppression of spontaneous emission<sup>23</sup>, that is, an excited atom located inside the lattice will not be able to emit its photon. This is the condition for a forbidden photonic band to be *omnidimensional*. Omnidirectional bands need three-dimensional lattices. Nevertheless, the reduction of the spontaneous emission rate has already been observed in [316, 729], which can be interpreted as  $1D$  photonic crystals.

#### 19.4.2.6 Impurities

The formula (19.196) allows the calculation of the impact of localized defects in numerical simulations. For example, it is instructive to look at the intensity profile along the structure in the presence of a localized lattice defect. In Fig. 19.20(c) we observe an intensity peak located at the 100-th atomic layer, exactly where the defect was introduced. This peak corresponds to a localized evanescent wave. Photons can not propagate freely through the lattice: they prefer to tunnel between lattice defects rather than propagate by radiation.

The curves (a-b) of Fig. 19.20 illustrate how an empty photonic band fills up with localized states with well-defined energies when noise is added to the periodicity of the lattice. This situation is similar to that in semi-conductors doped by donor and acceptor states.

### 19.4.3 Photonic bands in the Bloch and the coupled dipoles models

The transfer matrix model is limited in several respects:

1. Firstly, being intrinsically  $1D$ , the model does not apply to  $2D$  or  $3D$  lattices.
2. Also, it does not incorporate the possibility of transverse disorder or effects linked to the finite transverse extension of the atomic layers, for example, the

<sup>23</sup>For the same reason, resonant dipole-dipole interactions are suppressed [418].

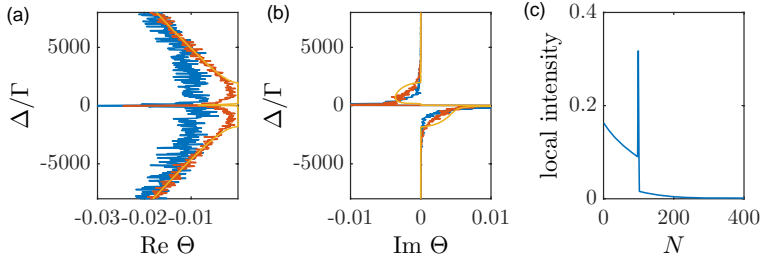


Figure 19.20: (code) (a,b) Dispersion relation as in Fig. 19.18, but in the presence of randomly distributed defects. (c) Intensity profile along the lattice with a defect located in the  $100^{\text{esima}}$  atomic layer.

limitation of the number of layers participating in multiple reflection ('walk-off') [643] or the impact of an imperfect mode matching [641].

In contrast, the coupled dipoles model offers several advantages. An optical lattice is, after all, nothing more than a periodically ordered diluted sample of atoms. Hence, we can apply the coupled dipoles model introduced in Sec. 19.1.2 [601, 600]. The advantages of this model are its applicability to 3D systems and finite and disordered lattices. It also allows the inclusion of all kinds of inhomogeneities such as, for example, the spatial intensity distribution of a focused incident laser, or the deviation of the laser beam penetrating an atomic cloud due to refraction. On the other hand, the model only lends itself to heavy numerical simulations, limiting it to some 10000 atoms.

### 19.4.3.1 The Bloch model and forbidden electronic bands

The *Bloch model* is another model to describe 3D periodic systems [21]. It was introduced in Chp. 5.4 for 1D optical lattices. Its disadvantages are that it supposes infinite lattices and the absence of defects.

The Bloch model is commonly used to describe the scattering of electron waves in a solid, where the band gap originates from the Coulomb interaction of the electron with the atoms of the solid crystal. In contrast, in photonic crystals, the modes with high (low) frequency  $\omega$  concentrate their energy in spatial regions with low (high) dielectric index  $\epsilon$ . Close to geometric (Mie) resonances this causes a repulsion in the density distribution of photonic states, and the opening of a gap separating high frequency bands (air bands) from low frequency bands.

In optical lattices the photons interact with the atomic resonances. Photons and electrons are distinguished by their different dispersion relations and by the fact that electronic waves are scalar and photonic waves are vectorial. The electrons of a crystal are bound to an energy surface and follow the lines of the dispersion relation without leaving the metal. In contrast, photons are usually injected into the structure, which gives an additional degree of freedom. Therefore, any point in the phase diagram can be reached and the dispersion relation only informs, where at which point the transmission is stronger.

	photonic crystal	metal
lattice structure	atoms in a stationary wave	atoms in a crystal
particles	photons	electrons in a metal
equations of motion	Maxwell	Schrödinger
dispersion relation	$\hbar k/c$	$\hbar k^2/2m$
tune	Bragg angle and frequency	voltage
band gap origin	$\text{Im } \alpha$ absorption by atoms	$e^-$ interacting with the atomic nuclei
band gap width	$< \omega_0 - \omega_{dip}$	interaction energy

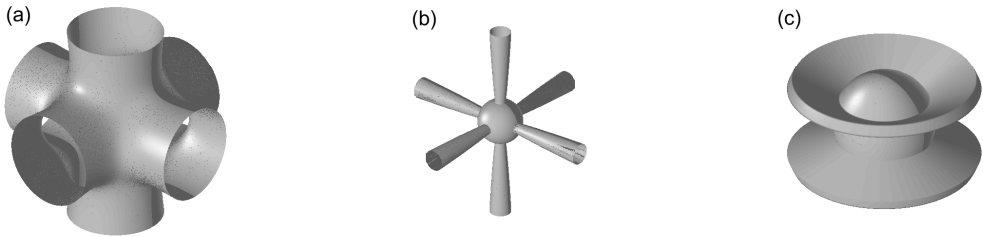


Figure 19.21: Attempt of an artistic illustration of the isoenergetic surfaces for electrons in a metal (left), photons in a 3D optical lattice (center), and photons in a 1D optical lattice (right). The interaction of atoms with the lattice is much weaker than the interaction of electrons with the metal, except close to resonances. Therefore, photonic bands are much narrower than electronic bands.

## 19.4.4 Exercises

### 19.4.4.1 Ex: Factor structure of a 1D lattice

Calculate the structure factor of the density distribution (19.162) and the square  $|S_{\mathbf{k}_0}(\mathbf{k})|^2$ .

### 19.4.4.2 Ex: Structure factor in spherical coordinates

Write the structure factor (19.162) in spherical coordinates.

### 19.4.4.3 Ex: Reflection in the dilute cloud limit

Verify the calculation (19.182).

### 19.4.4.4 Ex: Reflection in the dense cloud limit

Verify the representation (19.186).

### 19.4.4.5 Ex: Photonic band spectra

Plot the 1D-photonic band gap spectrum in a standing wave as a function of  $\Delta_{pr}$  and  $n$ .

**19.4.4.6 Ex: Intensity drop inside photonic bands**

Plot the intensity of the probe on its passage through the 1D optical lattice.

**19.4.4.7 Ex: Intensity drop inside photonic bands in the presence of disorder**

Simulate the intensity of the probe on its passage through the 1D optical lattice in the presence of disorder.

**19.4.4.8 Ex: Photonic bands with sidebands**

Plot the intensity of the probe on its passage through the 1D optical lattice as a function of detuning in the presence of modulation sidebands.

**19.4.4.9 Ex: Photonic bands versus absorption**

Compare the signatures of band gaps with absorption.

**19.4.4.10 Ex: Structure of a diamond lattice**

A geometric configuration of point-like scatterers that can exhibit a broad omnidirectional photonic bandgap is the one of a diamond lattice [138, 605, 21]. In this exercise we will study such a diamond-shaped lattice.

- Produce a geometric representation of the primitive cell and a Wigner-Seitz cell.
- Study the optical lattice generated by the following configuration of incident lasers,

$$\mathbf{k}_0 = \frac{\pi}{a}(0, -2, -1) \quad , \quad \mathbf{k}_1 = \frac{\pi}{a}(2, 0, 1) \quad , \quad \mathbf{k}_2 = \frac{\pi}{a}(0, 2, -1) \quad , \quad \mathbf{k}_3 = \frac{\pi}{a}(-2, 0, 1)$$

with  $k_{laser} = \omega_{laser}/c = \sqrt{5}\pi/a$ .

- Calculate the forbidden band according to [138, 605, 21].

**19.5 Further reading****19.5.1 on the coupled dipoles model**

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- A.A. Svidzinsky et al., *Evolution of collective  $N$  atom states in single photon superradiance: Effect of virtual Lamb shift processes* [\[DOI\]](#)
- A.A. Svidzinsky et al., *Cooperative spontaneous emission of  $N$  atoms: Many-body eigenstates, the effect of virtual Lamb shift processes, and analogy with radiation of  $N$  classical oscillators* [\[DOI\]](#)
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- R. Röhlsberger et al., *The collective Lamb shift in nuclear c-ray superradiance* [DOI]
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- S.E. Skipetrov et al., *Absence of Anderson Localization of Light in a Random Ensemble of Point Scatterers* [DOI]
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### 19.5.2 on Bragg scattering

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- G. Vandegrift et al., *The Moessbauer effect explained* [DOI]
- D. Mogilevtsev et al., *Light propagation and Anderson localization in disordered superlattices containing dispersive metamaterials Effects of correlated disorder* [DOI]
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- D. Petrosyan, *Tunable photonic band gaps with coherently driven atoms in optical lattices* [\[DOI\]](#)
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#### 19.5.4 on noise analysis of Bragg scattering

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## Chapter 20

# Coupling of atoms and optical cavities and the CQED regime

So far we have considered the coherent dynamics between atoms and radiation fields in free space, and we extended the theory to take into account the dissipative coupling to the electromagnetic vacuum by spontaneous emission and atomic motion. The vacuum represents a homogeneous and isotropic reservoir characterized by a continuous white energy spectrum. The situation changes completely when we place the atom inside an optical cavity which breaks the translational and rotational symmetries and imprints a resonance structure into the density of photonic states. Obviously, the cavity will profoundly change the atomic coupling to the electromagnetic vacuum, and hence the way in which the atom reacts to incident light, as much with respect to light scattering as with respect to optical forces.

In this chapter we will focus on the dynamics of the optical field modes of a cavity pumped by incident laser beams. In Sec. 20.1 we study the behavior of empty cavities, and in Sec. 20.2 we turn our attention to the impact of atoms (or macroscopic scatterers) on the cavity dynamics. The impact of optical cavities on the internal and the motional dynamics of the atoms is the subject of the Chp. 22.6.1.

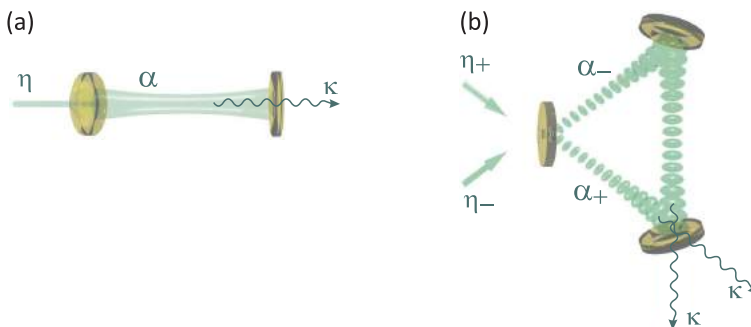


Figure 20.1: Scheme of (a) a linear cavity and (b) a ring cavity with optical modes  $\alpha_{\pm}$  pumped by incident light fields  $\eta_{\pm}$  and decaying into the void with rate  $\kappa$ .

## 20.1 Light fields in cavities without atoms

We will consider the degree of freedom to be studied in this chapter, which is the electric field amplitude of a light field developing in a mode of an optical cavity, as a classical entity. The quantization of the electromagnetic field will be discussed in the context of cavity QED in Sec. 22.5. Therefore, there is no need to stress quantum mechanics to derive the fundamental equations of motion, and a classical derivation is shown in Sec. 20.2.3. Nevertheless, for reasons of consistency with later discussions, where quantization is required, we will reproduce here the standard procedure, which consists in constructing the Hamiltonian for the relevant degrees of freedom. The degree of freedom under study being a mode of a cavity, we will label it by the field operator  $\hat{a}$  normalized to the electric field strength  $\vec{\mathcal{E}}_1$  generated by a single photon, such that  $|\langle \hat{a} \rangle|^2 = n$  represents the number of photons in the cavity.

In this first section of this chapter we will only consider a bare cavity not containing any matter which could interact with light. The mode of a linear cavity or the two counterpropagating modes of a ring cavity are pumped by incident laser light. We will first set up the equations of motion for the cavity fields and then discuss the main quantities characterizing a cavity, such as free spectral range, mode volume, decay rate, and single-photon field strength. Finally, we will calculate the density of states of cavities.

### 20.1.1 Master equation

The Hamiltonian of a laser-pumped linear cavity mode  $\hat{a}$  coupled to the continuum of a heat bath represented by operators  $\hat{a}_\omega$  is ( $\hbar = 1$ ),

$$\begin{aligned}
 \hat{H} &= \hat{H}_{cavity} + \hat{H}_{bath} + \hat{H}_{cavity:bath} + \hat{H}_{laser:cavity} \\
 \hat{H}_{cavity} &= \omega_0 \hat{a}^\dagger \hat{a} \\
 \hat{H}_{bath} &= \sum_{\omega} \omega \hat{a}_\omega^\dagger \hat{a}_\omega \\
 \hat{H}_{cavity:bath} &= \sum_{\omega} g_{cavity:bath} \hat{a}_\omega^\dagger \hat{a} + h.c. \\
 \hat{H}_{laser:cavity} &= \eta \hat{a}^\dagger + h.c.
 \end{aligned} \tag{20.1}$$

with  $[\hat{a}_\omega, \hat{a}_{\omega'}^\dagger] = \delta_{\omega, \omega'}$ . The part of the Hamiltonian  $\hat{H}_{laser:cavity}$  describes pumping of the cavity with an external light field matched to the cavity mode. The standard procedure consists in setting up the quantum Liouville equation for the total density operator  $\hat{\rho}_{total} = \hat{\rho}_{cavity} \otimes \hat{\rho}_{bath}$ , assuming a *quantum Wiener process*, and tracing the over the bath's degrees of freedom [258, 147]. From this procedure, as shown in Sec. 16.2.4, we derive a master equation for the reduced density operator  $\hat{\rho}$ .

The inevitable coupling of the cavity to the environment, described by  $\hat{H}_{cavity:bath}$ , leads to irreversible losses. These losses can be described as spontaneous decay to the continuous vacuum heat bath. The irreversibility of the process is readily understood in terms of the phase space offered by the vacuum being much larger. In fact, whenever discrete states are coupled to a continuum, the equilibrium is very much on the side of the continuum, that is, *discrete states decay*. Since an optical cavity can be considered

a *temperature reservoir*  $T$ , where,

$$\bar{n} = \frac{1}{1 - e^{-\hbar\omega/k_B T}}, \quad (20.2)$$

is the mean thermal photon number, the *Lindblad operator* is,

$$\begin{aligned} \mathcal{L}_{bath}\hat{\rho} = & \frac{\kappa}{2}(\bar{n} + 1)(2\hat{a}\hat{\rho}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}) + \frac{\kappa}{2}\bar{n}(2\hat{a}^\dagger\hat{\rho}\hat{a} - \hat{a}\hat{a}^\dagger\hat{\rho} - \hat{\rho}\hat{a}\hat{a}^\dagger) \\ & + \beta(2\bar{n} + 1)(2\hat{a}^\dagger\hat{a}\hat{\rho}\hat{a}^\dagger\hat{a} - (\hat{a}^\dagger\hat{a})^2\hat{\rho} - \hat{\rho}(\hat{a}^\dagger\hat{a})^2). \end{aligned} \quad (20.3)$$

We have already shown this in Exc. 16.2.6.1. The constants are the *cavity decay rate*  $\kappa$  and the pump rate  $\beta$ . Note that at room temperature in the microwave regime,  $\bar{n}$  may be as large as a few hundred photons, whereas in the optical regime we may neglect the thermal excitation,

$$\begin{cases} \dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \mathcal{L}_{cav} \\ \mathcal{L}_{cav}\hat{\rho}(t) = -\kappa\{\hat{a}^\dagger\hat{a}\hat{\rho}(t) - 2\hat{a}\rho(t)\hat{a}^\dagger + \hat{\rho}(t)\hat{a}^\dagger\hat{a}\} \end{cases}. \quad (20.4)$$

The expectation values are given by a *quantum Langevin equation* [147],

$$\dot{\alpha} = \langle \dot{\hat{a}} \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{a}] \rangle - \kappa \langle \hat{a} \rangle = (-\kappa - i\Delta_c)\alpha + \eta, \quad (20.5)$$

whose solution is easy to derive,

$$\alpha(t) = \left( \alpha(0) - \frac{\eta}{\kappa + i\Delta_c} \right) e^{(-\kappa - i\Delta_c)t} + \frac{\eta}{\kappa + i\Delta_c}, \quad (20.6)$$

or, using the electric field normalized to the amplitude of the field generated by a single photon,  $\vec{\mathcal{E}}_{cav}^+ = \vec{\mathcal{E}}_1\alpha$ ,

$$\begin{aligned} \vec{\mathcal{E}}_{cav}(z, t) &= \text{Re} \left[ \vec{\mathcal{E}}_1 e^{i(kz - \omega t)} \alpha(t) + \vec{\mathcal{E}}_1 e^{i(-kz - \omega t)} \alpha(t) \right] \\ &= 2\vec{\mathcal{E}}_1 \cos kz \text{Re} [e^{-i\omega t} \alpha(t)] \\ &= 2\vec{\mathcal{E}}_1 \cos kz \text{Re} \left[ \left( \alpha(0) - \frac{\eta}{\kappa + i\Delta_c} \right) e^{(-\kappa - i\omega_c)t} + \frac{\eta}{\kappa + i\Delta_c} e^{-i\omega t} \right]. \end{aligned} \quad (20.7)$$

The result (20.7) shows that, letting  $\eta = 0$ , we see that the cavity field decays with the time constant  $\kappa$  from the stationary situation.  $\kappa$  also corresponds to the HWHM of the *field intensity*,  $|\alpha(|\Delta_c| = \kappa)|^2 = \frac{1}{2}|\alpha(0)|^2$ . Note, that the intensity decays as  $2\kappa$ , and the HWHM of the *field amplitude* is  $|\alpha(|\Delta_c| = \sqrt{3}\kappa)| = \frac{1}{2}|\alpha(0)|$ .

**Example 88 (Evolution of the modes of a linear cavity):** (20.7) also shows that a cavity initially filled with a strong resonant light field  $|\alpha(0)| \gg \eta/\kappa$  begins to oscillate at its own frequency  $\omega_c$ , before the pump dominates and imposes its own frequency  $\omega$ . This is illustrated in Fig. 20.2. .

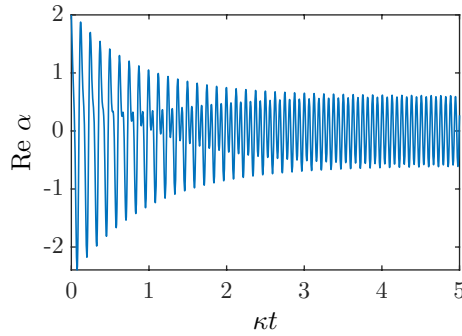


Figure 20.2: (code) Transient oscillations in a cavity pumped out of resonance.

Frequently, we are interested in the light reflected from a cavity. The reflective response of the cavity to an incident pump beam  $E_{in}$  is,

$$\vec{\mathcal{E}}_{refl}^+ = r_{in}\vec{\mathcal{E}}_{in}^+ + t_{in}\vec{\mathcal{E}}_{cav}^+ . \quad (20.8)$$

Also we may want to consider a temporal variation of the input field, for example of its detuning,  $\Delta_c(t)$ . In such cases, the equation (20.5) can not be integrated easily, and we need to resort to numerical methods. The simplest (and least convergent) method in a Newtonian iteration like,

$$\vec{\mathcal{E}}_{refl}^+(t + dt) = \vec{\mathcal{E}}_{refl}^+(t) + dt t_{in} \left[ (-\kappa - i\Delta_c(t))\vec{\mathcal{E}}_{cav}^+(t) + \eta\vec{\mathcal{E}}_{in}^+(t) \right] . \quad (20.9)$$

We will study in Exc. 20.1.5.1 how a sudden change of the pump laser detuning may lead to *ringing* with a fixed frequency  $\Delta_c$ . In Exc. 20.1.5.2 we will show, how it is possible to empty an optical cavity in times shorter than  $1/\kappa$ .

### 20.1.2 Dynamics of an empty ring cavity

In case of an ring cavity, we have two counterpropagating modes  $\alpha_{\pm}$ , which may be independently pumped by laser beams  $\eta_{\pm}$ . Hence, the quantum Langevin equation (20.5) must be generalized to,

$$\dot{\alpha}_{\pm}(t) = (-\kappa - i\Delta_c)\alpha_{\pm} + \eta_{\pm} , \quad (20.10)$$

and the general solution (20.6) to,

$$\alpha_{\pm}(t) = \left( \alpha_{\pm}(0) - \frac{\eta_{\pm}}{\kappa + i\Delta_c} \right) e^{(-\kappa - i\Delta_c)t} + \frac{\eta_{\pm}}{\kappa + i\Delta_c} . \quad (20.11)$$

The two counterpropagating field modes will, provided they have the same polarization, interfere and form a standing light wave. In contrast to linear cavities, the phase of this standing wave is represents a degree of freedom, as it depends on the phases of the two field modes  $\alpha_{\pm}$ , which in turn can be controlled by the incident

laser fields  $\eta_{\pm}$ . To better understand the behavior of the phase as a function of the pump beams, we analyze the interference of the two modes, which is described by,

$$\alpha_+ \alpha_-^* = \left( \alpha_+(0) \alpha_-^*(0) - \frac{\eta_-^* \alpha_+(0)}{\kappa - i\Delta_c} - \frac{\eta_+ \alpha_-^*(0)}{\kappa + i\Delta_c} + \frac{\eta_+ \eta_-^*}{\kappa^2 + \Delta_c^2} \right) e^{-2\kappa t} + \frac{\eta_+ \eta_-^*}{\kappa^2 + \Delta_c^2} + \left( \alpha_+(0) \frac{\eta_-^*}{\kappa - i\Delta_c} - \frac{\eta_+ \eta_-^*}{\kappa^2 + \Delta_c^2} \right) e^{(-\kappa - i\Delta_c)t} + \left( \alpha_-^*(0) \frac{\eta_+}{\kappa + i\Delta_c} - \frac{\eta_+ \eta_-^*}{\kappa^2 + \Delta_c^2} \right) e^{(-\kappa + i\Delta_c)t}. \quad (20.12)$$

To simplify this expression, we assume a symmetric pump,  $\eta_{\pm} = \eta e^{\pm i\phi}$ . We are interested in the reaction of the field's phase to a sudden change of  $\phi$ . Now, we define the initial stationary conditions for  $\phi = 0$  to be  $\alpha_{\pm}(0) = \frac{\eta}{\kappa + i\Delta_c}$  and obtain,

$$\alpha_+ \alpha_-^* = \frac{\eta^2}{\kappa^2 + \Delta_c^2} \left[ (1 - e^{i\phi})^2 e^{-2\kappa t} + e^{2i\phi} + 2e^{i\phi} (1 - e^{i\phi}) e^{-\kappa t} \cos \Delta_c t \right]. \quad (20.13)$$

In resonance,  $\Delta_c = 0$ , the expression (20.13) simplifies to,

$$\alpha_+ \alpha_-^* = \frac{\eta^2}{\kappa^2} \left[ (1 - e^{-\kappa t}) e^{i\phi} + e^{-\kappa t} \right]^2. \quad (20.14)$$

This results shows that the cavity phase adjusts itself to the pump field in exponential time  $\kappa^{-1}$ :

$$\tan \theta = \frac{\text{Im } \alpha_+ \alpha_-^*}{\text{Re } \alpha_+ \alpha_-^*} = \frac{(1 - e^{-\kappa t})^2 \sin 2\phi + 2(1 - e^{-\kappa t}) e^{-\kappa t} \sin \phi}{(1 - e^{-\kappa t})^2 \cos 2\phi + 2(1 - e^{-\kappa t}) e^{-\kappa t} \cos \phi + e^{-2\kappa t}}. \quad (20.15)$$

For small phase slips  $\phi \ll \pi$ , this reduces to,

$$\theta = 2\phi(1 - e^{-\kappa t}) \quad , \quad \dot{\theta} \simeq \kappa(2\phi - \theta) \quad , \quad \ddot{\theta} \simeq -\kappa\dot{\theta}. \quad (20.16)$$

Hence, the pump represents a friction force for the phase.

Out of resonance but with negligible decay,  $\kappa \simeq 0$ , the expression (20.13) simplifies to,

$$\alpha_+ \alpha_-^* = \frac{\eta^2}{\Delta_c^2} \left[ 1 + 2(e^{2i\phi} - e^{i\phi})(1 - \cos \Delta_c t) \right] + , \quad (20.17)$$

such that,

$$\tan \theta = \frac{2(\sin 2\phi - \sin \phi)(1 - \cos \Delta_c t)}{1 + 2(\cos 2\phi - \cos \phi)(1 - \cos \Delta_c t)}, \quad (20.18)$$

which, for very small angles  $\phi$ , reduces to,

$$\theta \simeq 4\phi \sin^2 \frac{1}{2} \Delta_c t. \quad (20.19)$$

### 20.1.2.1 Transfer function of a ring cavity

Cavities have a finite response time to frequency or amplitude fluctuations of the pump light. To study this, we assume the light pumping a ring cavity to be subject to a phase modulation with frequency  $\Omega$  and amplitude  $\phi_0$ , that is, the quantum Langevin equation (20.5) is,

$$\left( \partial_t + \kappa + i\Delta_c \right) \alpha_{\pm} = \eta e^{\pm i\phi_0 \sin \Omega t}, \quad (20.20)$$



and has the solution,

$$\alpha_{\pm}(t) = e^{(-\kappa - i\Delta_c)t} \left( \alpha_{\pm}(0) + \eta \int_0^T e^{(\kappa + i\Delta_c)\tau \pm i\phi_0 \sin \Omega \tau} d\tau \right). \quad (20.21)$$

For small amplitude oscillations, we can expand the pump term into a Fourier series of Bessel functions,

$$\begin{aligned} \alpha_{\pm}(t) &= e^{(-\kappa - i\Delta_c)t} \left( \alpha_{\pm}(0) + \eta \int_0^T \left( e^{(\kappa + i\Delta_c)\tau} \pm \frac{\phi_0}{2} e^{(\kappa + i\Delta_c)\tau + i\Omega\tau} \mp \frac{\phi_0}{2} e^{(\kappa + i\Delta_c)\tau - i\Omega\tau} \right) d\tau \right) \\ &= e^{(-\kappa - i\Delta_c)t} \alpha_{\pm}(0) + \eta \frac{1 - e^{(-\kappa - i\Delta_c)t}}{\kappa + i\Delta_c} \pm \frac{\phi_0}{2} \frac{e^{i\Omega t} - e^{(-\kappa - i\Delta_c)t}}{\kappa + i\Delta_c + i\Omega} \mp \frac{\phi_0}{2} \frac{e^{-i\Omega t} - e^{(-\kappa - i\Delta_c)t}}{\kappa + i\Delta_c - i\Omega} \\ &= \frac{\eta}{\kappa + i\Delta_c} \pm \frac{\phi_0 \eta}{2} \frac{e^{i\Omega t} - e^{(-\kappa - i\Delta_c)t}}{\kappa + i\Delta_c + i\Omega} \mp \frac{\phi_0 \eta}{2} \frac{e^{-i\Omega t} - e^{(-\kappa - i\Delta_c)t}}{\kappa + i\Delta_c - i\Omega} \\ &= \frac{\eta}{\kappa} \pm i\phi_0 \eta \frac{\kappa \sin \Omega t - \Omega \cos \Omega t + \Omega e^{-\kappa t}}{\kappa^2 + \Omega^2}. \end{aligned} \quad (20.22)$$

In the last two steps, we defined for simplicity,  $\alpha_{\pm}(0) = \frac{\eta}{\kappa + i\Delta_c}$  and set  $\Delta_c = 0$ . After some initial transients, when  $t \gg \kappa^{-1}$ , we can write,

$$\begin{aligned} \alpha_{\pm} \alpha_{\pm}^* &= \frac{\eta^2}{\kappa^2} + \phi_0^2 \eta^2 \left( \frac{\kappa \sin \Omega t - \Omega \cos \Omega t}{\kappa^2 + \Omega^2} \right)^2 \\ \alpha_{\pm} \alpha_{\mp}^* &= \left( \frac{\eta}{\kappa} \pm i\phi_0 \eta \frac{\kappa \sin \Omega t - \Omega \cos \Omega t}{\kappa^2 + \Omega^2} \right)^2, \end{aligned} \quad (20.23)$$

giving in analogy to (20.15),

$$\theta = \arctan \frac{2\phi_0(\kappa^2 + \Omega^2)(\kappa^2 \sin \Omega t - \kappa\Omega \cos \Omega t)}{(\kappa^2 + \Omega^2)^2 - \phi_0^2(\kappa^2 \sin \Omega t - \kappa\Omega \cos \Omega t)^2} \simeq 2\phi_0 \frac{\kappa^2 \sin \Omega t - \kappa\Omega \cos \Omega t}{\kappa^2 + \Omega^2}.$$

At low frequencies,  $\Omega \ll \kappa$ , the phase of the cavity field goes as,  $\theta(\phi_0) \simeq 2\phi_0 \sin \Omega t$ , and for high frequencies,  $\Omega \gg \kappa$ , as,  $\theta(\phi_0) \simeq -2\phi_0 \frac{\kappa}{\Omega} \cos \Omega t$ . Thus, we observe a low-pass behavior of the phase excursions of the cavity field with a cut-off frequency,  $\kappa^{-1}$ :

$$\theta_m \simeq \frac{2\phi_0}{1 + \Omega/\kappa}. \quad (20.24)$$

### 20.1.3 Characterization of the bare cavity

We first consider a linear cavity of length  $L$  pumped by a laser without any scatterer located inside the cavity. The cavity spectrum is an equidistant comb of eigenfrequencies separated by,

$$\delta_{f_{sr}} \equiv \tau_{rt}^{-1} = \frac{c}{2L}. \quad (20.25)$$

The *free spectral range*  $\delta_{f_{sr}}$  is given in units of a real frequency.  $\tau_{rt}^{-1}$  is the time for a photon to make a round trip in the cavity. The amplitude *decay rate of the cavity*,

$$\kappa = \tau_{\kappa}^{-1} = \frac{\pi \delta_{f_{sr}}}{F}. \quad (20.26)$$

The intensity decay rate of the cavity, measured by 'cavity ring-down' is  $\kappa_{int} = 2\kappa$ . Note, that  $\kappa_{int}$  is also the FWHM width of the intensity transmission spectrum <sup>1</sup>, such that the finesse

$$F = \frac{\delta_{fsr}}{\kappa_{int}/2\pi} \quad (20.27)$$

is simply the ratio between the free spectral range and the FWHM of the cavity intensity transmission curve, both measured in Hertz.

**Example 89 (Finesse of a cavity):** For example, for a cavity of length  $L = 10$  cm an intensity decay time of  $\tau_{int} = 20$   $\mu$ s is measured, and we want to evaluate the finesse. We begin calculating the free spectral range  $\delta_{fsr} = c/2L \approx 1.5$  GHz. Since the cavity field decays like  $E(t) = E_0 e^{-\kappa t}$  and the intensity like  $I(t) = E_0^2 e^{-2\kappa t}$ , we get  $\kappa = 1/\tau_{int} = 1/2\tau_{int} \approx (2\pi) 4$  kHz. Finally, the finesse is  $F = \pi\delta_{fsr}/\kappa \approx 189000$ .

For a cavity with a given geometry filled with a Gaussian mode of light with power  $P$ , the intensity is determined by Gaussian optics <sup>2</sup>,

$$I(\mathbf{r}) = \frac{2P}{\pi w^2(z)} e^{-2\rho^2/w^2(z)} \quad \text{and} \quad w(z) = w_0 \sqrt{1 + \left(\frac{\lambda z}{\pi w_0^2}\right)^2}. \quad (20.28)$$

Defining the *mode volume* via  $I(0)V_m \equiv \int I(\mathbf{r})dV$  and evaluating the spatial integral over the Gaussian mode along the cavity, we obtain,

$$\boxed{V_m = \frac{\pi}{4} L w_0^2}. \quad (20.29)$$

Defining the amplitude of the electric field generated by a *single photon* via,

$$I(\mathbf{r}) = n\varepsilon_0 c \mathcal{E}_1^2(\mathbf{r}), \quad (20.30)$$

where  $n$  is the number of photons in the cavity, we calculate for the energy stored in the cavity,

$$\begin{aligned} \int \varepsilon_0 |\vec{\mathcal{E}}_1(\mathbf{r})|^2 dV &= \varepsilon_0 \int \frac{I(\mathbf{r})}{n\varepsilon_0 c} \rho d\rho d\phi dz = \frac{1}{nc} \int \frac{2P}{\pi w^2(z)} e^{-2\rho^2/w^2(z)} \rho d\rho d\phi dz \quad (20.31) \\ &= \frac{1}{nc} \frac{P}{2} L = \frac{1}{nc} \frac{n\hbar\omega\delta_{fsr}}{2} L = \frac{\hbar\omega}{2}. \end{aligned}$$

Hence,

$$|\vec{\mathcal{E}}_1(0)| = \sqrt{\frac{I(0)}{n\varepsilon_0 c}} = \sqrt{\frac{1}{n\varepsilon_0 c} \frac{2P}{\pi w_0^2}} = \sqrt{\frac{1}{n\varepsilon_0 c} \frac{Ln\hbar\omega\delta_{fsr}}{2V_m}}.$$

Inserting the expression (20.25) for the free spectral range of a cavity we get,

$$\boxed{|\vec{\mathcal{E}}_1(0)| = \sqrt{\frac{\hbar\omega}{2\varepsilon_0 V_m}}}. \quad (20.32)$$

<sup>1</sup>See script on *Electrodynamics* (2020), Sec. 7.3.5 and Exc. 7.3.6.17.

<sup>2</sup>See script on *Electrodynamics* (2020), Sec. 7.4.1 and Exc. 7.4.3.1.

The light power can now be expressed as,

$$P = \frac{\pi\omega_0^2}{2} I(0) = \frac{2V_m}{L} n\varepsilon_0 c |\mathcal{E}_1^2(0)| = 2V_m \delta_{fsr} n\varepsilon_0 \frac{\hbar\omega}{2\varepsilon_0 V_m} = \delta_{fsr} n \hbar\omega . \quad (20.33)$$

We assume that the cavity is pumped by a laser beam. To estimate the pump rate, we assume that the power  $P_{input}$  be measured in transmission. The coefficient  $\eta$  for resonant pumping is related to the number  $n$  of photons inside the cavity,

$$n = |\alpha|^2 = \frac{\eta^2}{\kappa^2} . \quad (20.34)$$

The intracavity field is resonantly amplified by the finesse,

$$\alpha = \sqrt{\frac{F}{\pi}} \alpha_{input} = \sqrt{\frac{\delta_{fsr}}{\kappa}} \alpha_{input} . \quad (20.35)$$

This gives,

$$\eta = \kappa\alpha = \kappa \sqrt{\frac{I}{c\hbar\omega}} V_m = \sqrt{\kappa\delta_{fsr}} \alpha_{input} = \sqrt{\kappa\delta_{fsr}} \sqrt{\frac{I_{input}}{c\hbar\omega}} V_m . \quad (20.36)$$

In practice, the pump rate will depend on the quality of the phase matching of the Gaussian beams and the impedance matching (in case of partially absorbing mirrors).

We will pursue the characterization of ring cavities including their interaction with scattering atoms in Sec. 20.2.2.

## 20.1.4 Density of states in cavities

Let us now calculate the density of states  $\rho(\omega, \mathbf{k})$  of an optical cavity. It is defined by,

$$\int_{\mathcal{R}} \rho(\omega, \mathbf{k}) d\omega d\Omega = \frac{1}{(2\pi)^3} \int d^3\mathbf{x} d^3\mathbf{k} , \quad (20.37)$$

where  $\mathcal{R}$  denotes the boundary imposed by the cavity. For free space photons we calculate,

$$4\pi \int \rho_{free}(\omega, \mathbf{k}) d\omega = \frac{V}{(2\pi)^3} \int k^2 \sin\theta d\theta d\phi dk = \frac{Vk^3}{6\pi^2} = \frac{V\omega^3}{6\pi^2 c^3} , \quad (20.38)$$

such that,

$$\rho_{free}(\omega, \mathbf{k}) = \rho_{free}(\omega) = \frac{V\omega^2}{(2\pi c)^3} , \quad (20.39)$$

is isotropic. This corresponds to the density-of states of a radiating blackbody (1.53).

### 20.1.4.1 The role of cavity geometry

For light in a cavity, the density of states is modified with respect to free space, because it becomes frequency-dependent and anisotropic. The frequency dependence is expressed by the Airy formula,

$$\mathcal{L}(\omega) \equiv \frac{I_{cav}}{I_{in}} = \frac{\sqrt{1 + (2F/\pi)^2}}{1 + (2F/\pi)^2 \sin^2 kL} , \quad (20.40)$$

which will be derived in Excs. 20.1.5.3 and 20.1.5.4, and the anisotropy by,

$$\mathcal{R}(\hat{\mathbf{e}}_k) = 1 \quad \forall \quad \hat{\mathbf{e}}_k \in \Omega_{cav} , \quad (20.41)$$

where  $\Omega_{cav}$  is the solid angle covered by the cavity mode. The formula,

$$\rho_{cav}(\omega, \mathbf{k}) = \rho_{free}(\omega)[1 - \mathcal{R}(\hat{\mathbf{e}}_k)] + \rho_{free}(\omega)\mathcal{L}(\omega)\mathcal{R}(\hat{\mathbf{e}}_k) \quad (20.42)$$

expresses that the density of states is nothing more than the *structure factor* of the cavity.

#### 20.1.4.2 Confocal cavities

For a confocal cavity the solid angle is easy to calculate [316, 317]. Denoting by  $b$  is the clear aperture of the cavity mirrors, we get,

$$\Omega_{cav,con} = 2 \int_0^{2\pi} \int_0^{\arcsin(2b/L)} \sin\theta d\theta d\phi = 4\pi \left( 1 - \sqrt{1 - 4\frac{b^2}{L^2}} \right) . \quad (20.43)$$

Expanding the root for small  $b \ll L$ , we get,

$$\boxed{\Omega_{cav,con} \simeq \frac{8\pi b^2}{L^2}} . \quad (20.44)$$

For non-degenerate geometries the functions  $\mathcal{L}$  and  $\mathcal{R}$  depend on the order  $mn$  of the transverse Gaussian modes:

$$\mathcal{L}_{mn}(\omega) = \frac{\sqrt{1 + (2F/\pi)^2}}{1 + (2F/\pi)^2 \sin^2(kL + \varphi_{mn})} \quad \text{and} \quad \mathcal{R}_{mn}(\hat{\mathbf{e}}_k) = 1 \quad \forall \quad \hat{\mathbf{e}}_k \in \Omega_{mn} ,$$

where  $\varphi_{mn}$  is the frequency shift of the transverse modes.

#### 20.1.4.3 Expansion into Hermite-Gaussian modes

More correctly,  $\hat{\mathbf{e}}_k \in \Omega_{mn}$  means that we must weigh the density of states by the structure factor of the mode volume, which is nothing more than the Fourier transform of the cavity mode function,

$$\boxed{\mathcal{R}_{mn}(\hat{\mathbf{e}}_k) = \int_{\hat{\mathbf{e}}_k \in \Omega_{mn}} d^2k = \int_{\mathbb{R}^2} \mathcal{F} \left[ \frac{u_{mn}(\mathbf{r})}{\hbar\omega} \right] d^2k} . \quad (20.45)$$

For a Hermite-Gaussian mode with waist  $w(z)$ ,

$$u_{mn}(\mathbf{r}) = \hbar\omega \frac{w_0}{w} e^{-2(x^2+y^2)/w^2} H_m(\sqrt{2}x/w)^2 H_n(\sqrt{2}y/w)^2 . \quad (20.46)$$

The Hermite polynomials are the eigenfunctions of the Fourier transform,

$$\mathcal{F}[e^{-x^2/2} H_n(x)] = (-i)^n e^{-k^2/2} H_n(k) . \quad (20.47)$$

Hence,

$$\begin{aligned} \mathcal{F} \left[ \frac{1}{\hbar\omega} u_{mn}(\mathbf{r}) \right] &= \frac{1}{\hbar\omega} \frac{w_0}{w} \mathcal{F} \left[ e^{-2(x^2+y^2)/w^2} H_m(\sqrt{2}x/w)^2 H_n(\sqrt{2}y/w)^2 \right] \\ &= \frac{1}{\hbar\omega} \frac{w_0}{w} \mathcal{F} \left[ e^{-2x^2/w^2} H_m(\sqrt{2}x/w)^2 \right] \mathcal{F} \left[ e^{-2y^2/w^2} H_n(\sqrt{2}y/w)^2 \right] \\ &= \frac{1}{\hbar\omega} \frac{w_0}{w} e^{-2k_x^2 w^2} H_m(\sqrt{2}k_x w)^2 e^{-2k_y^2 w^2} H_n(\sqrt{2}k_y w)^2 \xrightarrow{m,n=0} \frac{1}{\hbar\omega} \frac{w_0}{w} e^{-2(k_x^2+k_y^2)w^2}. \end{aligned} \quad (20.48)$$

Finally,

$$\begin{aligned} \mathcal{R}_{mn}(\hat{\mathbf{e}}_k) &= \int \mathcal{F} \left[ \frac{u_{mn}(\mathbf{r})}{\hbar\omega} \right] d\left(\frac{k_x}{k}\right) d\left(\frac{k_y}{k}\right) \\ &= \frac{1}{\hbar\omega} \frac{w_0}{w} \int e^{-2k_x^2 w^2} H_m(\sqrt{2}k_x w)^2 d\left(\frac{k_x}{k}\right) \int e^{-2k_y^2 w^2} H_n(\sqrt{2}k_y w)^2 d\left(\frac{k_y}{k}\right). \end{aligned} \quad (20.49)$$

For the TEM<sub>00</sub> mode, we get,

$$\mathcal{R}_{00}(\hat{\mathbf{e}}_k) = \frac{\pi}{2k^2 w^2}, \quad (20.50)$$

using  $P = \int I_{mn}(\mathbf{r}) dx dy = \frac{1}{2} \pi w^2 I_0$ . This coincides with the intuition, that for the TEM<sub>00</sub>, the aperture is simply the divergence angle of the Gaussian mode.

The solid angle of a Gaussian mode in a non-degenerate cavity is calculated via,

$$\Omega_{cav} = 2 \cdot \frac{\pi w(z)^2}{z^2} = 2 \cdot \frac{\pi w_0^2}{z^2} \left( 1 + \left( \frac{\lambda z}{\pi w_0^2} \right)^2 \right). \quad (20.51)$$

In the far field, we get,

$$\boxed{\Omega_{cav} \xrightarrow{z \rightarrow \infty} \frac{8\pi}{k^2 w_0^2}}. \quad (20.52)$$

**Example 90 (Solid angle for Hermite-Gaussian modes in a confocal cavity):** For confocal cavities, we must add  $\sum_{mn} \mathcal{F} \left[ \frac{1}{\hbar\omega} u_{mn}(\mathbf{r}) \right]$  up to a limit, where the maximum  $H_m(\sqrt{2}kw)$  is cut by the finite aperture of the mirrors of the cavity. Empirically, we find that  $H_n(\xi)^2 e^{-\xi^2}$  has its maximum at  $\xi_{\max} = 13.7 \cdot n^{1/2}$ . From the condition  $u_{mn}(x, y, L) = 0$  for  $xy > a^2$ , we obtain,

$$\begin{aligned} x_{\max} y_{\max} &< a^2 \\ (13.7 \cdot n^{1/2})^2 &= \frac{\sqrt{2} x_{\max}}{w(L)} \frac{\sqrt{2} y_{\max}}{w(L)} < \frac{2a^2}{w(L)^2} \rightarrow \frac{a^2 k^2 w_0^2}{2L^2}, \end{aligned}$$

using  $w(L) = w_0 \sqrt{1 + \left( \frac{\lambda L}{\pi w_0^2} \right)^2} \rightarrow \frac{\lambda L}{\pi w_0}$ . Finally,

$$\sum_{mn} \mathcal{F} \left[ \frac{1}{\hbar\omega} u_{mn}(\mathbf{r}) \right] = \frac{\pi}{2k^2 w^2} \sum_{13.7^2 m, n < a^2 k^2 w_0^2 / 2L^2} = \frac{\pi}{2k^2 w^2} \frac{1}{13.7^2} \frac{a^2 k^2 w_0^2}{2L^2} = \frac{1}{13.7^2} \frac{\pi a^2}{4L^2}.$$

## 20.1.5 Exercises

### 20.1.5.1 Ex: Quick ullage of an optical cavity

Consider a linear cavity resonantly pumped by a laser beam until a stationary state is reached. Suddenly, the phase of the incident light is changed by  $180^\circ$ . Based on equation (20.6), analyze the evolution of the light field inside the cavity.

### 20.1.5.2 Ex: Ringing of an optical cavity

Consider a linear cavity with resonant frequency  $\omega_c$  and the decay rate  $\kappa$  pumped by a laser beam whose frequency is swept linearly over a range  $\omega \in [-10\kappa, 10\kappa]$ . Prepare a numerical simulation varying the time  $\Delta t$  of the sweep.

### 20.1.5.3 Ex: Derivation of the Airy formula

Derive the Airy formula (20.40).

### 20.1.5.4 Ex: Airy formula for ring cavities

Derive the Airy formulas for a ring cavity laser-pumped through an incoupling mirror with reflectivity  $r_{ic}$  and comprising two more high-reflecting mirrors with reflectivity  $r_{hr}$ . Calculate (a) the intracavity intensity, (b) the intensity of the light reflected from the incoupler, and (c) the intensity of the light transmitted through the first encountered high reflector. For each for intensity study the cases that (i) the ring cavity is resonant and (ii) off-resonance. Also study the limit  $r_{hr} \rightarrow 1$ . Disregard absorption losses.

### 20.1.5.5 Ex: Filling rate for long cavities

Using the solution (20.6) try to calculate the transmission of a 15 km long cavity of finesse  $F = 1000$  as a function of time, when it is pumped by a suddenly switched on laser. Analyze the results in the light of local causality.

## 20.2 Interaction of atoms with cavities

Until now we disregarded the possibility that the atoms in the ensemble be correlated. In Sec. 15.1 we have shown how to describe the dynamics of a single two-level atom driven by a quantized electromagnetic field and embedded in an electromagnetic vacuum under the assumption that the driving field be a plane wave and the vacuum be isotropic. In the following, we want to relax these conditions. We proceed by generalizing Eq. (15.7) by replacing the plane wave  $e^{i\mathbf{k}\cdot\mathbf{r}}$  by a mode function  $u_{\mathbf{k}}(\mathbf{r})$  and by allowing the coupling constant (15.17)  $g_{\mathbf{k}}$  to depend on  $\mathbf{k}$ . Furthermore, we will extend the formalism to the presence of several atoms. We will study *ab initio* atoms subject to cooperative environments imposed by the presence of other atoms or the presence of cavities. We note that the role of cavities can be understood as generating mirror images with which the atom under consideration interacts. We restrict to non-interacting atoms, that is, free atoms or atoms trapped in external potentials that only interact with each other via re-scattering of an incident radiation field, i.e. no

collisions and no properties requiring symmetrization of their wavefunctions. Both the atomic excitation and the radiation fields may decay.

In Sec. 20.2.1 we study a single atom or two atoms in a cooperative environment (e.g. a cavity). In particular, we will find that spontaneous emission is affected by the presence of a cavity. A wider discussion of scattering from correlated atoms will be presented in Sec. 21.1. Then in Sec. 20.2.2 we will introduce some parameters characterizing the interaction between atoms and cavities. In particular, we will relate the important notions of the *cooperativity* of several atoms and the structure factor for light scattering, with the cavity-to-free space scattering ratio, the finesse and the density-of-states of a cavity, simply by pointing out that a cavity multiplies the number of atoms interacting with a light modes by the number of its mirror images. Finally, in Secs. 20.2.3 to 20.2.5 we study the impact of cavities on the atomic motion.

## 20.2.1 Spontaneous emission in a cooperative environment

### 20.2.1.1 Atoms in a cooperative environment

The quantization of the electromagnetic field has been presented in Sec. 15.1.1 for the case of plane wave radiation modes. In the following, we want to generalize the treatment to arbitrary field modes characterized by mode functions  $\mathbf{u}_{\mathbf{k}\lambda}(\mathbf{r})$  labeled by a wavevector and a polarization. These are classical vector functions satisfying the vector Helmholtz equation and the transversality condition,

$$[\nabla^2 + k_\lambda^2]\mathbf{u}_{\mathbf{k}\lambda}(\mathbf{r}) = 0 \quad \text{and} \quad \nabla \cdot \mathbf{u}_{\mathbf{k}\lambda}(\mathbf{r}) = 0, \quad (20.53)$$

with  $k_\lambda = \omega_{\mathbf{k}\lambda}/c$  [487]. These classical functions are chosen to form an orthonormal set,

$$\int_V \mathbf{u}_{\mathbf{k}\lambda}^*(\mathbf{r}) \cdot \mathbf{u}_{\mathbf{k}'\lambda'}(\mathbf{r}) d^3r = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'}. \quad (20.54)$$

In free space, the plane wave approximation is generally good,

$$\mathbf{u}_{\mathbf{k}\lambda}^{free}(\mathbf{r}) = \frac{\vec{\epsilon}_\lambda}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (20.55)$$

where  $\vec{\epsilon}_{\mathbf{k}\lambda}$  is a polarization vector such that  $\mathbf{k} \cdot \vec{\epsilon}_{\mathbf{k}\lambda} = 0$  and  $V$  is the photon quantization volume.

Let us now rewrite the quantized transverse vector potential of the radiation field (15.7) as,

$$\hat{\mathbf{A}}(\mathbf{r}, t) = \sum_{\mathbf{k}\lambda} \sqrt{\frac{\hbar}{2\omega_{\mathbf{k}\lambda}\epsilon_0}} [\mathbf{u}_{\mathbf{k}\lambda}(\mathbf{r}) \hat{a}_{\mathbf{k}\lambda}(t) + \mathbf{u}_{\mathbf{k}\lambda}^*(\mathbf{r}) \hat{a}_{\mathbf{k}\lambda}^\dagger(t)]. \quad (20.56)$$

The quantum properties of the electric and magnetic field operators are determined by the bosonic annihilation and creation operators,  $\hat{a}_{\mathbf{k}\lambda}(t)$  and  $\hat{a}_{\mathbf{k}\lambda}^\dagger(t)$ , respectively, with usual commutation relations:  $[\hat{a}_{\mathbf{k}\lambda}(t), \hat{a}_{\mathbf{k}'\lambda'}(t)] = 0$  and  $[\hat{a}_{\mathbf{k}\lambda}(t), \hat{a}_{\mathbf{k}'\lambda'}^\dagger(t)] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'}$ .

For weak-coupling between the atoms and the field, one has the contributions to

the Hamiltonian,

$$\begin{aligned} \hat{H}_{atom} &= \hbar\omega_0\hat{\sigma}^z \\ \hat{H}_{field} &= \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}[\hat{a}_{\mathbf{k}\lambda}^\dagger(t)\hat{a}_{\mathbf{k}\lambda}(t) + \frac{1}{2}] \\ \hat{H}_{atom:field} &= -i\hbar \sum_{\mathbf{k},\lambda} (\hat{\sigma}^+ + \hat{\sigma}^-)[g_{\mathbf{k}\lambda}(\mathbf{r})\hat{a}_{\mathbf{k}\lambda} - g_{\mathbf{k}\lambda}^*(\mathbf{r})\hat{a}_{\mathbf{k}\lambda}^\dagger] \end{aligned}, \quad (20.57)$$

and,

$$g_{\mathbf{k}\lambda}(\mathbf{r}) \equiv \sqrt{\frac{\omega_{\mathbf{k}}}{2\varepsilon_0\hbar}} \mathbf{d} \cdot \mathbf{u}_{\mathbf{k}\lambda}(\mathbf{r}) \quad (20.58)$$

is a complex function associated with the coupling strength between the atom and the field.

By solving the Heisenberg equations of motion for the atomic and field operators within the Born and Markov approximations (or using the procedure leading to the expression (15.117)), one obtains the spontaneous emission rate on a transition  $|e\rangle \rightarrow |g\rangle$  of frequency  $\omega_0$ :

$$\Gamma(\mathbf{r}) = 2\pi \sum_{\mathbf{k},\lambda} |g_{\mathbf{k}\lambda}(\mathbf{r})|^2 \delta(\omega_{\mathbf{k}} - \omega_0). \quad (20.59)$$

which is the same result obtained by the Weisskopf-Wigner theory [487]. To evaluate the sum we need go to a continuous  $k$ -space via,

$$\sum_{\mathbf{k},\lambda} \rightarrow \lim_{V \rightarrow \infty} \sum_{\lambda} \frac{V}{8\pi^3} \int d^3k. \quad (20.60)$$

Hence, in free space, inserting the mode function (20.56),

$$\begin{aligned} \Gamma(\mathbf{r}) &= \frac{\pi\omega_0}{\varepsilon_0\hbar} \sum_{\mathbf{k},\lambda} |\mathbf{d} \cdot \mathbf{u}_{\mathbf{k}\lambda}(\mathbf{r})|^2 \delta(\omega_{\mathbf{k}} - \omega_0) \\ &= \frac{\hbar\omega_0}{8\pi^2\varepsilon_0\hbar^2} \lim_{V \rightarrow \infty} \sum_{\lambda} \int d^3k |\mathbf{d} \cdot \vec{\epsilon}_{\mathbf{k}\lambda}|^2 \delta(\omega_{\mathbf{k}} - \omega_0) \\ &= \lim_{V \rightarrow \infty} \sum_{\lambda} \int \frac{|\mathbf{d} \cdot \vec{\epsilon}_{\mathbf{k}\lambda}|^2 \bar{\mathcal{E}}_{\mathbf{k}}^2}{\hbar^2} 2\pi\delta(\omega_{\mathbf{k}} - \omega_0) \frac{V}{8\pi^3c} k^2 d\Omega_{\mathbf{k}} d\omega_{\mathbf{k}}. \end{aligned} \quad (20.61)$$

Plugging in the density of states for free space (1.53), we finally get,

$$\Gamma(\mathbf{r}) = \sum_{\lambda} \int \frac{|\mathbf{d} \cdot \vec{\epsilon}_{\mathbf{k}\lambda}|^2 \bar{\mathcal{E}}_{\mathbf{k}}^2}{\hbar^2} 2\pi\delta(\omega_{\mathbf{k}} - \omega_0) \rho(\omega_{\mathbf{k}}, \mathbf{k}) d\Omega_{\mathbf{k}} d\omega_{\mathbf{k}}, \quad (20.62)$$

where the density of states can now be arbitrarily shaped by the presence of boundary conditions, such as optical cavities or dielectric or metallic surfaces.

**Example 91 (Two atoms):** Let us now consider two excited atoms labeled by  $q = 1, 2$ , located at  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , and described by two of their eigenstates,  $\{|g_q\rangle, |e_q\rangle\}$ . As usual,  $|g_q\rangle$  is the eigenstate with lowest energy ( $E_{g_q} = -\frac{1}{2}\hbar\omega_q$ )



and longer lifetime, i.e. the ground state, whereas  $|e_q\rangle$  is the eigenstate with highest energy ( $E_{e_q} = +\frac{1}{2}\hbar\omega_q$ ). In presence of an external electromagnetic field, the Hamiltonian of the two atom-field system in the electric dipole approximation is,

$$\hat{H} = \sum_{q=1,2} [\hat{H}_{atom}^{(q)} + \hat{H}_{atom:field}^{(q)}] + \hat{H}_{field},$$

where  $\hat{H}_{atom}^{(q)} \equiv \hbar\omega_q\hat{s}_q^z$  is the atomic Hamiltonian, with  $\hat{s}_q^z \equiv \frac{1}{2}(|e_q\rangle\langle e_q| - |g_q\rangle\langle g_q|)$  being the energy operator of the  $q$ -th atom, and  $\hat{H}_{atom:field}^{(q)} \equiv -\hat{\mathbf{d}}_q \cdot \hat{\mathcal{E}}(\mathbf{r}_q)$  is the atom-field interaction Hamiltonian. The electric dipole moment operator satisfies  $\langle e_q|\hat{\mathbf{d}}_q|e_q\rangle = \mathbf{0} = \langle g_q|\hat{\mathbf{d}}_q|g_q\rangle$  and has non-vanishing off-diagonal elements, i.e. the eigenstates have no permanent dipole moment. We define the dipole-moment matrix element as  $\mathbf{d}_q \equiv \langle e_q|\hat{\mathbf{d}}_q|g_q\rangle$ . The description of the field is identical to the case of one atom (20.55).

For weak-coupling between the atoms and the field, the interaction Hamiltonian becomes,

$$\hat{H}_{atom:field} = -i\hbar \sum_{\mathbf{k},\lambda} \sum_{q=1,2} (\hat{s}_q^+ + \hat{s}_q^-) [g_{\mathbf{k}\lambda}(\mathbf{r}_q)\hat{a}_{\mathbf{k}\lambda} - g_{\mathbf{k}\lambda}^*(\mathbf{r}_q)\hat{a}_{\mathbf{k}\lambda}^\dagger],$$

where  $\hat{s}_q^+ \equiv |e_q\rangle\langle g_q|$  and  $\hat{s}_q^- \equiv |g_q\rangle\langle e_q|$  are the electric dipole raising and lowering operators, respectively, satisfying the well-known commutation and anti-commutation relations:  $[\hat{s}_q^+, \hat{s}_q^-] = 2\hat{s}_q^z\delta_{qq'}$ ,  $[\hat{s}_q^z, \hat{s}_q^\pm] = \pm\hat{s}_q^\pm\delta_{qq'}$ , and  $[\hat{s}_q^+, \hat{s}_q^-]_{\pm} = 0$  with  $(\hat{s}_q^\pm)^2 = 0$ .

By solving the Heisenberg equations of motion for the atomic and field operators within the Born and Markov approximations, one obtains the spontaneous emission rate on a transition  $|e_q\rangle \rightarrow |g_q\rangle$  of frequency  $\omega_q$ :

$$\Gamma_q = 2\pi \sum_{\mathbf{k},\lambda} |g_{\mathbf{k}\lambda}(\mathbf{r}_q)|^2 \delta(\omega_{\mathbf{k}} - \omega_q) = \frac{\pi\omega_q}{\varepsilon_0\hbar} \sum_{\mathbf{k},\lambda} |\mathbf{d}_q \cdot \mathbf{u}_{\mathbf{k}\lambda}(\mathbf{r}_q)|^2 \delta(\omega_{\mathbf{k}} - \omega_q),$$

which is the same result obtained by the Weisskopf-Wigner theory [487]. In addition, due to the coupling between the atoms through the vacuum field, one also has the cross-damping spontaneous emission rate:

$$\Gamma_q(\mathbf{r}_1, \mathbf{r}_2) = \Gamma_q(\mathbf{r}_2, \mathbf{r}_1) = \frac{\pi\omega_0}{\varepsilon_0\hbar} \sum_{\mathbf{k},\lambda} \text{Re} [\mathbf{d}_1 \cdot \mathbf{u}_{\mathbf{k}\lambda}(\mathbf{r}_1)\mathbf{u}_{\mathbf{k}\lambda}^*(\mathbf{r}_2) \cdot \mathbf{d}_2^*] \delta(\omega_{\mathbf{k}} - \omega_q),$$

which shows explicitly the cooperative effect of the dipole-dipole interaction in the spontaneous emission rate.

### 20.2.1.2 Modification of the natural linewidth by cavities

The *cooperativity parameter* of a cavity is defined as the rate at which an atom emits into the volume of a cavity mode normalized to the rate at which it would scatter into free space,

$$\Upsilon \equiv \frac{\Gamma_{cav}}{\Gamma_{free}}. \quad (20.63)$$

In a cavity, spontaneous emission is strongly modified [316, 317, 318]. An atom interacting with a cavity will spontaneously emit into the cavity mode at an increased (reduced) rate, depending on whether the cavity is resonant or out of resonance. The

natural width due to spontaneous decay and the line shift are calculated by integration over the coupling force between the atom and every available field mode [see (20.61)],

$$\begin{aligned} \Gamma &= \iint \frac{|\mathbf{d}_{eg} \cdot \vec{\epsilon}_{\mathbf{k}}|^2 |\vec{\mathcal{E}}_{\mathbf{k}}|^2}{\hbar^2} 2\pi \delta(\omega_0 - \omega_{\mathbf{k}}) \rho(\omega_{\mathbf{k}}, \mathbf{k}) d\Omega_{\mathbf{k}} d\omega_{\mathbf{k}} \\ \Delta\omega &= \sum_i \iint \frac{|\mathbf{d}_{ei} \cdot \vec{\epsilon}_{\mathbf{k}}|^2 |\vec{\mathcal{E}}_{\mathbf{k}}|^2}{\hbar^2} \frac{1}{\omega_{ei} - \omega_{\mathbf{k}}} \rho(\omega_{\mathbf{k}}, \mathbf{k}) d\Omega_{\mathbf{k}} d\omega_{\mathbf{k}} \end{aligned}, \quad (20.64)$$

with the field amplitude per photon,  $|\vec{\mathcal{E}}_{\mathbf{k}}| = \sqrt{\hbar\omega_{\mathbf{k}}/2\varepsilon_0 V}$ , derived in (20.32), and the index  $i$  running over all internal atomic states. These formulas are simply applications of second-order perturbation theory (6.16) and of Fermi's golden rule (6.112) for transition probabilities both weighed with dynamic structure factor of the cavity.

We use the number of modes per unit of frequency range and per unit of solid angle in free space derived in (20.39) ( $\rho/V$  is the density of states),

$$\rho_{free}(\omega_{\mathbf{k}}) = \frac{V\omega_{\mathbf{k}}^2}{(2\pi)^3 c^3}. \quad (20.65)$$

Setting  $\theta_{\mathbf{k}}$  as the angle between the atomic dipole moment and the cavity axis (which is not in place, yet, as we are still in free space),  $\mathbf{d} \cdot \hat{\epsilon}_{\mathbf{k}} = d \cos \alpha_{\mathbf{k}} = d \cos(90^\circ - \theta_{\mathbf{k}}) = d \sin \theta_{\mathbf{k}}$ ,

$$\begin{aligned} \Gamma_{free} &= \int \frac{d^2 \sin^2 \theta_{\mathbf{k}}}{\hbar^2} \frac{\hbar\omega_0}{2\varepsilon_0 V} 2\pi \frac{V\omega_0^2}{(2\pi)^3 c^3} \sin \theta d\theta d\phi \\ &= \frac{d^2 k^3}{4\pi\varepsilon_0 \hbar} \int_0^\pi \sin^3 \theta d\theta = \frac{d^2 k^3}{3\pi\varepsilon_0 \hbar}. \end{aligned} \quad (20.66)$$

Since the integration covers the whole solid angle of space  $4\pi$  and the free space is isotropic, there is no preferred orientation, and we can perform the integration setting  $\theta \equiv \theta_{\mathbf{k}}$ . The result coincides with earlier calculations (13.43).

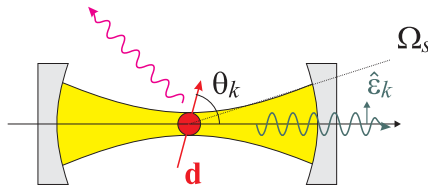


Figure 20.3: Illustration of cooperativity in a cavity. An excited atom can decay by emitting light into a cavity mode or into free space. Note that the cavity is not pumped directly by an incident laser beam.

Now, we put the cavity in place, but tune it off resonance, such that no photons can be emitted into the solid angle covered by the cavity. That is, in the presence of the cavity, the solid angle of free space into which photons can be emitted is restricted. We repeat the calculation (20.66), but now we are not free to choose the axis of the

coordinate system arbitrarily. Instead, we assume that  $\theta_{\mathbf{k}}(\theta, \phi) \simeq \text{const}$  over the small solid angle covered by the cavity,  $\theta, \phi \in \Omega_{cav}$ ,

$$\begin{aligned} \Gamma_{free \notin cav} &= \int_{\hat{\mathbf{e}}_{\mathbf{k}} \notin cav} \frac{d^2 \sin^2 \theta_{\mathbf{k}}}{\hbar^2} \frac{\hbar \omega_0}{2\varepsilon_0 V} 2\pi \frac{V \omega_0^2}{(2\pi)^3 c^3} \sin \theta d\theta d\phi \\ &\simeq \Gamma_{free} - \frac{d^2 k^3 \sin^2 \theta_{\mathbf{k}}}{8\pi^2 \varepsilon_0 \hbar} \int_{\hat{\mathbf{e}}_{\mathbf{k}} \in cav} \sin \theta d\theta d\phi = \Gamma_{free} \left( 1 - \frac{3}{8\pi} \Omega_{cav} \sin^2 \theta_{\mathbf{k}} \right). \end{aligned} \quad (20.67)$$

Finally, we study the situation, when the cavity is in place but now tuned on resonance. Then the density of states in the photon emission directions  $\mathbf{k} \in \text{cavity}$  is modulated by the Airy function (20.40),

$$\rho_{cav}(\omega_{\mathbf{k}}, \mathbf{k}) = \rho_{free}(\omega_{\mathbf{k}}) \mathcal{L}(\omega_{\mathbf{k}}). \quad (20.68)$$

That is, photons can be emitted into the cavity mode with increased probability. Once again we repeat the calculation (20.66), but now inserting the density of states of the cavity,

$$\begin{aligned} \Gamma_{cav} &= \int_{\hat{\mathbf{e}}_{\mathbf{k}} \in cav} \frac{d^2 \sin^2 \theta_{\mathbf{k}}}{\hbar^2} \frac{\hbar \omega_0}{2\varepsilon_0 V} 2\pi \mathcal{L}(\omega_0) \frac{V \omega_0^2}{(2\pi)^3 c^3} \sin \theta d\theta d\phi \\ &\simeq \frac{d^2 k^3 \sin^2 \theta_{\mathbf{k}}}{8\pi^2 \varepsilon_0 \hbar} \mathcal{L}(\omega_0) \int_{\hat{\mathbf{e}}_{\mathbf{k}} \in cav} \sin \theta d\theta d\phi = \Gamma_{free} \mathcal{L}(\omega_0) \frac{3}{8\pi} \Omega_{cav} \sin^2 \theta_{\mathbf{k}}, \end{aligned} \quad (20.69)$$

where, in the last step, we substituted the free space decay rate (20.66). An analogous calculation for the *cooperative Lamb shift*  $\Delta\omega_{cav}$  is left to the Exc. 20.2.6.1:

$$\begin{array}{l} \Gamma_{cav} = \Gamma_{free} \frac{3}{8\pi} \Omega_{cav} \sin^2 \theta_{\mathbf{k}} \mathcal{L}(\omega_0) \\ \Delta\omega_{cav} = \Gamma_{free} \frac{3}{32\pi} \Omega_{cav} \sin^2 \theta_{\mathbf{k}} \frac{\mathcal{L}'(\omega_0)}{\mathcal{L}(\omega_0)} 2\delta_{fsr} \end{array}. \quad (20.70)$$

The quantities  $\Gamma_{cav}$  and  $\Gamma_{free \in cav}$  are scattering rates into complementary solid angles. Now, the total spontaneous emission rate, which determines the lifetime of the radiating excited state and the spectral width of the transition is simply the sum of the partial scattering rates,

$$\begin{aligned} \Gamma &= \Gamma_{free \notin cav} + \Gamma_{cav} \\ &= \Gamma_{free} \left( 1 - \frac{3}{8\pi} \Omega_{cav} \right) \sin^2 \theta_{\mathbf{k}} + \Gamma_{free} \mathcal{L}(\omega_0) \frac{3}{8\pi} \Omega_{cav} \sin^2 \theta_{\mathbf{k}} \\ &= \Gamma_{free} \left[ 1 + (\mathcal{L}(\omega_0) - 1) \frac{3}{8\pi} \Omega_{cav} \right] \sin^2 \theta_{\mathbf{k}}. \end{aligned} \quad (20.71)$$

Assuming for simplicity,  $\theta_{\mathbf{k}} = \pi/2$ , we find the extremes of the spontaneous emission rate,  $\Gamma_{enh}$  and  $\Gamma_{inh}$ , when the cavity is on or off resonance. With a resonant high finesse cavity the emission is obtained via  $kL \rightarrow 0$ ,

$$\Gamma_{enh} = \Gamma_{free} \left[ 1 + \left( \sqrt{1 + \left( \frac{2F}{\pi} \right)^2} - 1 \right) \frac{3}{8\pi} \Omega_{cav} \right] \simeq \Gamma_{free} \left( 1 + \frac{3}{4\pi^2} F \Omega_{cav} \right). \quad (20.72)$$

assuming high finesse,  $F \gg 1$ . With a non-resonant cavity, the emission is obtained via  $kL \rightarrow \pi/2$ ,

$$\Gamma_{inh} = \Gamma_{free} \left[ 1 + \left( \frac{1}{\sqrt{1 + \left( \frac{2F}{\pi} \right)^2}} - 1 \right) \frac{3}{8\pi} \Omega_{cav} \right] \simeq \Gamma_{free} \left( 1 - \frac{3}{8\pi} \Omega_{cav} \right). \quad (20.73)$$

For a small solid angle, we can expect a big increase of the scattering into the cavity, but without noticeable inhibition of the total decay,  $\Gamma_{inh} \simeq \Gamma_{free}$ .

If the atoms are saturated by an incident laser, they scatter light into the cavity at a rate (apart from a factor  $\frac{1}{2}$ ),

$$\Gamma_{cav} = \Gamma_{free} \mathcal{L}(\omega_0) \frac{3}{8\pi} \Omega_{cav} . \quad (20.74)$$

Without cavity the emission into the same solid angle is obtained via  $F \rightarrow 0$ ,

$$\Gamma_{free \in cav} = \Gamma_{free} \frac{3}{8\pi} \Omega_{cav} . \quad (20.75)$$

The scattering will fill the cavity with photons, until the leakage equalizes the pumping. When the balance is reached,  $\Gamma_{cav}$  will also be the rate at which photons are emitted by the cavity mode. We calculate an example in Exc. 20.2.6.2.

### 20.2.1.3 Purcell factor for confocal and concentric cavities

Using the solid angle of a confocal cavity (20.46), the cooperativity parameter is,

$$\Upsilon \simeq \frac{3F}{4\pi^2} \Omega_{cav} = \frac{3F}{4\pi^2} \frac{8\pi b^2}{L^2} , \quad (20.76)$$

where  $b$  is the clear aperture of the cavity mirrors. That is,

$$\boxed{\Upsilon = \frac{F}{\pi} \frac{6b^2}{L^2}} . \quad (20.77)$$

### 20.2.1.4 Purcell factor for the TEM<sub>00</sub> cavity mode

With the solid angle (20.52) calculated for a this TEM<sub>00</sub> cavity mode we calculate the *cooperativity parameter*,

$$\begin{aligned} \Upsilon &\equiv \frac{\Gamma_{cav}}{\Gamma_{free}} = \mathcal{L}(\omega_0) \frac{3}{8\pi} \Omega_{cav} = \sqrt{1 + \left(\frac{2F}{\pi}\right)^2} \frac{3}{8\pi} \Omega_{cav} \\ &\simeq \frac{3F}{4\pi^2} \Omega_{cav} = \frac{\Gamma_{enh}}{\Gamma_{free}} - 1 = \frac{3F}{4\pi^2} \frac{8\pi}{k^2 w_0^2} , \end{aligned} \quad (20.78)$$

that is,

$$\boxed{\Upsilon = \frac{F}{\pi} \frac{6}{k^2 w_0^2}} , \quad (20.79)$$

which is also called *Purcell factor*.

Now, exploiting the relationships (20.52), (20.79), and (20.26),

$$\Omega_{cav} = \frac{8\pi}{k^2 w_0^2} , \quad \Upsilon = \frac{F}{\pi} \frac{6}{k^2 w_0^2} , \quad \frac{F}{\pi} = \frac{\delta_{fsr}}{\kappa} , \quad (20.80)$$

and defining a new quantity,

$$g^2 = \Upsilon \kappa \Gamma_{free} , \quad (20.81)$$

which we will call the atom-field coupling strength, we may rewrite the prefactor  $\Gamma_{free} \frac{3}{8\pi} \Omega_{cav}$  for the case of Gaussian cavity modes,

$$\Gamma_{free} \frac{3}{8\pi} \Omega_{cav} = \frac{g^2}{2\delta_{fsr}}. \quad (20.82)$$

Close to a cavity resonance,  $kL = \omega/2\delta_{fsr} = (\omega_a + \Delta_a)/2\delta_{fsr} = 2\pi N + \Delta_a/2\delta_{fsr}$ , the sine appearing in the Airy function (20.40) may be expanded  $\sin kL = \sin \Delta_a/2\delta_{fsr} \simeq \Delta_a/2\delta_{fsr}$ . Furthermore, assuming a high finesse,  $F \gg 1$ , the Airy function simplifies to,

$$\mathcal{L}(\omega_0) = \frac{\sqrt{1 + (2F/\pi)^2}}{1 + (2F/\pi)^2 \sin^2 \frac{\omega}{2\delta_{fsr}}} \simeq \frac{2F/\pi}{1 + \Delta_a^2/\kappa^2}. \quad (20.83)$$

Inserting this into the formulae (20.70), where we set  $\theta_{\mathbf{k}} = \frac{\pi}{2}$ ,

$$\boxed{\begin{aligned} \Gamma_{cav} &\simeq \frac{g^2 \kappa}{\Delta_a^2 + \kappa^2} \\ \Delta\omega_{cav} &\simeq \frac{-2g^2 \Delta_a}{\Delta_a^2 + \kappa^2} \end{aligned}}. \quad (20.84)$$

Obviously, the atom-field coupling strength  $g$  plays a central role in the modification of the emission spectra of atoms interaction with cavities. Therefore, we will have to study this quantity more deeply in the next sections.

**Example 92 (Cooperativity of non-degenerate and confocal cavities):** For example, for a non-degenerate linear cavity with finesse  $F = 110000$  and waist  $w_0 = 50 \mu\text{m}$  at 689 nm, the cooperativity is relatively weak,  $\Upsilon \simeq 1$ . Still, at this cooperativity, half of the spontaneously emitted photons go into a tiny solid angle represented by the cavity. Confocal or concentric cavities may present more favorable geometries [316, 317, 318]. With  $N_0 = 10^4$  saturated strontium

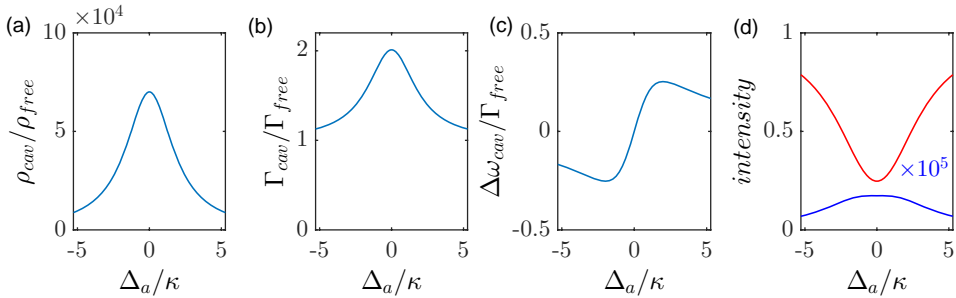


Figure 20.4: (code) Spontaneous emission on the strontium atom cooling transition ( $\lambda = 689 \text{ nm}$ ,  $\Gamma = (2\pi) 7.6 \text{ kHz}$ ) in a  $L = 3.6 \text{ cm}$  long cavity with  $F = 110000$  and  $w_0 = 50 \mu\text{m}$ . (a) Cooperativity  $\mathcal{L}(\omega)$  from Eq. (20.40) as a function of the detuning of the cavity. (b) Linewidth  $\Gamma_{cav}$  from (20.70)(ii) and (c) frequency shift of the strontium transition from Eq. (20.70)(ii). (d) Spontaneous emission into the cavity (blue) and into the open space (red).

atoms, the light power scattered into the cavity is  $P_j = 20 \text{ fW}$ . Estimation

the cavity transmission by  $T \simeq \pi/F$ , we expect that a number of  $T \frac{P_{cav}}{\hbar\omega} = 10^7 \text{ s}^{-1}$  photons can be detected by a photodetector recording the photon number leaking out of the cavity.

### 20.2.2 Characterization of the atom-field coupling

In Sec. 20.1.3 we started introducing a number of quantities characterizing empty cavities. We will now pursue this task including their interaction with atoms. In particular, we will introduce three important quantities allowing us to measure the degree of quantization of the system: the cooperativity  $\Upsilon$ , the saturation parameter  $s$ , and the cavity resolution  $r$ .

#### 20.2.2.1 The atomic dipole moment

As usual, the interaction strength of an atom with a light field is measured by the atom-field coupling constant, which is precisely HALF the single photon Rabi frequency. Using relationships derived in Sec. 20.1.3 and the expression (13.38) for the atomic dipole moment  $d$ , we find,

$$g \equiv \frac{d\vec{\mathcal{E}}_1(0)}{\hbar} = \sqrt{\frac{3\pi\Gamma\omega}{2k^3V_m}} = \sqrt{\frac{3\Gamma\delta_{fsr}}{k^2w^2}}, \tag{20.85}$$

where  $\vec{\mathcal{E}}_1(0)$  the electric field produced by a single photon inside the cavity mode volume  $V_m$  calculated in (20.29) and  $\Gamma$  is the spontaneous decay rate. See also (watch talk).

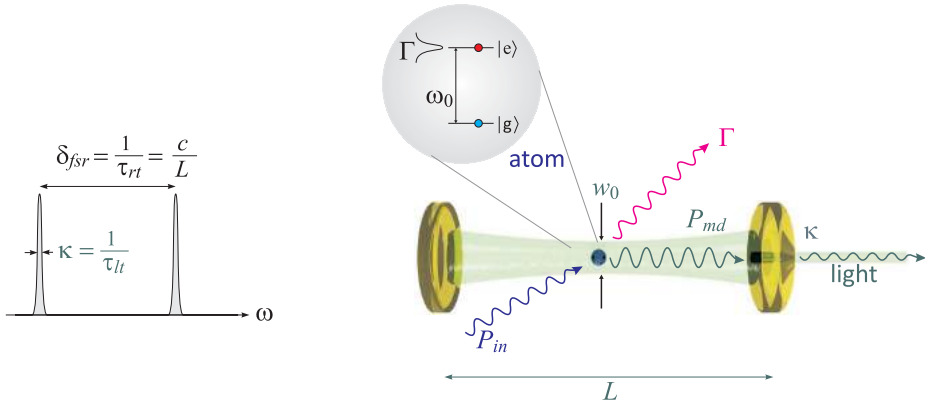


Figure 20.5: Relevant parameters for an atom interacting with a cavity.

#### 20.2.2.2 Single atom reflection coefficient

Based on the complex atomic polarizability ,

$$\frac{\alpha_{pol}}{\epsilon_0} \simeq \frac{6\pi}{k^3} \frac{-1}{i + 2\Delta/\Gamma}, \tag{20.86}$$

the *single atom reflection coefficient* is defined as,

$$\beta_{\Delta} = \frac{k}{\pi w^2} \left| \frac{\text{Re } \alpha_{pol}}{\varepsilon_0} \right| = \frac{6}{k^2 w^2} \frac{2\Gamma |\Delta_a|}{4\Delta_a^2 + \Gamma} \xrightarrow{|\Delta| \gg \Gamma} \frac{6}{k^2 w^2} \frac{\Gamma}{2|\Delta_a|}, \quad (20.87)$$

where  $\Delta_a = \omega - \omega_0$ . The resonant reflection coefficient can be interpreted in terms of a phase shift that depends on the matching between the resonant optical cross-section of the atom,  $\sigma_0 = 3\lambda^2/2\pi$ , and the cross section of the optical mode,

$$\beta_0 = \frac{\sigma_0}{\pi w^2} = \frac{6}{k^2 w^2} = \frac{2g^2}{\delta_{fsr}\Gamma}. \quad (20.88)$$

The frequency shift accumulated during a round trip in the cavity,  $\delta_{fsr}\beta_0$ , becomes noticeable, when it exceeds the linewidth of the cavity  $\kappa$ . From this condition, we obtain the optical depth for a single passage through the atomic sample multiplied by the finesse of the cavity, which is precisely the *cooperativity parameter*,

$$\Upsilon \equiv \frac{\delta_{fsr}\beta_0}{\kappa} = \frac{F}{\pi} \frac{6}{k^2 w^2} = \frac{2g^2}{\kappa\Gamma}. \quad (20.89)$$

The sensitivity to the atom number can be measured in terms of a *critical atom number*  $N_{crt}$ , which the system can resolve. It goes to infinity as the resonant single atom reflection coefficient disappears,  $\beta_0 \rightarrow 0$ , and converges to zero when  $\beta_0 \rightarrow 1$ ,

$$N_{crt} = \frac{4\pi}{F\beta_0} = 4\pi \frac{k^2 w^2}{6F} = 2\pi \frac{\Gamma \delta_{fsr}}{Fg^2} = \frac{2\kappa\Gamma}{g^2} = \frac{4}{\Upsilon}. \quad (20.90)$$

The total reflection coefficient is increased by the number of atoms  $N$  and the number of photon round trips  $F$  in the cavity, which gives out of resonance,

$$NF\beta_{\Delta} \simeq NF \frac{6}{k^2 w^2} \frac{\Gamma}{2\Delta_a} = NF \frac{g^2}{\Delta_a} \frac{kV}{\omega\pi w^2} = NU_0 \frac{L}{c} F = \frac{NU_0}{\kappa}, \quad (20.91)$$

where we introduced the *light-shift* produced by a single off-resonant photon and the Rayleigh scattering rate produced by a single photon,

$$U_0 \simeq \frac{g^2}{\Delta_a} \quad \text{and} \quad \gamma_0 \simeq \frac{g^2\Gamma}{\Delta_a^2}. \quad (20.92)$$

Using the dipole moment  $d = \sqrt{3\pi\varepsilon_0\hbar\Gamma/k^3}$  and defining the electric field amplitude per photon  $\mathcal{E}_1$  by the photon number  $n$ , the power  $P$ , and the intensity  $I = \varepsilon_0 c n_{ph} \mathcal{E}_1^2 = 2P/\pi w_0^2$ , we calculate for the single-photon Rabi frequency (or atom-field coupling strength),

$$g = \frac{d\mathcal{E}_1}{\hbar} = \sqrt{\frac{1}{\hbar^2} \frac{3\pi\varepsilon_0\hbar\Gamma}{k^3} \frac{I}{\varepsilon_0 c n_{ph}}} = \sqrt{\frac{1}{\hbar^2} \frac{3\pi\varepsilon_0\hbar\Gamma}{k^3} \frac{1}{\varepsilon_0 c n_{ph}} \frac{2P}{\pi w_0^2}} = \sqrt{\frac{6}{k^2 w_0^2} \Gamma \frac{P}{n_{ph}\hbar\omega}}. \quad (20.93)$$

The single-photon light shift (or atom-atom coupling strength) is,

$$U_0 = \frac{g^2}{|\Delta_a|} = \frac{6}{k^2 w_0^2} \frac{\Gamma}{|\Delta_a|} \frac{P}{n_{ph}\hbar\omega} = \beta_{\Delta} \frac{P}{n_{ph}\hbar\omega}, \quad (20.94)$$

and the single-photon Rayleigh scattering rate,

$$\gamma_0 = \frac{g^2\Gamma}{\Delta_a^2} = \frac{6}{k^2w_0^2} \frac{\Gamma^2}{\Delta_a^2} \frac{P}{n_{ph}\hbar\omega}. \quad (20.95)$$

In a cavity the flux  $\delta_{fsr} = P/n_{ph}\hbar\omega$  is just the photon round trip rate (or free spectral range).  $1/\delta_{fsr}$  is the time a photon interacts with an atom. In free space, this does not make sense to me, because I don't know how define the mode volume. I can however consider the interaction of a photon with an extended sample of length  $L$ . In this case, a photon interacts with the sample for the time  $L/c$ , so that,

$$U_0 = \frac{g^2}{|\Delta_a|} = \frac{6}{k^2w_0^2} \frac{\Gamma}{|\Delta_a|} \frac{c}{L} = \beta\Delta \frac{c}{L}, \quad (20.96)$$

and

$$\gamma_0 = \frac{g^2\Gamma}{\Delta_a^2} = \frac{6}{k^2w_0^2} \frac{\Gamma^2}{\Delta_a^2} \frac{c}{L}. \quad (20.97)$$

This means, we can use the CARL equations derived for a ring cavity by just substituting  $\kappa = \delta_{fsr} = c/L$ , where  $L$  is now not the cavity but the sample length.

### 20.2.2.3 Optical density

Lambert-Beer's law relates the amplitude of the field transmitted to the incident (see also Eq. (24.139)),

$$\frac{\vec{\mathcal{E}}_t}{\vec{\mathcal{E}}_0} = \exp \left[ i\sigma(\Delta_a) \left( \frac{i}{2} - \frac{\Delta_a}{\Gamma} \right) \int_{-\infty}^{\infty} n(\mathbf{r}) dz \right] = e^{-b/2} e^{i\varphi}. \quad (20.98)$$

I.e. the field is shifted by an amount  $\varphi$  and absorbed by an amount  $b$ . The exponent (called optical density) can be rewritten, if we assume a number of  $N$  atoms homogeneously distributed over a cylinder with length  $L$  and radius  $\bar{r} = w_0$ ,

$$\begin{aligned} OD &= i\sigma(\Delta_a) \left( \frac{i}{2} - \frac{\Delta_a}{\Gamma} \right) \int_{-\infty}^{\infty} n(\mathbf{r}) dz = \sigma_0 \frac{\Gamma^2}{\Delta_a^2} \left( -\frac{1}{2} - \frac{i\Delta_a}{\Gamma} \right) \int_0^L \frac{N}{\pi\bar{r}^2 L} dz \quad (20.99) \\ &= \sigma_0 \frac{\Gamma^2}{\Delta_a^2} \left( -\frac{1}{2} - \frac{i\Delta_a}{\Gamma} \right) \frac{N}{\pi w_0^2} = \frac{6N}{k^2w_0^2} \frac{\Gamma^2}{\Delta_a^2} \left( -\frac{1}{2} - \frac{i\Delta_a}{\Gamma} \right) \\ &= \frac{6N}{k^2w_0^2} \left( -\frac{1}{2} \frac{\Gamma^2}{\Delta_a^2} - \frac{i\Gamma}{\Delta_a} \right) = N \frac{L}{c} (-\gamma_0 - iU_0). \end{aligned}$$

Hence, the parameters  $N\gamma_0$  and  $NU_0$  are nothing else that the optical density per photon round trip time  $\delta_{fsr} = c/L$ ,

$$\boxed{OD = \frac{-N(\gamma_0 + iU_0)}{\delta_{fsr}}}. \quad (20.100)$$



### 20.2.2.4 Collective cooperativity

While the strong coupling regime of the CQED requires  $\Upsilon > 1$  with a single atom, collective cooperativity is reached with  $N$  atoms if  $N\Upsilon > 1$  [104, 148]. In this case, the atomic ensemble couples to the mode like a single 'super-atom', the coupling force being magnified to  $g_N = g_1\sqrt{N}$ . We have already obtained this result within the Jaynes-Cummings model for two indistinguishable atoms coupling to the same light mode and forming a *Dicke state* (see Sec. 21.4.5).

### 20.2.2.5 Saturation parameter in cavities

The *saturation parameter* for a single photon is given by,

$$s = \frac{g^2}{\Gamma^2} . \quad (20.101)$$

Therefore, the number of photons needed to saturate an atomic transition is,

$$n_{sat} = \frac{\Gamma^2}{2g^2} = \frac{\Gamma}{\delta_{fsr}} \frac{k^2 w^2}{6} = \frac{1}{2s} . \quad (20.102)$$

We see, that there is a *symmetry* between  $\Upsilon$  and  $s$ , that is, between  $N_{crt}$  and  $n_{sat}$ . The regime  $N\Upsilon > 1$  denotes the collective behavior of  $N$  atoms in the same way as  $n_{sat} > 1$  indicates saturation. While  $\Upsilon$  depends only on the phase matching between the atomic antenna and the cavity,  $s$  also depends on the cavity mode volume and the natural decay rate.

### 20.2.2.6 Cavity resolution parameter

Comparing the photonic recoil, which is given by,

$$\omega_{rec} = \frac{\hbar k^2}{2m} , \quad (20.103)$$

with the resolution power of a cavity  $\kappa$ , we can define the *resolution parameter*,

$$r \equiv \frac{\omega_{rec}}{\kappa} . \quad (20.104)$$

With the three parameters defined in Eqs. (20.89), (20.101), and (20.104) we are able to measure the degree of quantization of the degrees of freedom involved in the matter-light interaction in a cavity. The cooperativity  $\Upsilon$  measures the resolvability of single atoms in the atomic cloud, which depends on the phase matching between the atomic antenna (i.e. its optical cross section) and the focus of the optical mode. The saturation parameter  $s$  measures the resolvability of single photons in the cavity. And the cavity resolution parameter  $r$  measures the resolvability of the Doppler-shift due to the atomic center-of-mass motion caused by the absorption of a single photon. If one wants to operate in an environment, where all degrees of freedom involved in the atom-light interactions are fully quantized, the atoms need to be placed into a cavity whose characteristic quantities are all large,  $\Upsilon, s, r \gg 1$ .

In Exc. 20.2.6.3 we compare the coupling force and other characteristic parameters for various combinations of atomic species and optical cavities. In Exc. 20.2.6.4 we calculate the number of photons in a cavity pumped in or out of resonance.

### 20.2.3 Ring cavity dynamics in the presence of an atom

The equations of motion (20.10) describe the evolution of the light fields in counterpropagating modes of a ring cavity. Without scatterer located in the mode volume, the modes evolve independently. In contrast, a scatterer (e.g. an atom or a beamsplitter) may redistribute photons between the modes, whose dynamics thereby becomes coupled.

We will in the following assume the scatterer as immobile, except for Sec. 20.3.2, where we consider a vibrating scatterer. Immobile scatterers can, for example, be heavy masses, such as imperfections on the surfaces of the mirrors of the cavity (scratches, dust particles, etc.), which can scatter light both, out of the cavity and into the reverse cavity mode. In *laser gyroscopes* this backscattering may induce a locking of counterpropagating modes and hamper their proper operation.

#### 20.2.3.1 Classical derivation of coupled atom-cavity equations

The equations of motion (20.10) describe the light fields classically. Hence, it is not surprising that they can be derived with entirely classical arguments. Here, we will show this for a ring cavity in the presence of an atom sitting at a fixed position  $z$  on the cavity's optical axis. We understand the atom as a beamsplitter located within the mode volume of the resonator and partially reflecting and transmitting incident light with reflection and transmission coefficients  $(r_\beta, t_\beta) = (\imath\beta, 1 + \imath\beta)$  such that  $r_\beta^2 + t_\beta^2 = 1$ . Transmitted (forward scattered) photons may be phase-shifted, while reflected photons are backscattered into the counterpropagating mode of the resonator.

Similarly, we treat the incoupling mirror as a beamsplitter with coefficients  $(r_{in}, t_{in})$ . The incident field  $E_{in}$  produces, in the cavity, field amplitudes of  $\alpha_\pm$  for the co- and counterpropagating waves. As in (20.7), we normalize the amplitudes by the numbers of photons  $n_\pm \equiv |\alpha_\pm|^2$ . After a round-trip time  $\tau = \delta_{f_{sr}}^{-1}$  through the mode volume we have in the position of the incoupling mirror the field,

$$\begin{aligned}\alpha_+(t + \tau) &= r_{in}(1 + \imath\beta)e^{\imath kL}\alpha_+(t) + \imath\beta r_{in}^2 e^{2\imath kL - 2\imath kz}\alpha_-(t) + t_{in}\alpha_+^{in}(t) \\ \alpha_-(t + \tau) &= r_{in}(1 + \imath\beta)e^{\imath kL}\alpha_-(t) + \imath\beta e^{2\imath kz}\alpha_+(t) + t_{in}(1 + \imath\beta)e^{\imath kL}\alpha_-^{in}(t).\end{aligned}\quad (20.105)$$

$L$  is the total length of the ring cavity. Obviously, we have  $kL = \omega/\delta_{f_{sr}}$ . In the vicinity of a resonance we have,  $\Delta_c \ll \delta_{f_{sr}}$ , and the quantity  $\omega/\delta_{f_{sr}}$  is almost integer,  $\omega \simeq 2\pi N\delta_{f_{sr}} - \Delta_c$ , such that we can expand the exponential,  $e^{\imath kL} = 1 - \imath\Delta_c/\delta_{f_{sr}}$ . Thus, we obtain,

$$\begin{aligned}\tau\dot{\alpha}_+ &= -[1 - r_{in}(1 + \imath\beta)e^{\imath kL}]\alpha_+ + \imath\beta r_{in}^2 e^{-2\imath kz}\alpha_- + t_{in}\alpha_+^{in} \\ \tau\dot{\alpha}_- &= -[1 - r_{in}(1 + \imath\beta)e^{\imath kL}]\alpha_- + \imath\beta e^{2\imath kz}\alpha_+ + t_{in}(1 + \imath\beta)\alpha_-^{in}.\end{aligned}\quad (20.106)$$

We now connect the transmission of the coupling mirror  $t_{in}$  with the decay constant  $\kappa$  assuming that the light can only leave the cavity through this mirror. We define,

$$\kappa \equiv \frac{T}{\tau}\quad (20.107)$$

as the part of the light lost during one round trip. Thus,  $t_{in} = \sqrt{T} \simeq \sqrt{\pi/F} = \sqrt{\kappa/\delta_{fsr}}$ . Besides that,  $t_{in}$  is very small, such that,

$$t_{in}^2 = 1 - r_{in}^2 \simeq 2(1 - r_{in}) . \quad (20.108)$$

Thus, the first factor is,

$$\begin{aligned} \delta_{fsr} [1 - r_{in}(1 + \imath\beta)e^{\imath kL}] &\simeq \delta_{fsr} - \delta_{fsr}(1 - t_{in}^2/2)(1 + \imath\beta)(1 + \imath\Delta_c/\delta_{fsr}) \\ &\simeq \kappa/2 + \imath\beta - \imath\Delta_c \simeq -\kappa/2 . \end{aligned} \quad (20.109)$$

It gives the cavity losses for the two modes during one round trip. We assume here that losses can only occur via the coupling mirror. However, all losses can be included in a single appropriate  $\kappa$ . There are usually other losses due to scattering on the surface of the mirrors or absorption by the atoms. Finally, we obtain for weak atomic reflection and in resonance, that is, for  $\beta \ll \kappa$  and  $\Delta_c = 0$  the system of equations,

$$\begin{aligned} \dot{\alpha}_+ &= -\kappa\alpha_+ + \imath\delta_{fsr}\beta(1 - t_{in}^2)e^{-2\imath kz}\alpha_- + \sqrt{\kappa\delta_{fsr}}\alpha_+^{in} \\ \dot{\alpha}_- &= -\kappa\alpha_- + \imath\delta_{fsr}\beta e^{2\imath kz}\alpha_+ + (1 + \imath\beta)\sqrt{\kappa\delta_{fsr}}\alpha_-^{in} \end{aligned} \quad (20.110)$$

To calculate the value of  $\beta$ , we need the reflection coefficient of a single atom. It depends on the polarizability,

$$r_\beta = \frac{k}{\pi w^2} \frac{\alpha_{pol}}{\varepsilon_0} \left( = \frac{\sigma_0}{\pi w^2} \frac{\Gamma}{2\Delta_a} \right) . \quad (20.111)$$

The optical potential to which the atom is exposed is,

$$\phi = \frac{I}{2c} \frac{\alpha_{pol}}{\varepsilon_0} , \quad (20.112)$$

where we write the intensity of light as,

$$I = 2\varepsilon_0 c E_1^2 |\alpha_+ e^{\imath kZ} + \alpha_- e^{-\imath kZ}| . \quad (20.113)$$

We normalize once more to the field generated by a single photon,  $E_1 = \sqrt{\hbar\omega/2\varepsilon_0 V_m}$  with the mode volume,  $V_m = \frac{\pi}{2} L w^2$ . On the other hand, the potential can be determined directly through the Rabi frequency,

$$\phi(\mathbf{r}) = \frac{\hbar\Omega(\mathbf{r})^2}{4\Delta_a} , \quad (20.114)$$

The Rabi frequency  $\Omega(\mathbf{r})^2 = 4g^2|\alpha_+ e^{\imath kZ} + \alpha_- e^{-\imath kZ}|^2$  is normalized to the frequency of Rabi generated by a photon  $g$ . Using the frequency shift (light-shift) by photon (20.92),  $U_0 = \frac{g^2}{\Delta_a}$ , we can also write,

$$\phi(\mathbf{r}) = \hbar U_0 |\alpha_+ e^{\imath kZ} + \alpha_- e^{-\imath kZ}|^2 . \quad (20.115)$$

A comparison of the above equations gives,

$$r_\beta = \frac{\imath U_0}{\delta_{fsr}} . \quad (20.116)$$

With an atom in the resonator, we have,

$$\beta = \frac{iU_0}{\delta_{fsr}}. \quad (20.117)$$

We define for convenience,  $\eta_{\pm} = \sqrt{\kappa\delta_{fsr}}\alpha_{\pm}^{in}$  and we suppose, that  $t_{in} \ll 1$ ,  $r_{\beta} \ll 1$  and  $\beta \ll 1$ . This ultimately leads to the result,

$$\dot{\alpha}_{\pm} = -\kappa\alpha_{\pm} - iU_0 e^{\mp 2ikz} \alpha_{\mp} + \eta_{\pm}. \quad (20.118)$$

**Example 93 (Classical CARL equations):** If we were to treat the atomic position  $z$  as a degree of freedom, we could calculate the classical potential of the stationary light wave, and therefore the dipole force,

$$F = -\nabla\phi = -\hbar U_0 \nabla_{Z=z} |\alpha_+ e^{ikZ} + \alpha_- e^{-ikZ}|^2, \quad (20.119)$$

and, consequently, derive the dynamics of the scatterer via,

$$m\ddot{z} = -2i\hbar k U_0 (\alpha_+ \alpha_-^* e^{2ikz} - \alpha_+^* \alpha_- e^{-2ikz}). \quad (20.120)$$

This will be studied in Chp. 22.6.1. In the remaining sections of this chapter we will assume the atom to be located at a fixed position.

In the above derivation we assumed, for simplicity, the pump laser on resonance with the cavity,  $\Delta_c = 0$ . Relaxing this condition, an analogous derivation yields <sup>3</sup>,

$$\dot{\alpha}_{\pm} = (-\kappa + i\Delta_c - iU_0)\alpha_{\pm} - iU_0 e^{\mp 2ikz} \alpha_{\mp} + \eta_{\pm}. \quad (20.121)$$

## 20.2.4 Stationary solutions and spectra

Considering the atom fixed in space,  $\dot{x} = 0 = \dot{p}$ , we can concentrate on solving the equations of motion (20.121) only for the fields. As a first approach, we look for stationary solutions, being aware that they do not always exist, as we will see later in the discussion of the proper CARL effect. In the Exc. 20.2.6.5 we derive the stationary solutions of the equations:

$$\alpha_{\pm} = \frac{[\kappa - i(\Delta_c - U_0)]\eta_{\pm} - iU_0 e^{\mp 2ikz} \eta_{\mp}}{[\kappa - i(\Delta_c - U_0)]^2 + U_0^2}. \quad (20.122)$$

With the abbreviations,

$$\chi \equiv \kappa - i(\Delta_c - U_0), \quad \xi \equiv e^{-2ikz} \frac{\eta_-}{\eta_+} \quad (20.123)$$

the stationary solution can be written,

$$\alpha_{\pm}(\infty) = \eta_{\pm} \frac{\chi - iU_0 \xi^{\pm 1}}{\chi^2 + U_0^2}. \quad (20.124)$$

We note that a phase shift  $\phi$  in the pump fields only shifts the phase of the quantity  $\xi = e^{-2ikx - 2i\phi} \frac{\eta_-}{\eta_+}$ .

<sup>3</sup>Note, that we have not allowed for spontaneous emission by the atomic scatterer out of the cavity mode. This approximation is only good far from resonance,  $\Delta_a \gg \Gamma$ . We will see in Sec. 22.1.3, how to generalize the equations of motion for near resonance cases.

### 20.2.4.1 Splitting of the cavity resonance

The equation (20.121) can be written as follows,

$$i\dot{\vec{\alpha}} = W\vec{\alpha} + i\vec{\eta}, \quad (20.125)$$

where  $\vec{\alpha}$  and  $\vec{\eta}$  regroup the amplitudes  $\alpha_{\pm}$  and  $\eta_{\pm}$ . This equation takes the form of a Schrödinger equation, where,

$$W \equiv \begin{pmatrix} U_0 - \Delta_c - i\kappa & U_0 e^{-2ikz} \\ U_0 e^{2ikz} & U_0 - \Delta_c - i\kappa \end{pmatrix} \quad (20.126)$$

would be the Hamiltonian describing the coupling between counterpropagating modes. The eigenvalues of this matrix are,

$$W^{(1,2)} = 2U_0 - \Delta_c - i\kappa, \quad -\Delta_c - i\kappa. \quad (20.127)$$

This *normal mode splitting*<sup>4</sup> of the cavity results from the coupling of the two cavity modes  $\hat{a}_{\pm}^{\dagger}\hat{a}_{\pm}$ . Obviously, the energies and widths of the eigenvalues do not depend neither on the pump intensities  $\eta_{\pm}$  nor the  $z$ -position of the atom. On the other hand, the spectral behavior of  $\alpha_{\pm}$ , and hence the observable quantities, such as the transmission

$$T_{\pm} \equiv \left| \frac{\kappa\alpha_{\pm}}{\eta_{\pm}} \right|^2 \quad (20.128)$$

depend on these parameters. In the Exc. 20.2.6.7 we will calculate the spectrum by the condition  $0 = \partial_{\Delta_c} \alpha_{\pm}(\infty)$ .

In the following, we will discuss two relevant cases: unidirectional pumping and symmetrical pumping.

### 20.2.4.2 Unidirectional pumping

For unilateral pumping,  $\eta_{-} = 0$ , the equation (20.124) simplifies to,

$$\alpha_{+}(\infty) = \eta_{+} \frac{\chi}{\chi^2 + U_0^2} \quad \text{and} \quad \alpha_{-}(\infty) = \eta_{+} \frac{iU_0 e^{2ikz}}{\chi^2 + U_0^2}. \quad (20.129)$$

These formulas show that, for weak coupling,  $U_0 \ll \kappa$ , the counterpropagating mode receives little light. On the other side, for strong coupling (or very high finesse) and  $\Delta_c = 0$ , the intensity is equally distributed,  $|\alpha_{+}|^2 = |\alpha_{-}|^2 = \frac{\eta_{\pm}^2}{2\kappa}$ <sup>5</sup>. We calculate the splitting of normal modes in Exc. 20.2.6.8.

The counterpropagating modes form, by interference, a standing light wave giving rise to a dipole potential in the form of a one-dimensional optical lattice. Defining the phase  $\theta$  through,

$$\alpha_{+} \equiv |\alpha_{+}| \quad \text{and} \quad \alpha_{-} \equiv |\alpha_{-}| e^{-i\theta}, \quad (20.130)$$

<sup>4</sup>The splitting is not exactly the *vacuum Rabi splitting*, which occurs when the excitation can not be eliminated adiabatically. The vacuum Rabi splitting results from the Jaynes-Cummings [680, 161] and is caused by the coupling of internal and external states  $\hat{a}^{\dagger}\hat{\sigma}$ .

<sup>5</sup>This observation explains why perturbing effects such as backscattering from mirrors imperfections are dramatically magnified when the finesse is high.

we verify by the equation (20.7),

$$E^+(z, t) = E_1|\alpha_+(t)|e^{ikz} + E_1|\alpha_-(t)|e^{-i\theta(t)}e^{-ikz}, \quad (20.131)$$

and,

$$\begin{aligned} \frac{1}{2\varepsilon_0 c E_1^2} \iota(z, t) &= \frac{1}{E_1^2} E^+(z, t) E^-(z, t) \\ &= |\alpha_+(t)|^2 + |\alpha_-(t)|^2 + 2|\alpha_+(t)||\alpha_-(t)| \cos(2kz + \theta). \end{aligned} \quad (20.132)$$

That is, the phase indicates the positions of the potential maxima. Inserting the stationary solution for unilateral pumping (20.129), we derive the expression,

$$\tan \theta = \frac{\text{Im } \alpha_+(\infty) \alpha_-^*(\infty)}{\text{Re } \alpha_+(\infty) \alpha_-^*(\infty)} = \frac{\text{Im } \chi \iota e^{-2ikz}}{\text{Re } \chi \iota e^{-2ikz}} = \frac{\kappa \cos 2kz + (U_0 - \Delta_c) \sin 2kz}{\kappa \sin 2kz - (U_0 - \Delta_c) \cos 2kz}. \quad (20.133)$$

Or in other words, the phase of light determines the equilibrium position of the atom (or vice versa). Two cases are interesting: (i) For  $\Delta_c = 0$  and  $U_0 \gg \kappa$  the condition (20.133) turns into  $\tan \theta = -\tan 2kx$ . In this case, the phase of the backscattered field adjusts in such a way, that the atom stays at the valleys of the anti-nodes. (ii) For  $\Delta_c = U_0$  (or alternatively, when  $\kappa \gg U_0, \Delta_c$ ) the condition (20.133) turns into  $\tan \theta = -\tan(2kx + \frac{\pi}{2})$ , such that the atom is at half height of the potential slope, exactly at the position, where it is able to backscatter the maximum of photons from the pumped mode  $\alpha_+$  to the mode  $\alpha_-$ .

**Example 94 (Resonant case):** Assuming that the cavity is in resonance,  $\Delta_c = 0$ , and pumped in a single direction,  $\eta_- = 0$ , neglecting spontaneous emission,  $\gamma_0 = 0$ , and assuming low backscattering rates,  $U_s \ll \kappa$ ,

$$\alpha_+(\infty) \simeq \frac{\eta_+}{\kappa} \quad \text{and} \quad |\alpha_-(\infty)| = \frac{U_s}{\kappa} |\alpha_+(\infty)|.$$

Looking at short times, we find that the dynamics of the unpumped mode is delayed, since,

$$\dot{\alpha}_+(0) \simeq \eta_+ \quad \text{and} \quad \dot{\alpha}_-(0) \simeq -iU_s \alpha_+ e^{-2ikr_s},$$

giving,

$$\alpha_+(0) \simeq \eta_+ t \quad \text{and} \quad \alpha_-(0) \simeq -iU_s \eta_+ \frac{t^2}{2} e^{-2ikr_s}.$$

The complete solution of the equations (20.128) with unidirectional pumping,  $\eta_- = 0$ , will be derived in Exc. 20.2.6.9.

### 20.2.4.3 Symmetric pumping

Now, we assume equal intensities for the pumps,  $\eta_{\pm}(t) = \eta e^{\pm i\phi(t)}$ , such that  $\xi = e^{-2ikz - i\phi}$ . Then, equation (20.124) simplifies to,

$$\alpha_{\pm}(\infty) = \eta_{\pm} \frac{\chi - iU_{\gamma} \xi^{\pm}}{\chi^2 + U_{\gamma}^2} = \eta \frac{\chi - iU_{\gamma} e^{\mp 2ikz \mp i\phi}}{\chi^2 + U_{\gamma}^2}. \quad (20.134)$$

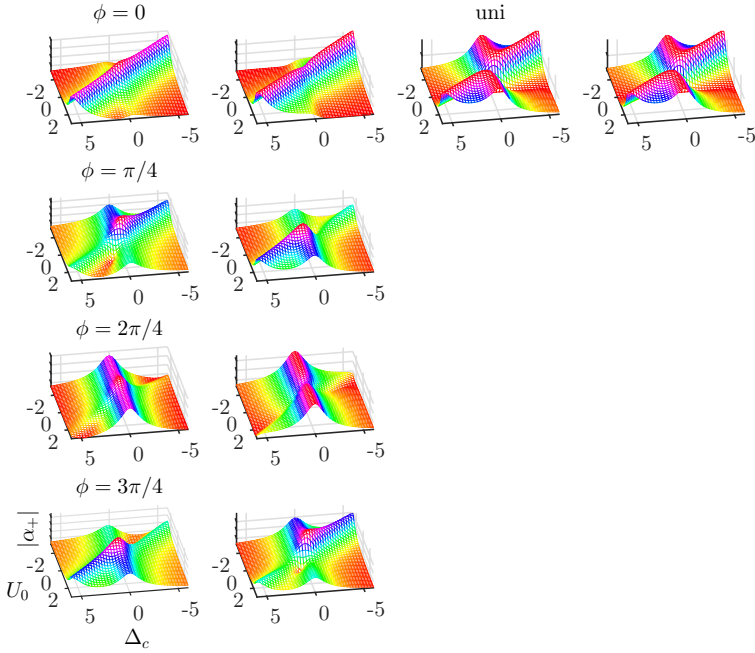


Figure 20.6: (code) (columns 1 and 2) Steady state field values according to (20.122) for bidirectional pumping with a single scatterer located at  $\phi$ . (columns 3 and 4) Same for unidirectional pumping. Here the location of the scatterer does not matter.

The potential is calculated in the same way as in (20.132). The coherences are,

$$\begin{aligned}
 \alpha_{\pm}(\infty)\alpha_{\pm}^*(\infty) &= \eta^2 \frac{(\kappa - i\Delta_c \mp 2U_0 e^{\mp ikz} \sin kz)(\kappa + i\Delta_c \mp 2U_0 e^{\pm ikz} \sin kz)}{(\kappa^2 + 2U_0\Delta_c - \Delta_c^2)^2 + 4\kappa^2(U_0 - \Delta_c)^2} \\
 \alpha_{\pm}(\infty)\alpha_{\mp}^*(\infty) &= \eta^2 \frac{\kappa^2 + (\Delta_c \mp 2iU_0 e^{\mp ikz} \sin kz)^2}{(\kappa^2 + 2U_0\Delta_c - \Delta_c^2)^2 + 4\kappa^2(U_0 - \Delta_c)^2} \quad , \quad (20.135) \\
 e^{\pm 2ikz} &= \frac{\alpha_{\mp}\alpha_{\pm}^*}{|\alpha_{\mp}\alpha_{\pm}^*|}
 \end{aligned}$$

such that the relative phase of the counter-propagating waves adjusts itself to,

$$\tan \theta = \frac{\text{Im } \alpha_{+}(\infty)\alpha_{-}^*(\infty)}{\text{Re } \alpha_{+}(\infty)\alpha_{-}^*(\infty)} = \frac{\kappa^2 \sin 2\phi + 4U_0^2 \sin^2(kz + \phi) \sin 2kz}{\kappa^2 \cos 2\phi - 4U_0^2 \sin^2(kz + \phi) \cos 2kz} \quad . \quad (20.136)$$

The quantity  $\eta^2/\kappa^2$  denotes the number of intracavity photons. According to the formula (20.136), for a weak atom-field coupling,  $U_0 \ll \kappa$ , the phase adjusts itself to the external pumps,  $\theta \rightarrow 2\phi$ , while for strong coupling, it adjusts to the position of the atom,  $\theta \rightarrow 2kz$ .

**Example 95 ('Pulling' of the optical mode by the atom):** We study the case  $U_0 \simeq \kappa$  considering  $\gamma_0 = 0 = \Delta_c$  and a particular external phase [255],

$$\phi = \pi/2,$$

$$\alpha_{\pm}(\infty) = \pm i\eta \frac{\kappa + iU_0 \pm U_0 e^{\mp 2ikz}}{\kappa^2 + 2i\kappa U_0} \quad (20.137)$$

$$\theta(\infty) = \arctan \frac{-4U_0^2 \cos^2 kz \sin 2kz}{\kappa^2 + 4U_0^2 \cos^2 kz \cos 2kz} \simeq \arctan \frac{-8U_0^2}{\kappa^2 + 4U_0^2} kz ,$$

expanding the last formula around  $kz = 0$ . Fig. 20.7 shows how, with the increase in the coupling force between the field and the atoms,  $U_0$ , the phase tends to lock to the atomic position. However, the phase imposed by the external pump competes for this privilege. Curiously, this is independent of laser power, but depends only on the ratio between  $U_0$  and  $\kappa$ .

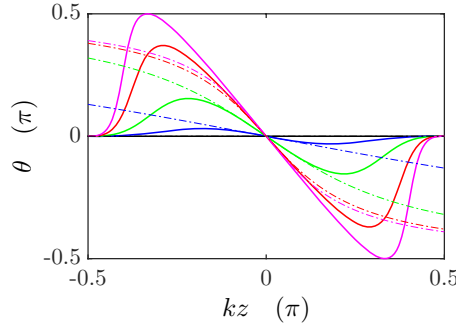


Figure 20.7: (code) 'Pulling' of the phase by the atoms for  $U_0/\kappa = 0, 0.2, 0.5, 1$  and  $\sqrt{2}$ . The solid curves show the exact phase, the 'dash-dotted' curves the linear approximation (20.141).

#### 20.2.4.4 Time-dependent solution without pump

To calculate the homogeneous time-dependent solution of the equation of motion of the ring cavity with  $\eta_{\pm} = 0$ , we solve the Schrödinger equation (20.125) the way we learned in quantum mechanics. We start by diagonalizing the matrix (20.126),

$$\begin{aligned} W &= \begin{pmatrix} U_0 - i\kappa & U_0 e^{-2ikz} \\ U_0 e^{2ikz} & U_0 - i\kappa \end{pmatrix} \\ &= \begin{pmatrix} e^{-2ikz} & -e^{-2ikz} \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 2U_0 - i\kappa & 0 \\ 0 & -i\kappa \end{pmatrix} \begin{pmatrix} e^{-2ikz} & -e^{-2ikz} \\ 1 & 1 \end{pmatrix}^{-1} = UE_W U^{-1} , \end{aligned} \quad (20.138)$$

where  $E_W$  is the matrix of eigenvalues and  $U$  a unitary transformation. So,

$$\begin{aligned} \vec{\alpha} &= e^{-iWt} \vec{\alpha}_0 = U e^{-iE_W t} U^{-1} \vec{\alpha}_0 \\ &= e^{-\kappa t - iU_0 t} \begin{pmatrix} \cos U_0 t & -ie^{-2ikz} \sin U_0 t \\ -ie^{2ikz} \sin U_0 t & \cos U_0 t \end{pmatrix} \vec{\alpha}_0 . \end{aligned} \quad (20.139)$$

We'll see an alternative calculation in Exc. 20.2.6.10. We calculate the coherence by,

$$\begin{aligned} \alpha_+(t)\alpha_-^*(t) &= e^{-2\kappa t} \left[ \alpha_{0+}\alpha_{0-} (\cos^2 U_0 t + e^{-4ikz} \sin^2 U_0 t) + \frac{1}{2}(\alpha_{0+}^2 - \alpha_{0-}^2) i e^{-2ikz} \sin 2U_0 t \right] \\ &\xrightarrow{z \rightarrow 0} e^{-2\kappa t} \left[ \alpha_{0+}\alpha_{0-} + \frac{1}{2}(\alpha_{0+}^2 - \alpha_{0-}^2) i \sin 2U_0 t \right] , \end{aligned} \quad (20.140)$$



making the transition to the Lamb-Dicke regime by  $z \rightarrow 0$ . The phase of the standing wave is,

$$\tan \theta = \frac{\text{Im } \alpha_+(t)\alpha_-^*(t)}{\text{Re } \alpha_+(t)\alpha_-^*(t)} \xrightarrow{z \rightarrow 0} \frac{\alpha_{0+}^2 - \alpha_{0-}^2}{2\alpha_{0+}\alpha_{0-}} \sin 2U_0 t . \quad (20.141)$$

We see that, in resonance and without pumping, the field adjusts its phase to the atom and also decays with the rate  $\kappa$ , while the atom redistributes the photons between modes with the (Rabi-)frequency  $2U_0$ . The formula (20.141) does not show any damping of the phase dynamics in the Lamb-Dicke regime. Thus, in the absence of pumping, the cavity dissipation reduces only the field amplitudes, but does not damp the adjustment of the phase to the atomic position.

### 20.2.4.5 Time-dependent solution with fixed pump

To find the complete solution of the inhomogeneous Schrödinger equation (20.125), we first calculate the stationary solution,

$$\vec{\alpha}(\infty) = -iW^{-1}\vec{\eta} . \quad (20.142)$$

This particular solution of the inhomogeneous equation, added to the general solution of the homogeneous equation, gives the general solution of the inhomogeneous Schrödinger equation,

$$\vec{\alpha}(t) = e^{-iWt}\vec{\alpha}(0) + (1 - e^{-iWt})\vec{\alpha}(\infty) . \quad (20.143)$$

We derive and analyze this solution in the Exc. 20.2.6.11.

## 20.2.5 Forced atomic vibration in a ring cavity

We now assume, that the atom is forced to vibrate by an external force. The vibration is described by,

$$kz = kz_0 \sin \omega t . \quad (20.144)$$

We consider small modulation excursions,  $1 \gtrsim kz_0 = \frac{kv}{\omega} = \frac{2\omega_{rec}}{\omega}$ , which is equivalent to saying that the oscillation frequency should exceed to recoil shift. In this (Lamb-Dicke) regime the Bessel-expansion yields,

$$e^{\pm 2ikz_0 \sin \omega t} = \sum_n J_n(\pm 2kz_0) e^{in\omega t} \simeq J_0(2kz_0) \pm 2iJ_1(2kz_0) \sin \omega t \simeq 1 \pm 2ikz_0 \sin \omega t . \quad (20.145)$$

The differential equations for the two counterpropagating ring cavity-field (20.121) can then be written:

$$\dot{\alpha}_{\pm} = (\mathbf{L} - 2i\mathbf{X} \sin \omega t)\alpha_{\pm} + \eta_{\pm} , \quad (20.146)$$

where,

$$\mathbf{L} = \begin{pmatrix} -\kappa - iU_0 & -iU_0J_0 \\ -iU_0J_0 & -\kappa - iU_0 \end{pmatrix} \quad \text{and} \quad \mathbf{X} = \begin{pmatrix} 0 & -iU_0J_1 \\ iU_0J_1 & 0 \end{pmatrix} . \quad (20.147)$$

We insert the ansatz  $\alpha_{\pm} = \sum_n \alpha_{\pm}^{(n)} e^{in\omega t}$ , where  $\dot{\alpha}_{\pm}^{(n)} = 0$ , into the equations and project onto the basis  $e^{in\omega t}$ :

$$\begin{aligned} in\omega x \sum_n \alpha_{\pm}^{(n)} e^{in\omega t} &= (\mathbf{L} - \mathbf{X}(e^{i\omega t} - e^{-i\omega t})) \sum_n \alpha_{\pm}^{(n)} e^{in\omega t} + \eta_{\pm} \\ \implies (\mathbf{L} - in\omega) \alpha_{\pm}^{(n)} + \mathbf{X}(\alpha_{\pm}^{(n+1)} - \alpha_{\pm}^{(n-1)}) &= -\eta_{\pm} \delta_{n0} . \end{aligned} \quad (20.148)$$

We define operators  $\mathbf{S}_n^{\uparrow\downarrow}$  by  $\alpha_{\pm}^{(n+1)} = \mathbf{S}_n^{\uparrow} \alpha_{\pm}^{(n)}$  for  $n \geq 0$  and  $\alpha_{\pm}^{(n-1)} = \mathbf{S}_n^{\downarrow} \alpha_{\pm}^{(n)}$  for  $n \leq 0$  and obtain,

$$[\mathbf{L} - in\omega + \mathbf{X}(\mathbf{S}_n^{\uparrow} - \mathbf{S}_n^{\downarrow})] \alpha_{\pm}^{(n)} = -\eta_{\pm} \delta_{n0} . \quad (20.149)$$

For  $n = 0$ , we get,

$$\alpha_{\pm}(\infty) = \alpha_{\pm}^{(0)} = -[\mathbf{L} + \mathbf{X}(\mathbf{S}_0^{\uparrow} - \mathbf{S}_0^{\downarrow})]^{-1} \eta_{\pm} . \quad (20.150)$$

If we substitute in equation (20.148)  $\alpha_{\pm}^{(n)} = \mathbf{S}_{n-1}^{\uparrow} \alpha_{\pm}^{(n-1)} = \mathbf{S}_{n+1}^{\downarrow} \alpha_{\pm}^{(n+1)}$ , we get for  $n \geq 0$ ,

$$\mathbf{S}_{n-1}^{\uparrow} = [\mathbf{L} - in\omega + \mathbf{X}\mathbf{S}_n^{\uparrow}]^{-1} \mathbf{X} \quad \text{and} \quad \mathbf{S}_{n+1}^{\downarrow} = [\mathbf{L} - in\omega - \mathbf{X}\mathbf{S}_n^{\downarrow}]^{-1} \mathbf{X} . \quad (20.151)$$

By recursive substitution of the lower into the upper equation, the stationary solution can now be written by means of continued fractions,

$$\mathbf{S}_0^{\uparrow\downarrow} \equiv \frac{1}{\mathbf{L} - i\omega \pm \mathbf{X} \frac{1}{\mathbf{L} - 2i\omega \pm \mathbf{X} \frac{1}{\dots}} \mathbf{X}} \mathbf{X} . \quad (20.152)$$

$\alpha_{\pm}(\infty)$  in Eq. (20.150) gives us the stationary solution of the differential equation, time-averaged over an oscillation period.

If we are deep in the Lamb-Dicke regime, we need only consider the first order of the continued fractions. We set  $\mathbf{S}_1^{\uparrow\downarrow} = \mathbf{1}$  and obtain the simplified equations,

$$\begin{aligned} \mathbf{S}_0^{\uparrow} &= [\mathbf{L} - i\omega + \mathbf{X}]^{-1} \mathbf{X} \quad \text{and} \quad \mathbf{S}_0^{\downarrow} = [\mathbf{L} - i\omega - \mathbf{X}]^{-1} \mathbf{X} \\ \alpha_{\pm}^{(0)} &= -[\mathbf{L} + \mathbf{X}(\mathbf{S}_0^{\uparrow} - \mathbf{S}_0^{\downarrow})]^{-1} \eta_{\pm} \\ \alpha_{\pm}^{(1)} &= \mathbf{S}_0^{\uparrow} \alpha_{\pm}^{(0)} \quad \text{and} \quad \alpha_{\pm}^{(-1)} = \mathbf{S}_0^{\downarrow} \alpha_{\pm}^{(0)} . \end{aligned} \quad (20.153)$$

Explicitly,

$$\begin{aligned} \mathbf{S}_0^{\uparrow\downarrow} &= \frac{U_0 k z_0}{(\kappa + iU_0 + i\omega)^2 + U_0^2(1 - k^2 x_0^2)} \begin{pmatrix} -U_0(1 \pm k z_0) & i(\kappa + iU_0 + i\omega) \\ -i(\kappa + iU_0 + i\omega) & -U_0(-1 \pm k z_0) \end{pmatrix} \\ \mathbf{S}_0^{\uparrow} - \mathbf{S}_0^{\downarrow} &= \frac{-2U_0^2 k^2 x_0^2}{(\kappa + iU_0 + i\omega)^2 + U_0^2(1 - k^2 x_0^2)} \mathbb{I}_2 \\ \alpha_{\pm} &= \alpha_{\pm}^{(0)} + \alpha_{\pm}^{(1)} e^{i\omega t} + \alpha_{\pm}^{(-1)} e^{-i\omega t} . \end{aligned} \quad (20.154)$$

Finally,

$$\boxed{\alpha_{\pm} = -[1 + \mathbf{S}_0^{\uparrow} e^{i\omega t} + \mathbf{S}_0^{\downarrow} e^{-i\omega t}][\mathbf{L} + \mathbf{X}(\mathbf{S}_0^{\uparrow} - \mathbf{S}_0^{\downarrow})]^{-1} \eta_{\pm}} . \quad (20.155)$$

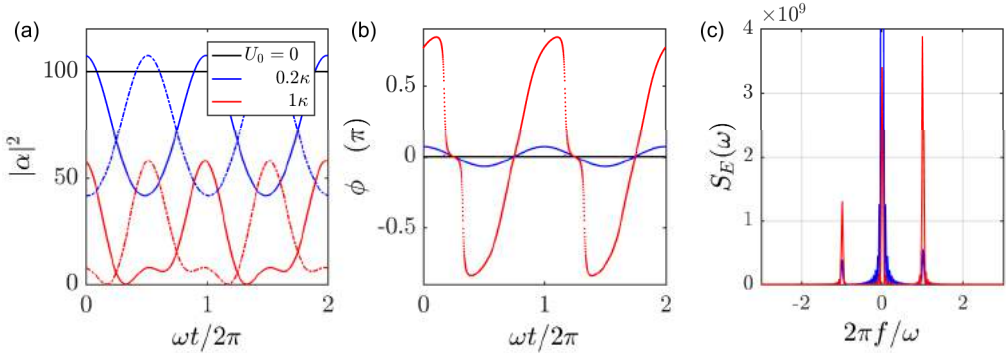


Figure 20.8: (code) (a) Photon number and (b) phase shift of the cavity in response to a modulated atomic position. The parameters are  $kz_0 = 1$ ,  $\kappa = (2\pi) 20$  kHz,  $\omega = 2.5\kappa$ , and  $\eta_{\pm} = 10\kappa$ . (c) Spectrum recorded behind a cavity mirror with the transmittivity  $t_{hr}$ . The spectrum is obtained as the Fourier transform of the  $g^{(1)}(\tau)$  correlation function of the transmitted field  $E_{out} = t_{hr}e^{ik_a}E_{cav}$ , where  $e^{ik_a}$  is a fixed phase factor depending on the mirror position  $a$  (see Sec. ??).

The Fig. 20.8 shows how the phase of the ring cavity behaves in time for various atom-field coupling constants.

It is interesting to study the oscillatory response of the cavity-field to a forced atomic vibration, because it yields information about the cavity backaction. In fact, as shown above, the vibrating atom imprints sidebands to the intracavity refractive index [603, 5]. The sidebands appear in the cavity transmission spectrum. A more sophisticated method to detect the backaction could be to watch the response in the beat signal to a periodic modulation of the incoupled fields with a vibrating atom,

$$\dot{\alpha}_{\pm} = (-\kappa - iU_0)\alpha_{\pm} - iU_0e^{\mp 2ikz_0 \sin \omega t}\alpha_{\mp} + \eta e^{\pm i\phi_0 \sin \omega_{\phi} t}. \quad (20.156)$$

We would expect a clear signature for resonance,  $\omega_{\phi} = \omega$ . The sidebands of the modulated pump would be coupled in, if they coincide. Instead of monitoring the cavity field, we could search the signature of the backaction in the atomic response. We will come back to this, when we discuss collective effects and the frequency shift of the center-of-mass motion. Do Exc. 20.2.6.14.

## 20.2.6 Exercises

### 20.2.6.1 Ex: Cooperative Lamb shift in a cavity

Calculate the cooperative Lamb shift in a cavity from the second formula (20.64) and plot the result as a function of the cavity detuning.

### 20.2.6.2 Ex: Cooperative amplification for a rubidium gas in a cavity

Consider an non-degenerate cavity characterized by  $\delta_{f_{sr}} = 2$  GHz,  $F = 80$ , and  $w_0 = 6 \mu\text{m}$ . In order to benefit from the cooperativity of the cavity, the atoms must be within a volume axially delimited by the Rayleigh length and radially by the

diameter of the mode near its waist.

- Calculate the Rayleigh length for a wavelength of 780 nm and the mode volume.
- For a given partial pressure of rubidium at room temperature of  $p \approx 10^{-5}$  Pa, calculate the average number of atoms within the mode volume.
- Of these atoms only those with an axial Doppler shift below  $kv_z < \kappa$  emit resonantly into the cavity. Calculate the number of these atoms from the Maxwell-Boltzmann distribution.
- Calculate the cooperative amplification of the emission rate into the cavity.

### 20.2.6.3 Ex: Characteristic parameters for various atom-cavity systems

Complete the following table calculating  $\kappa$ ,  $V_m$ ,  $\omega_r$ ,  $g_1$ ,  $\Upsilon$ ,  $s$ , and  $r$ ,

	rubidium	strontium
$\Gamma$	6 MHz	6.8 kHz
$\mathcal{F}$	250000	250000
$L$	100 $\mu\text{m}$	3 cm
$w_0$	20 $\mu\text{m}$	70 $\mu\text{m}$

### 20.2.6.4 Ex: Number of photons in a cavity

- How many photons are in the mode of a cavity with finesse  $F = 80000$  (i) in resonance e (ii) out of resonance?
- What power must be injected to produce 1 photon inside the cavity?
- Resonant backscattering by the cavity mirrors can scatter photons into the reverse mode. Typically,  $P_-/P_+ \simeq 0.005$ . Hence,  $n_{-,cav}^{on} = 1.5 \times 10^7$  and  $n_{-,cav}^{off} = 0.01$ . Using advanced techniques it is possible to reduce the number of backscattered photons by factor of  $> 20$ . Assuming that the losses due to backscattering are  $S = 1$  ppm. Can the resonant backscattering by the mirrors destroy a BEC?
- What is the amplitude of the CARL signal in terms of photons?

### 20.2.6.5 Ex: Stationary solution of the equations of motion with spontaneous emission

Spontaneous emission can be included in the equations of motion via the substitution  $U_0 \rightarrow U_\gamma \equiv U_0 - \nu\gamma_0$ , with  $U_0$  and  $\gamma_0$  defined in (20.92).

- Write down the equations of motion generalized from (20.121) and
- derive their stationary solution.

### 20.2.6.6 Ex: PDH-probing atoms in a ring cavity

Calculate the steady-state reflection of a phase-modulated laser beam from a ring cavity neglecting backscattering from the atoms. Demodulate the reflection signal with the modulation frequency.

### 20.2.6.7 Ex: Normal mode spectrum

Derive the normal mode spectrum of ring cavity pumped in one direction by applying the condition  $0 = \partial_{\Delta_c} \alpha_{\pm}(\infty)$  to the stationary solution (20.124).

**20.2.6.8 Ex: Normal mode splitting**

Consider the generalized equations of motion generalized by including spontaneous emission (see Exc. 20.2.6.5) and assume one-way pumping,  $\eta_- = 0$ . For this system,

- write down the stationary solution for  $\alpha_+$  and
- calculate the transmission of the cavity in the direction of mode  $\alpha_+$  as a function of the detunings  $\Delta_a$  and  $\Delta_c$  and the number of atoms.

Transmission spectra can be recorded under various boundary conditions. Calculate the transmission

- keeping the laser at a fixed frequency  $\omega$  and varying the cavity length  $\omega_c$ ;
- tuning a cavity resonance to the atomic transition,  $\omega_c = \omega_a$ , and varying the laser frequency  $\omega$ ;
- keeping the cavity constant at an *arbitrary* frequency  $\omega_c$  and varying the laser frequency  $\omega$ ;
- keeping the laser locked to the cavity,  $\omega = \omega_c + NU_0$ , and now ramping the cavity across the atomic resonance.

**20.2.6.9 Ex: Ring cavity pumped in one direction**

Derive the complete solution of the equations (20.121).

**20.2.6.10 Ex: Position of the phase without pumping of the cavity**

Solve the Schrödinger equation (20.126) by inserting ansatz,

$$\vec{\alpha} = \vec{\alpha}_1 e^{-\lambda_1 t} + \vec{\alpha}_2 e^{-\lambda_2 t} ,$$

where  $\lambda_1 = \kappa + 2iU_0$  e  $-\lambda_2 = \kappa$  are the eigenvalues of the matrix (20.126).

**20.2.6.11 Ex: Dynamics of a standing wave in a symmetrically pumped ring cavity**

Solve and discuss the equation (20.143).

**20.2.6.12 Ex: Stationary position of the atom in a unidirectionally pumped ring cavity**

What is the steady state position of an atom interacting with the modes of a unidirectionally pumped ring cavity?

**20.2.6.13 Ex: Equations of motion for intensities and coherences**

Derive from the equations (20.121) the equations of motion for intermodal coherences  $\alpha_+ \alpha_+^*$ ,  $\alpha_- \alpha_-^*$ ,  $\alpha_+ \alpha_-^*$ , and  $\alpha_- \alpha_+^*$ .

**20.2.6.14 Ex: Backaction of atomic vibration on the modes of a symmetrically pumped ring cavity**

- Calculate the Lamb-Dicke parameter for gravitation-induced Bloch oscillations in a strontium gravimeter, as well as the modulation index. Is the continued fractions

method applicable?

b. Study the dynamics of the counterpropagating light modes of a ring cavity in the presence of an atom whose position is periodically modulated with a given frequency by numerical integration of the equations of motion (20.121). Compare with the results obtained by the method of continued fractions proposed in Sec. 20.2.5.

## 20.3 Further reading

A.N. Poddubny et al., *Microscopic model of Purcell enhancement in hyperbolic metamaterials* [DOI]

Wenlong Gao et al., *Topological Photonic Phase in Chiral Hyperbolic Metamaterials* [DOI]

Haibin Wu et al., *Observation of Intracavity Electromagnetically Induced Transparency and Polariton Resonances in a Doppler-Broadened Medium* [DOI]

Xiaodong Zeng et al., *Spontaneous emission interference enhancement with a  $\mu$ -negative metamaterial slab* [DOI]

Xiaodong Zeng et al., *Enhancement of the vacuum Rabi oscillation via surface plasma modes in single-negative metamaterials* [DOI]

F. Dubin et al., *Photon Correlation versus Interference of Single-Atom Fluorescence in a Half-Cavity* [DOI]

U. Dorner et al., *Laser-driven atoms in half-cavities* [DOI]

P. Lambropoulos et al., *Fundamental quantum optics in structured reservoirs* [DOI]

### 20.3.1 on cavities

B. Yurke et al., *Quantum network theory* [DOI]

C.W. Gardiner et al., *A multimode quantum theory of a degenerate parametric amplifier in a cavity* [DOI]

### 20.3.2 on superradiant lasing

R. H. Dicke, *Coherence in Spontaneous Radiation Processes* [DOI]

M. Tavis et al., *Exact solution for an  $N$ -molecule-radiation-field Hamiltonian* [DOI]

J. Krause et al., *Quantum theory of the micromaser: Symmetry breaking via off-diagonal atomic injection* [DOI]

A.F. Huss et al., *Phase Correlation of Laser Waves with Arbitrary Frequency Spacing* [DOI]

B.M. Peden et al., *Nondestructive cavity QED probe of Bloch oscillations in a gas of ultracold atoms* [DOI]

- D. Meiser et al., *Prospects for a Millihertz-Linewidth Laser* [\[DOI\]](#)
- M.A. Norcia et al., *Strong coupling on a forbidden transition in strontium and non-destructive atom counting* [\[DOI\]](#)
- M.A. Norcia et al., *Cold-Strontium Laser in the Superradiant Crossover Regime* [\[DOI\]](#)
- M.A. Norcia et al., *Cavity-mediated collective spin-exchange interactions in a strontium superradiant laser* [\[DOI\]](#)
- A. Bychek et al., *Superradiant lasing in inhomogeneously broadened ensembles with spatially varying coupling* [\[DOI\]](#)

# Chapter 21

## Correlated atoms, entanglement and quantum gates

In the preceding chapters, we concentrated on understanding the interaction of *single* atoms with light fields. The models used were the Rabi and the Jaynes-Cummings model. In the following chapters, we will extend these models to several and many atoms <sup>1</sup>.

model	RWA	symmetry	atom #	photon #	section
Rabi	no	$\mathcal{P}$	1	$n$	14.2
Jaynes-Cummings	yes	$U(1)$	1	$n$	15.2
coupled dipoles			$> 1$	1	19.1.2
Dicke	no	$\mathcal{P}$	$> 1$	$n$	21.1
Tavis-Cummings	yes	$U(1)$	$> 1$	$n$	21.4.2, 21.2.4

It does not come as a surprise that totally new phenomena arise from the collective interaction of several atoms with a single light mode. For instance, the atomic cloud can evolve toward a spin-squeezed or an entangled state, or it can emit light in a super- and subradiant way. The interplay between collective processes and processes favoring an individualization of the atom-light interaction is subtle, and the different models used to understand the processes only grasp partial aspects. The difficulty arises from the complexity of the task of describing the dynamics of  $N$  evolving in a Hilbert space of dimension  $2^N$ . Approximations used to reduce the complexity of the Hilbert space come at the price of eventually losing some interesting features. On the other hand, they may also help to crystallize fundamental symmetries, which allow us to deepen our intuition on the collective behavior of the many-body system.

Famous models used in the description of collective scattering are (among others) the Dicke model, the Tavis-Cummings model, and the coupled dipoles model (see table above). The Dicke model (presented in Sec. 21.1) assumes a total indistinguishability of the atoms, the Tavis-Cummings (discussed in Sec. 21.3 and used for the purpose

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<sup>1</sup>Other models, such as the Ising model, the Heisenberg model, or the Bose-Hubbard model are not treated here.

$\mathcal{P}$  is the parity operator defined in Eq. (21.51). The unitary group  $U(1)$  corresponds to the circle group consisting of all complex numbers with absolute value 1 under multiplication.



of quantum computation) makes use of the rotating-wave approximation, and the coupled dipoles model (studied in Chp. 19.5.4) is based on the assumption that at most a single photon at a time interacts with the atomic ensemble.

New phenomena arise from the presence of optical cavities shaping the spatial and spectral distribution of electromagnetic vacuum modes (see Chp. 20.3.2) and from the consideration of photonic recoil (see Chp. 22.6.1 and Chp. 23.6).

## 21.1 The Dicke model in the mean-field approximation

As we have seen in Sec. 2.3.8, the Hilbert space increases exponentially with the numbers of particles considered, the dimension of the Hilbert space of  $N$  particles being  $2^N$ . This obviously represents a problem for numerical simulations, and simplifying models are needed. One of them is the famous Dicke model, where the  $N$  atoms are described as spin- $\frac{1}{2}$  particles and their collective interaction with a light field via a single collective spin  $\mathbf{S}$  with  $S = N/2$ . In this model, the dimension of the Hilbert space only scales polynomially as  $2S + 1$ .

In the next sections, we will introduce this model detailing its advantages and limitations and emphasizing its relations to super- and subradiance, spin squeezing and entanglement.

### 21.1.1 Dicke states

The *Dicke model* describes the coupling of a single light mode with a set of  $N$  two-level atoms [196, 327]. When the coupling between the light and matter crosses a critical value, the Dicke model shows a mean-field phase transition to a superradiant phase. The Hilbert space of the Dicke model is given by (the tensor product of) the states of the cavity and of the two-level atoms<sup>2</sup>. The Hilbert space of the cavity can be spanned by Fock states  $|n\rangle$ . Choosing the basis  $|-\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $|+\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , the states of each two-level atom  $j = 1, 2, \dots, N$  are defined through the spin operators  $\hat{\mathbf{s}}_j = (\hat{s}_j^x, \hat{s}_j^y, \hat{s}_j^z)$  acting only on an individual atom,

$$\begin{aligned}\hat{s}_j^x|\dots \pm \dots\rangle &= \frac{\hbar}{2}|\dots \mp \dots\rangle \\ \hat{s}_j^y|\dots \pm \dots\rangle &= \pm i\frac{\hbar}{2}|\dots \mp \dots\rangle \\ \hat{s}_j^z|\dots \pm \dots\rangle &= \mp\frac{\hbar}{2}|\dots \pm \dots\rangle,\end{aligned}\tag{21.1}$$

and satisfying the spin algebra,

$$[\hat{s}_j^x, \hat{s}_k^y] = i\hbar\hat{s}_j^z\delta_{j,k},\tag{21.2}$$

and related to the Pauli spin matrices via  $\hat{\mathbf{s}}_j = \frac{\hbar}{2}\hat{\sigma}_j$ . The Hamiltonian of the Dicke model is,

$$\hat{H} = \hbar\omega_c\hat{a}^\dagger\hat{a} + \hbar\omega_a\sum_{j=1}^N\hat{s}_j^z + 2\hbar g(\hat{a} + \hat{a}^\dagger)\sum_{j=1}^N\hat{s}_j^x.\tag{21.3}$$

<sup>2</sup>Dicke states have already been introduced in the context of the Jaynes-Cummings model in Sec. 21.4.5.

Frequently, the coupling strength is normalized to the atom number,  $g \equiv \lambda/\sqrt{N}$ . The coupling can be written as the sum of two terms: a co-rotating term that conserves the number of excitations and is proportional to  $\hat{a}\hat{\sigma}^+ + \hat{a}^\dagger\hat{\sigma}^-$  and a counter-rotating term proportional to  $\hat{a}\hat{\sigma}^- + \hat{a}^\dagger\hat{\sigma}^+$ .

The above Hamiltonian assumes that all the spins are identical, i.e. they have the same transition frequency, they do not interact with each other, and they equally couple to the radiation field (e.g. a cavity mode). For the simple system of only two not mutually interacting spins,  $\mathbf{s}_1$  and  $\mathbf{s}_2$ , simultaneously coupling to the same radiation field, the Dicke model has been introduced in Sec. 4.4.2. There, we have shown that the spin operators can be added,  $\hat{\mathbf{S}} = \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2$ , and the total system be represented in a coupled basis, where  $[\hat{s}_1 \cdot \hat{s}_2, \hat{\mathbf{S}}^2] = 0 = [\hat{s}_1 \cdot \hat{s}_2, \hat{S}_z^2]$ . This concept can be generalized to an arbitrary number of spins, that is, under the above assumption, one can define macroscopic collective spin operators,

$$\hat{S}_\alpha \equiv \sum_{j=1}^N \hat{s}_j^\alpha \quad \text{with} \quad [\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \quad (21.4)$$

and  $\alpha = x, y, z$ . Using these operators, one can rewrite the above Hamiltonian as

$$\hat{H} = \hbar\omega_c\hat{a}^\dagger\hat{a} + \hbar\omega_a\hat{S}_z + 2\hbar g(\hat{a} + \hat{a}^\dagger)\hat{S}_x, \quad (21.5)$$

and it is easy to see that,

$$[\hat{H}, \hat{\mathbf{S}}^2] = 0 \neq [\hat{H}, \hat{S}_z]. \quad (21.6)$$

That is, the Dicke Hamiltonian preserves the spin  $\langle \hat{\mathbf{S}}^2 \rangle$ , but interaction with a light field can change the projection  $\langle \hat{S}_z \rangle$ . We will see in the following that this fact as important consequences for interaction dynamics of atomic ensembles coupled to a single light mode.

### 21.1.1.1 Degeneracies of Dicke states

Let us now look at states having the same number  $N$  of energy packets counting free photons  $n$  and atomic excitations  $N - n$ . For example with  $N = 2$ , the following states are possible.

$ n\rangle$	$ S, M\rangle =   \frac{N}{2}, M \rangle$	$  \frac{N}{2} - 1, M \rangle; \#1$
0	$ 1, 1\rangle =  ++\rangle$	
1	$ 1, 0\rangle = \frac{1}{\sqrt{2}}( +-\rangle +  -+\rangle)$	$ 0, 0\rangle = \frac{1}{\sqrt{2}}( +-\rangle -  -+\rangle)$
2	$ 1, -1\rangle =  --\rangle$	

This shows the existence of a singlet state, which decouples from the triplet states, in particular the deexcited one. Hence, this state is stable or subradiant, as discussed in Sec. 4.4.2<sup>3</sup>.

For example with  $N = 3$  (see also Exc. 4.4.5.14),

$ n\rangle$	$ S, M\rangle =   \frac{N}{2}, M \rangle; \#1$	$  \frac{N}{2} - 1, M \rangle; \#2$
0	$  \frac{3}{2}, \frac{3}{2} \rangle =  +++ \rangle$	
1	$  \frac{3}{2}, \frac{1}{2} \rangle =  ++-\rangle +  +-+\rangle +  -++\rangle$	$  \frac{1}{2}, \frac{1}{2} \rangle$
2	$  \frac{3}{2}, -\frac{1}{2} \rangle =  +--\rangle +  -+-\rangle +  --+\rangle$	$  \frac{1}{2}, -\frac{1}{2} \rangle$
3	$  \frac{3}{2}, -\frac{3}{2} \rangle =  ---\rangle$	

<sup>3</sup>Note that while superradiance, as well as subradiance can be explained by classical radiator models, such as the coupled dipoles model.

Example with  $N$  arbitrary,

$ n\rangle$	$ S, M\rangle =  \frac{N}{2}, M\rangle; \#1$	$ \frac{N}{2} - 1, M\rangle; \#(N - 1)$	$ \frac{N}{2} - 2, M\rangle; \#\frac{N(N-3)}{2}$
0	$ \frac{N}{2}, \frac{N}{2}\rangle =  ++++\dots\rangle$		
1	$ \frac{N}{2}, \frac{N}{2} - 1\rangle = \sum_{perm.}   - + + + \dots \rangle$	$ \frac{N}{2} - 1, \frac{N}{2} - 1\rangle$	
2	$ \frac{N}{2}, \frac{N}{2} - 2\rangle = \sum_{perm.}   - - + + \dots \rangle$	$ \frac{N}{2} - 1, \frac{N}{2} - 2\rangle$	$ \frac{N}{2} - 2, \frac{N}{2} - 1\rangle$
$\vdots$	$\vdots$	$\vdots$	
$N$	$ \frac{N}{2}, -\frac{N}{2}\rangle =  -----\dots\rangle$		

We see that the Dicke states are not made to unambiguously label degenerate states. States  $|S, M\rangle$  with  $S < |M|$  are largely degenerate, and transitions between energetically degenerate states  $|S, M\rangle$  and  $|S, M'\rangle$  with  $M = M'$  but  $S \neq S'$  are prohibited. Now, we want to know, how many states  $|+\rangle^{N+}|-\rangle^{N-}$  are in a single Dicke state labeled by  $|S, M\rangle$ .

### 21.1.1.2 Mean-field approximation and light field elimination

The *mean-field approximation* consists in replacing the photonic operators by their expectation values, i.e. assuming classical light. This allows us to remove the light energy term from the Hamiltonian and replace the coupling strength by the  $n$ -photon Rabi frequency,  $\Omega = g\sqrt{n}$ . The Hamiltonian then becomes just a generalization of the one-atom Hamiltonian (14.77) to large spins,

$$\hat{H} = \hat{\mathbf{S}} \cdot \mathbf{G} = \hbar\Delta \hat{S}_z + \hbar\text{Re } \Omega \hat{S}_x + \hbar\text{Im } \Omega \hat{S}_y, \quad (21.7)$$

with  $\Omega = 2g\sqrt{n}$  and allowing for complex Rabi frequencies.

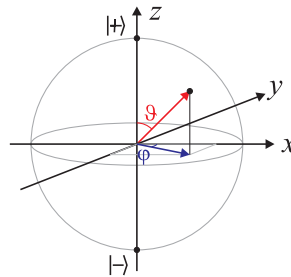


Figure 21.1: Illustration of the Bloch sphere.

In the absence of spontaneous emission, any pure single-atom state is given by,

$$|\psi\rangle = |\vartheta, \varphi\rangle = \cos \frac{\vartheta}{2} |+\rangle + e^{i\varphi} \sin \frac{\vartheta}{2} |-\rangle, \quad (21.8)$$

where the angles  $\vartheta$  and  $\varphi$  point to a location on the Bloch sphere characterizing the state of the atom. For example, an atom having been subject to a  $\frac{\pi}{2}$ -pulse ends up in the state  $|\frac{\pi}{2}, 0\rangle$ . The expectation value of the spin operator in this state is simply

obtained from,

$$\begin{aligned} \langle \vartheta, \varphi | \hat{S}_z | \vartheta, \varphi \rangle &= \cos^2 \frac{\vartheta}{2} \langle + | \hat{S}_z | + \rangle + \sin^2 \frac{\vartheta}{2} \langle - | \hat{S}_z | - \rangle = \frac{1}{2} \cos \vartheta \\ \langle \vartheta, \varphi | \hat{S}_+ | \vartheta, \varphi \rangle &= e^{i\varphi} \sin \frac{\vartheta}{2} \cos \frac{\vartheta}{2} \langle + | \hat{S}_+ | - \rangle = \frac{1}{2} e^{i\varphi} \sin \vartheta , \end{aligned} \quad (21.9)$$

yielding,

$$\langle \vartheta, \varphi | \hat{\mathbf{S}} | \vartheta, \varphi \rangle = \frac{1}{2} \begin{pmatrix} \cos \varphi \sin \vartheta \\ \sin \varphi \sin \vartheta \\ \cos \vartheta \end{pmatrix} . \quad (21.10)$$

We will also denote the probability of finding the system in state  $|\pm\rangle$  by,

$$p_{\pm} = \langle \hat{P}_{\pm} \rangle = |\langle + | \psi \rangle|^2 = \cos^2 \frac{\vartheta}{2} = 1 - p_{-} . \quad (21.11)$$

### 21.1.1.3 Collective spin states

Let us now study the system obeying the Hamiltonian (21.7) in detail. The spin operators  $\hat{\mathbf{S}}$  satisfy a SU(2) algebra explained in Sec. 4.3.2, i.e.  $\hat{\mathbf{S}} \times \hat{\mathbf{S}} = i\hat{\mathbf{S}}$ . The common eigenstates of  $\hat{\mathbf{S}}^2$  and  $\hat{S}_z$  are denoted by  $|S, M\rangle$ ,

$$\begin{aligned} \hat{S}_z &= \hat{S}_+ \hat{S}_- - \hat{S}_- \hat{S}_+ \quad \text{with} \quad \hat{S}_z |S, M\rangle = \hbar M |S, M\rangle \\ \hat{N}_{\pm} &\equiv \frac{1}{2} (N\mathbb{I} \pm \frac{1}{\hbar} \hat{S}_z) \quad \text{with} \quad \hat{N}_{\pm} |S, M\rangle = \frac{1}{2} (N \pm M) |S, M\rangle . \end{aligned} \quad (21.12)$$

From this we conclude that  $S = N/2$  is half the number of atoms and  $M$  the inversion.

We consider an ensemble of  $N = N_+ + N_-$  two-level atoms excited by a definite number of  $M$  photons, such that,

$$N = N_+ + N_- \quad \text{and} \quad 2M = N_+ - N_- . \quad (21.13)$$

Hence,  $N_{\pm} = \frac{N}{2} \pm M$  is the number of atoms in each of the two states. The  $N$  atoms can occupy  $2^N$  different collective states. However, when the atoms are identical and couple uniformly to the same light mode, all states where the same number of atoms is excited are energetically degenerate, and the total energy available to the system is,

$$E = M\hbar\omega_c . \quad (21.14)$$

The degeneracy of each many-body state with a given inversion  $M$  is given by the binomial coefficient,

$$\# = \binom{N}{\frac{N}{2} + M} = \binom{N}{N_+} = \binom{N}{N_-} \quad \text{such that} \quad \sum_{N_+=0}^N \binom{N}{N_+} = 2^N . \quad (21.15)$$

Therefore, we may set,

$$|S, M\rangle \equiv |+\rangle^{N_+} |-\rangle^{N_-} . \quad (21.16)$$

These states are called *Dicke states*<sup>4</sup>.

<sup>4</sup>In Sec. 4.4.3 we used for the coupling of two spins the notation  $|((s_1, s_2)s, m)\rangle$ . For coupling  $N$  spins, we should write in analogy,

$$|\overbrace{(\frac{1}{2}, \dots, \frac{1}{2})}^N, S, M\rangle \equiv |N, S, M\rangle .$$

Mostly, we will however drop the (constant) number  $N$ .

For the special case  $N = 2$  the transformation from the basis  $|+\rangle^{N+}|-\rangle^{N-}$ , used in the *Tavis-Cummings model*, to the basis  $|S, M\rangle$ , used in the Dicke model, is a unitary transformation. It has been extensively discussed in Sec. 4.4 at the example of two spins, whose complete Hilbert space can be expanded in the uncoupled or in the coupled basis. For  $N > 2$  the situation is more complicated, since the degeneracies of both models are different. It is important to be aware that  $S$  is not simply half the atom number, but runs over  $S = \frac{N}{2}, \frac{N}{2} - 1, \dots$ , depending on how the individual spins couple together. The degeneracy of an angular momentum state  $|S, M\rangle$  with a specific inversion  $M$  but undefined orbital momentum  $S$  is determined by the condition  $0 \leq S \leq M$ , and given by,

$$\# = \frac{N}{2} - |M| + 1. \quad (21.17)$$

For example, for  $N = 2$  the possible spin states are given by  $|s_1 - s_2| \leq S \leq s_1 + s_2$ . And for  $N = 5$ ,  $M = \frac{3}{2}$  is supported by  $S = \frac{3}{2}$  and  $\frac{5}{2}$ . Obviously, the degeneracy (21.17) is lower than (21.15) except for  $N = 2$ .

### 21.1.2 Coherent spin states

By the fact that the individual spins are additive and the Hamiltonian linear in the spin operators,  $\hat{H} \propto \hat{S}_z$ , we know that the Schrödinger equation will be satisfied by *product states*,

$$|\Psi_N\rangle = \prod_{k=1}^N |\vartheta_k, \varphi_k\rangle_k, \quad (21.18)$$

where  $|\vartheta_k, \varphi_k\rangle_k$  is the state of the  $k$ -th atom given by (21.8).

*Coherent spin states* now consist of  $N$  atoms, all being in the same state. In Exc. 21.1.6.1 we present another equivalent definition. Since the atoms are indistinguishable by the radiation field, we may as well drop the labeling index  $k$ ,

$$|\Psi_N\rangle = |\vartheta, \varphi\rangle^N = \sum_{k=0}^N \sqrt{\binom{N}{k}} \cos^{N-k} \frac{\vartheta}{2} |+\rangle^{N-k} e^{ik\varphi} \sin^k \frac{\vartheta}{2} |-\rangle^k, \quad (21.19)$$

in agreement with (16.50), or equivalently,

$$\boxed{|\vartheta, \varphi\rangle^N = \sum_{k=0}^{2S} \sqrt{\binom{2S}{k}} \cos^{2S-k} \frac{\vartheta}{2} e^{ik\varphi} \sin^k \frac{\vartheta}{2} |S, S-k\rangle}. \quad (21.20)$$

Hence, similarly to the coherent state of a harmonic oscillator, which consists of a Poissonian distribution of number states, the coherent spin state consists of a binomial distribution of  $N_+$  atoms in one state and  $N - N_+$  in the other. Note also, that by construction, the coherent spin states are **stretched**,  $S = N/2$ . That is, they can be represented by a vector of length  $N$  equal to the radius of the (generalized) Bloch sphere<sup>5</sup>. In other words,  $S$  is a conserved quantum number as already shown in (21.6), and this feature does not change under the influence of the Hamiltonian (21.7). These states are called superradiant. Nevertheless, other states  $|S, M\rangle$  are possible with  $S \leq \frac{N}{2}$ . These are squeezed, subradiant, or entangled states.

<sup>5</sup>An illustration of the generalized Bloch sphere is attempted in Fig. 21.10.

In the following we will study some of the properties of the coherent spin states. For instance, in Exc. 21.1.6.2 we calculate the expectation values coherent spin states,

$$\langle \Psi_N | \hat{\mathbf{S}} | \Psi_N \rangle = \langle \vartheta, \varphi |^N \hat{\mathbf{S}} | \vartheta, \varphi \rangle^N = S \begin{pmatrix} \cos \varphi \sin \vartheta \\ \sin \varphi \sin \vartheta \\ \cos \vartheta \end{pmatrix}. \quad (21.21)$$

Hence, the spin evolves on the surface of a Bloch sphere with radius  $\| |\Psi_N\rangle | \hat{\mathbf{S}} | \Psi_N \rangle \| = S = \frac{N}{2}$ . For the number of atoms in each state we expect,

$$\langle N_+ \rangle = \frac{N}{2} + \frac{1}{2\hbar} \langle \hat{S}_z \rangle = N \cos^2 \frac{\vartheta}{2} = N p_+ = N(1 - p_-) = N - \langle N_- \rangle. \quad (21.22)$$

### 21.1.2.1 Uncertainties and quantum projection noise in the Dicke model

Measuring the population of a coherently excited two-level system by projecting it onto an energy eigenstate introduces *quantum projection noise*. Although this inherent noise spoils the determination of the resonance frequency, it can to some extent be surpassed by *spin squeezing* [724]. The projection noise limit has been observed with ions [355, 347] and with atomic clouds [604]. The reduction of the noise by spin squeezing has been observed with ions [595], micromasers [572], and atomic clouds [301, 419]. Also, a weakly entangled state of two modes was observed for continuous spin variables [376]. Very strong squeezing spin can be obtained in a *Mott insulator* state, as demonstrated by [280].

First, we want to show that the Heisenberg uncertainty of a coherent spin state is nothing else than the quantum projection noise studied in Sec. 16.3.2. On one hand, we have,

$$\begin{aligned} \langle \vartheta, \varphi |^N (\Delta \hat{S}_z)^2 | \vartheta, \varphi \rangle^N &= \langle \vartheta, \varphi |^N \hat{S}_z^2 | \vartheta, \varphi \rangle^N - (\langle \vartheta, \varphi |^N \hat{S}_z | \vartheta, \varphi \rangle^N)^2 \\ &= \sum_{k=0}^N \binom{N}{k} \left( \frac{N}{2} - k \right)^2 p_+^{N-k} p_-^k - \left( \sum_{k=0}^N \binom{N}{k} \left( \frac{N}{2} - k \right) p_+^{N-k} p_-^k \right)^2 \\ &= \left( \frac{N^2}{4} - N^2 p_+ p_- + N p_+ p_- \right) - \left( \frac{N}{2} (p_+ - p_-) \right)^2 = N p_+ p_-. \end{aligned} \quad (21.23)$$

On the other hand, we have seen in (16.49),

$$\begin{aligned} (\Delta r)^2 &= \sum_{r=0}^N (r - N p_{\pm})^2 P_{N,r,\pm} \\ &= \sum_{k=0}^N \left( \frac{N}{2} - k + \frac{N}{2} (p_+ - p_-) \right)^2 \binom{N}{k} p_+^{N-k} p_-^k = N p_+ p_-. \end{aligned} \quad (21.24)$$

The Heisenberg uncertainty relation (2.88) applied to angular momentum operator satisfying  $[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$  states,

$$\Delta S_x \Delta S_y \geq \frac{\hbar}{2} |\hat{S}_z|. \quad (21.25)$$

Since there are no quantum correlations between the particles, the uncertainty of coherent spin states is additive (see Exc. 4.3.4.5),

$$(\Delta S_\alpha)^2 = \sum_{k=0}^N (\Delta s_k^\alpha)^2 . \quad (21.26)$$

**Example 96 (Uncertainty of a coherent spin state after a  $\frac{\pi}{2}$ -pulse):** A  $\frac{\pi}{2}$ -pulse applied to a cloud in the collective ground state generates the state  $|\vartheta, \varphi\rangle = |\frac{\pi}{2}, 0\rangle$ . This is somewhat analogous to the beam splitting of a photonic Fock state discussed in Sec. 15.6. Interestingly, a Fock state seems more natural for an atomic cloud, while the Glauber state is more natural for a photonic mode. For example, for the particular state  $|\frac{\pi}{2}, 0\rangle$  we find,

$$(\Delta S_x)^2 = 0 \quad \text{and} \quad (\Delta S_y)^2 = (\Delta S_z)^2 = \hbar^2 \frac{S}{2} .$$

We show this by an explicit calculation in Exc. 21.1.6.2.

Now, if appropriate quantum correlations are established between the individual spins, fluctuations may partly cancel out in one direction, while being increased in the other direction. This is the concept of spin squeezing. We will study this in the next section.

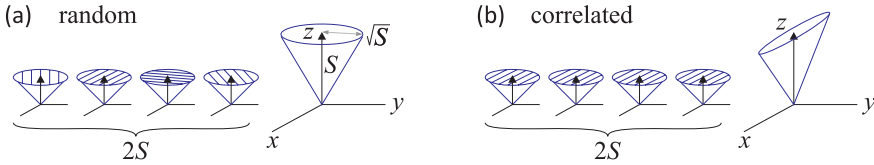


Figure 21.2: Illustration of the uncertainty in (a) a coherent state and (b) a spin-squeezed state.

### 21.1.3 Rotations, spin excitation and precession

A useful rule for the subsequent calculations, proved in Exc. 21.1.6.3, is the following,

$$e^{iF(\hat{S}_z)} \hat{S}_+ e^{-iF(\hat{S}_z)} = \hat{S}_+ e^{i[F(\hat{S}_z + \mathbb{I}) - F(\hat{S}_z)]} , \quad (21.27)$$

where  $F$  is an arbitrary function. For  $F(\hat{S}_z) \equiv \phi \hat{S}_z$  the unitary transform  $e^{iF(\hat{S}_z)}$  denotes a rotation about the  $z$ -axis, which we will study in the example below. For  $F(\hat{S}_z) \equiv \zeta \hat{S}_z^2$  it generates squeezing along the  $z$ -axis, which we will study in the next section. Furthermore, we define the rotation matrices about the Cartesian axis,

$$R_x(\gamma) \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \gamma & -\sin \gamma \\ 0 & \sin \gamma & \cos \gamma \end{pmatrix} , \quad R_y(\gamma) \equiv \begin{pmatrix} \cos \gamma & 0 & -\sin \gamma \\ 0 & 1 & 0 \\ \sin \gamma & 0 & \cos \gamma \end{pmatrix} ,$$

$$R_z(\gamma) \equiv \begin{pmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad (21.28)$$

for which it is possible to show (with  $\alpha = x, y, z$ ),

$$\boxed{R_\alpha(\gamma)\hat{\mathbf{S}} = e^{i\gamma\hat{S}_\alpha}\hat{\mathbf{S}}e^{-i\gamma\hat{S}_\alpha}}. \quad (21.29)$$

**Example 97 (Rotation about  $\hat{S}_z$ ):** Defining  $F(\hat{S}_z) \equiv \phi\hat{S}_z$  the relationship (21.27) tells us,

$$e^{i\phi\hat{S}_z}\hat{S}_+e^{-i\phi\hat{S}_z} = \hat{S}_+e^{i\phi},$$

and consequently,

$$e^{i\phi\hat{S}_z}\hat{\mathbf{S}}e^{-i\phi\hat{S}_z} = \begin{pmatrix} \frac{1}{2}(e^{i\phi}\hat{S}_+ + e^{-i\phi}\hat{S}_-) \\ \frac{1}{2i}(e^{i\phi}\hat{S}_+ - e^{-i\phi}\hat{S}_-) \\ \hat{S}_z \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \hat{\mathbf{S}} \equiv R_z(\phi)\hat{\mathbf{S}}.$$

Furthermore,

$$\begin{aligned} e^{i\phi\hat{S}_z}|\vartheta, \varphi\rangle^N &= \sum_{k=0}^{2S} \sqrt{\binom{2S}{k}} \cos^{N-k} \frac{\vartheta}{2} e^{ik\varphi} \sin^k \frac{\vartheta}{2} e^{i\phi(S-k)} |S, S-k\rangle \\ &= e^{i\phi S} \left( e^{i\phi} \cos \frac{\vartheta}{2} |+\rangle + e^{i(\varphi-\phi)} \sin \frac{\vartheta}{2} |-\rangle \right)^N = e^{i\phi S} |\vartheta, \varphi - \phi\rangle^N, \end{aligned}$$

and,

$$\begin{aligned} \langle \vartheta, \varphi |^N R_z(\phi)\hat{\mathbf{S}} | \vartheta, \varphi \rangle^N &= \frac{N}{2} \begin{pmatrix} \cos(\varphi + \phi) \sin \vartheta \\ \sin(\varphi + \phi) \sin \vartheta \\ \cos \vartheta \end{pmatrix} = \langle \vartheta, \varphi + \phi |^N \hat{\mathbf{S}} | \vartheta, \varphi + \phi \rangle^N \\ \langle \vartheta, \varphi |^N R_z(\varphi)R_y^{-1}(\theta)R_z^{-1}(\varphi)\hat{\mathbf{S}} | \vartheta, \varphi \rangle^N &= \frac{N}{2} \begin{pmatrix} \cos \varphi \sin(\theta + \vartheta) \\ \sin \varphi \sin(\theta + \vartheta) \\ \cos(\theta + \vartheta) \end{pmatrix} = \langle \vartheta + \theta, \varphi |^N \hat{\mathbf{S}} | \vartheta + \theta, \varphi \rangle^N. \end{aligned}$$

The rotation about the  $x$ -axis is derived in Exc. 21.1.6.4, and in Exc. 21.1.6.5 we write down the explicit rotation matrix for two atoms.

Rotations such as the ones described by  $R_\alpha(\gamma)$  are generated by the Dicke Hamiltonian (21.7), since the solution of the Schrödinger equation is,

$$\boxed{|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\Psi(0)\rangle = e^{-it\hat{S}_x \text{Re } \Omega_x - it\hat{S}_y \text{Im } \Omega_y - it\hat{S}_z \Delta} |\Psi(0)\rangle}. \quad (21.30)$$

The last example confirms that rotations do only transform coherent states into each other. Nevertheless, there are other unitary operations that transform coherent states into states that cannot be represented by coherent states. One example is squeezing.

## 21.1.4 Spin squeezing

### 21.1.4.1 Spin squeezing by one-axis twisting

Squeezing of spin is not as straightforward as squeezing of bosons, since the uncertainty relations are essentially different [397]. To study *spin-squeezing*, let us now specify the rule (21.27) for the particular case  $F(\hat{S}_z) = \zeta\hat{S}_z^2$ , defining the spin-squeezing operator,

$$\boxed{Q_z(\zeta)\hat{\mathbf{S}} \equiv e^{i\zeta\hat{S}_z^2}\hat{\mathbf{S}}e^{-i\zeta\hat{S}_z^2}}. \quad (21.31)$$



We get,

$$\begin{aligned} Q_z(\zeta)\hat{S}_+ &= e^{\iota\zeta\hat{S}_z^2}\hat{S}_+e^{-\iota\zeta\hat{S}_z^2} = \hat{S}_+e^{2\iota\zeta(\hat{S}_z+1/2)} \\ Q_z(\zeta)\hat{S}_- &= (Q_z(\zeta)\hat{S}_+)^\dagger = e^{-2\iota\zeta(\hat{S}_z+1/2)}\hat{S}_-, \end{aligned} \quad (21.32)$$

and hence,

$$Q_z(\zeta)\hat{\mathbf{S}} = e^{\iota\zeta\hat{S}_z^2}\hat{\mathbf{S}}e^{-\iota\zeta\hat{S}_z^2} = \begin{pmatrix} \frac{1}{2}(\hat{S}_+e^{2\iota\zeta(\hat{S}_z+1/2)} + e^{-2\iota\zeta(\hat{S}_z+1/2)}\hat{S}_-) \\ \frac{1}{2i}(\hat{S}_+e^{2\iota\zeta(\hat{S}_z+1/2)} - e^{-2\iota\zeta(\hat{S}_z+1/2)}\hat{S}_-) \\ \hat{S}_z \end{pmatrix}. \quad (21.33)$$

Since the unitary transform  $e^{\iota\zeta\hat{S}_z^2}$  commutes with  $\hat{S}_z$ , the prescription (21.31) does not immediately lead to squeezing along the  $z$ -axis. As shown in Exc. 21.1.6.6(a),

$$\langle \frac{\pi}{2}, 0 |^N e^{\iota\zeta\hat{S}_z^2}\hat{\mathbf{S}}e^{-\iota\zeta\hat{S}_z^2} | \frac{\pi}{2}, 0 \rangle^N = \begin{pmatrix} \frac{N}{2} \cos^{N-1} \zeta \\ 0 \\ 0 \end{pmatrix}. \quad (21.34)$$

Nevertheless, the prescription does generate quantum correlations in  $\hat{S}_x$  and  $\hat{S}_y$ , which can be transformed to squeezing by subsequently rotating the collective spin about the  $x$ -axis [397]. As shown in Exc. 21.1.6.7, a rotation by an angle  $\nu$  yields,

$$\overline{\langle \frac{\pi}{2}, 0 |^N e^{\nu\hat{S}_x} e^{\iota\zeta\hat{S}_z^2} \Delta \hat{S}_x^2 e^{-\iota\zeta\hat{S}_z^2} e^{-\nu\hat{S}_x} | \frac{\pi}{2}, 0 \rangle^N} = \frac{N}{4} [N(1 - \cos^{2N-2} \zeta) - \frac{N-1}{2} A] \quad (21.35)$$

$$\overline{\langle \frac{\pi}{2}, 0 |^N e^{\nu\hat{S}_x} e^{\iota\zeta\hat{S}_z^2} \Delta \hat{S}_{y,z}^2 e^{-\iota\zeta\hat{S}_z^2} e^{-\nu\hat{S}_x} | \frac{\pi}{2}, 0 \rangle^N} = \frac{N}{4} \{1 + \frac{N-1}{4} [A \pm \sqrt{A^2 + B^2} \cos(2\nu + 2\delta)]\},$$

with  $A \equiv 1 - \cos^{N-2} 2\zeta$ ,  $B \equiv 4 \sin \zeta \cos^{N-2} \zeta$ , and  $\delta \equiv \frac{1}{2} \arctan \frac{B}{A}$ . We study spin squeezing in Exc. 21.1.6.8 to 21.1.6.10. In Exc. 21.1.6.11 we investigate, whether double Fock states can lead to Heisenberg-limited interferometry, and in Exc. 21.1.6.12 we study entanglement witnesses with coherent spin states.

Obviously, since squeezed states are obtained from coherent states by unitary transform, they are still normalized,

$$\langle \vartheta, \varphi |^N e^{-\iota\zeta\hat{S}_z^2} e^{\iota\zeta\hat{S}_z^2} | \vartheta, \varphi \rangle^N = 1. \quad (21.36)$$

**Example 98 (Conditional spin-squeezing by non-demolition measurement):** Technically, spin-squeezed states can be generated in experiments by quantum non-demolition measurements [85, 159, 598].

## 21.1.5 The Holstein-Primakoff prescription

In the limit of large atom numbers the Dicke Hamiltonian can be approximated by a system of two coupled quantum oscillators. The mapping is done via the so-called *Holstein-Primakoff transformation*. The transformation is a mapping of the spin operators to boson creation and annihilation operators, effectively truncating their infinite-dimensional Fock space to finite-dimensional subspaces. Let us consider a spin

operator  $\hat{\mathbf{S}}$  defined by its commutation behavior  $[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$  and characterized by its eigenvectors  $|S, M\rangle$ ,

$$\hat{S}^2|S, M\rangle = \hbar^2 S(S+1)|S, M\rangle \quad , \quad \hat{S}_z|S, M\rangle = \hbar M|S, M\rangle \quad , \quad (21.37)$$

with the projection quantum number  $M = -S, -S+1, \dots, S-1, S$ . We consider a single particle of spin  $S$  and take the state  $|S, M = +S\rangle$  as a vacuum for a set of boson operators, and each subsequent state with lower projection quantum number as a boson excitation of the previous one,

$$|S, S-n\rangle \mapsto \frac{1}{\sqrt{n!}}(\hat{b}^\dagger)^n|0\rangle. \quad (21.38)$$

Each additional boson then corresponds to a decrease of  $M$  in the spin projection. Thus, the spin raising and lowering operators  $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$  satisfying so that  $[\hat{S}_+, \hat{S}_-] = 2\hbar\hat{S}_z$  correspond to bosonic annihilation and creation operators, respectively. The precise relations between the operators must be chosen to ensure the correct commutation relations for the spin operators. The resulting Holstein-Primakoff transformation can be written as,

$$\boxed{\hat{S}_+ = \hbar\sqrt{2S}\sqrt{1 - \frac{\hat{b}^\dagger\hat{b}}{2S}} \hat{b} \quad , \quad \hat{S}_- = \hbar\sqrt{2S} \hat{b}^\dagger \sqrt{1 - \frac{\hat{b}^\dagger\hat{b}}{2S}} \quad , \quad \hat{S}_z = \hbar(S - \hat{b}^\dagger\hat{b})} \quad . \quad (21.39)$$

The transformation is particularly useful in the case where  $S$  is large, when the square roots can be expanded as Taylor series, to give an expansion in decreasing powers of  $S$  [672, 71]. Do the Exc. 21.1.6.13.

The Holstein-Primakoff approximation allows us to rewrite the Hamiltonian (21.5) as,

$$\begin{aligned} \hat{H}_{HP} &= -\hbar\Delta_c\hat{a}^\dagger\hat{a} - \hbar\Delta_a\hat{S}_z + 2\hbar g(\hat{a} + \hat{a}^\dagger)\hat{S}_x & (21.40) \\ &= -\hbar\Delta_c\hat{a}^\dagger\hat{a} - \hbar\Delta_a(S - \hat{b}^\dagger\hat{b}) + 2\hbar g(\hat{a} + \hat{a}^\dagger)\sqrt{2S} \left( \sqrt{1 - \frac{\hat{b}^\dagger\hat{b}}{2S}} \hat{b} + \hat{b}^\dagger \sqrt{1 - \frac{\hat{b}^\dagger\hat{b}}{2S}} \right) \\ &\simeq -\hbar\Delta_c\hat{a}^\dagger\hat{a} - \frac{1}{2}\hbar\Delta_a\hat{b}^\dagger\hat{b} + 2\hbar g_N(\hat{a} + \hat{a}^\dagger)(\hat{b} + \hat{b}^\dagger) \quad , \end{aligned}$$

with the collective Rabi frequency  $g_N \equiv g\sqrt{N}$ . The Hamiltonian (21.40) describes two coupled quantum oscillators without rotating-wave approximation [232]<sup>6</sup>, a system which has already been discussed in Sec. 15.6.7 in the context of beamsplitters.

## 21.1.6 Exercises

### 21.1.6.1 Ex: Coherent spin states

Show that the coherent spin state is an eigenstate of the operator  $\hat{S}_{\vartheta, \varphi} \equiv \hat{S}_x \sin \vartheta \cos \varphi + \hat{S}_y \sin \vartheta \sin \varphi + \hat{S}_z \cos \vartheta$ .

<sup>6</sup>The Jaynes-Cummings model describes coupling of an atom to a harmonic oscillator mode [232]. In contrast ().

**21.1.6.2 Ex: Collective spin of a coherent spin state**

- Calculate the expectation values for all spin components of the collective spin  $\hat{\mathbf{S}}$  in a coherent spin state see also Exc. 4.3.4.8.
- Calculate the uncertainties for all spin components of the collective spin  $\hat{\mathbf{S}}$  in a coherent spin state.
- Apply the results to the particular state  $|\frac{\pi}{2}, 0\rangle^N$ .

**21.1.6.3 Ex: Unitary spin transformations**

Prove the relationship  $e^{iF(\hat{S}_z)}\hat{S}_+e^{-iF(\hat{S}_z)} = \hat{S}_+e^{i[F(\hat{S}_z+\mathbb{1})-F(\hat{S}_z)]}$ .

**21.1.6.4 Ex: Rotation about the  $x$ -axis**

How does the collective spin transform under rotation about the  $x$ -axis?

**21.1.6.5 Ex: Spin operators for two atoms**

Calculate explicitly for the case of two atoms the rotation matrices  $e^{i\gamma\hat{S}_\alpha}$  for  $\alpha = x, y, z$ . Check the relationship  $e^{i\gamma\hat{S}_\alpha}\hat{\mathbf{S}}e^{-i\gamma\hat{S}_\alpha} = R_\alpha(\gamma)\hat{\mathbf{S}}$  by explicit calculation.

**21.1.6.6 Ex: Spin squeezing**

- Calculate  $\langle \frac{\pi}{2}, 0 |^N e^{i\zeta\hat{S}_z^2}\hat{\mathbf{S}}e^{-i\zeta\hat{S}_z^2} | \frac{\pi}{2}, 0 \rangle^N$ .
- Calculate  $\langle \frac{\pi}{2}, 0 |^N e^{i\zeta\hat{S}_z^2}\Delta\hat{S}_x^2e^{-i\zeta\hat{S}_z^2} | \frac{\pi}{2}, 0 \rangle^N$ .

**21.1.6.7 Ex: Rotation of spin squeezed states****21.1.6.8 Ex: Spin squeezing with two atoms**

- For a system of two atoms, write down the coherent state  $|\vartheta, \varphi\rangle^2 = |\frac{\pi}{2}, 0\rangle^2$  in the Tavis-Cummings basis and in the Dicke state basis.
- Derive the matrix representation for the squeezing operator along the  $z$ -axis and apply this operator to the above coherent spin state.
- Compare spin squeezing with entanglement.

**21.1.6.9 Ex: Spin-squeezing via one-axis twisting**

For a Dicke state with  $N = 8$  atoms, program the matrix representations of the operators  $\hat{S}_\pm$ ,  $\hat{\mathbf{S}}$ ,  $R_\alpha(\theta)$ , and  $Q_\alpha(\zeta)$  for  $\alpha = x, y, z$  defined in the script, as well as the vector representation of the state  $|\vartheta, \varphi\rangle$ .

- Starting from the ground state  $|\vartheta, \varphi\rangle = |0, 0\rangle$ , simulate the following time evolution: (i)  $\frac{\pi}{2}$ -pulse with the Hamiltonian  $\hat{H} = \Omega\hat{S}_x$ , where  $\Omega$  is the Rabi frequency, (ii) interaction-free precession with the Hamiltonian  $\hat{H} = \Delta\hat{S}_z$  where  $\Delta$  is the detuning during a time  $T$ , (iii)  $\frac{\pi}{2}$ -pulse with the Hamiltonian  $\hat{H} = \Omega\hat{S}_x$ , (iv) projection of the energy axis. Plot the time evolution of the expectation values  $\langle \hat{S}_\alpha \rangle$  and  $\Delta\hat{S}_\alpha$ .

b. Starting from the ground state  $|\vartheta, \varphi\rangle = |0, 0\rangle$ , simulate the following time evolution: (i)  $\frac{\pi}{2}$ -pulse with the Hamiltonian  $\hat{H} = \Omega \hat{S}_y$ , where  $\Omega$  is the Rabi frequency, (ii) squeezing pulse along the  $z$ -axis with the squeezing parameter  $\zeta = 0.6$ , (iii)  $\frac{\pi}{2}$ -pulse with the Hamiltonian  $\hat{H} = \Omega \hat{S}_x$ . Plot the time evolution of the expectation values  $\langle \hat{S}_\alpha \rangle$  and  $\Delta \hat{S}_\alpha$ .

#### 21.1.6.10 Ex: Two-axis countertwisting

Study the Hamiltonian,

$$\hat{H} = \hbar\zeta(\hat{S}_{\pi/2, \pi/4}^2 + \hat{S}_{\pi/2, -\pi/4}^2 - \hat{S}_+^2 - \hat{S}_-^2)$$

with  $\hat{S}_{\vartheta, \varphi}$  defined in Exc. 21.1.6.1 in view of its squeezing features of an initial coherent spin state  $|0, \varphi\rangle$  [397].

#### 21.1.6.11 Ex: Interferometry with double Fock states

Discuss numerically whether, assuming as the initial state a double spin Fock state of the form  $|+\rangle^{N_1} |-\rangle^{N_2}$ , Heisenberg limited interferometry can be done within the Dicke model [99].

#### 21.1.6.12 Ex: Entanglement criteria

A sufficient entanglement criterion for an  $N$ -qubit state is, that it violates one of the following inequalities [688, 689],

$$\begin{aligned} \frac{(\Delta \hat{S}_z)^2}{\langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2} &\geq \frac{1}{N} \\ \langle \hat{S}_x^2 \rangle + \langle \hat{S}_y^2 \rangle + \langle \hat{S}_z^2 \rangle &\leq \frac{N(N+2)}{4} \\ \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle + \langle \Delta \hat{S}_z^2 \rangle &\geq \frac{N}{2} \\ \langle \hat{S}_k^2 \rangle + \langle \hat{S}_m^2 \rangle - \frac{N}{2} &\leq (N-1) \langle \Delta \hat{S}_n^2 \rangle \\ (N-1)[\langle \Delta \hat{S}_k^2 \rangle + \langle \Delta \hat{S}_m^2 \rangle] &\geq \langle \hat{S}_k^2 \rangle + \frac{N(N-2)}{4}, \end{aligned}$$

for  $(kmn) = (123)$ . Verify that, according to these criteria, coherent Dicke states are not entangled.

#### 21.1.6.13 Ex: Consistency of the Holstein-Primakoff transform

Verify that the relations (21.39) satisfy  $[\hat{S}_+, \hat{S}_-] \simeq 2\hbar \hat{S}_z$  and  $[\hat{S}_x, \hat{S}_y] \simeq \frac{\hbar}{2} \hat{S}_z$ .

## 21.2 Super- and subradiance in open systems

The abstract spin formalism developed in the last sections revealed propagators allowing us to rotate and squeeze coherent spin states, but it did not tell us how to implement them physically. For this, we need to solve equations of motion derived from Hamiltonians realizable in the laboratory. In the following sections, we will set

up the fundamental equations of motion (master or Heisenberg-Liouville) for open systems of  $N$  atoms subject to spontaneous emission collectively interacting with a single light mode subject to cavity decay and pumped by an external source.

We will discuss constants of motion of the Dicke and of the Tavis-Cummings model and phase transitions to superradiant states in the mean-field and in the Holstein-Primakoff approximation. Finally, we will present recent experimental realizations of Dicke phase transitions, namely superradiant self-ordering and superradiant lasing.

### 21.2.1 Models for open systems and phase transitions

We have already seen, that the spin quantum number  $S$  is preserved under the effect of the Dicke Hamiltonian (21.5). The spherical harmonics  $|S, M\rangle$  are orthonormal and the spin operators  $\hat{S}_\pm$  and  $\hat{S}_{x,y,z}$  or their combinations do not allow for transitions between states with different  $S$ ,

$$\begin{aligned} [\hat{H}, \hat{\mathbf{S}}^2] &= 0 \quad \text{with} \quad \hat{\mathbf{S}}^2 = \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+) + \hat{S}_z^2 \\ \text{but} \quad [\hat{H}, \hat{S}_z] &= i\hbar^2(\text{Im } \Omega \hat{S}_x - \text{Re } \Omega \hat{S}_y) \neq 0. \end{aligned} \quad (21.41)$$

Hence, under the effect of the Dicke Hamiltonian an initial state  $|N, S, M\rangle$  can only change its magnetic quantum number  $|N, S, M\rangle \rightarrow |N, S, M'\rangle$ , and the manifolds with a given  $S$  form closed sub-spaces (see Exc. 21.2.5.2). In other words, once we start in a superradiant state  $|N, S, M\rangle = |N, \frac{N}{2}, +\frac{N}{2}\rangle$ , spin conservation excludes subradiant states, which allowed us to restrict to the superradiant Dicke subspace. Transitions between Dicke subspaces are only possible via physical processes that act on individual atoms, e.g. decay or phase fluctuation processes, as we will see later [261].

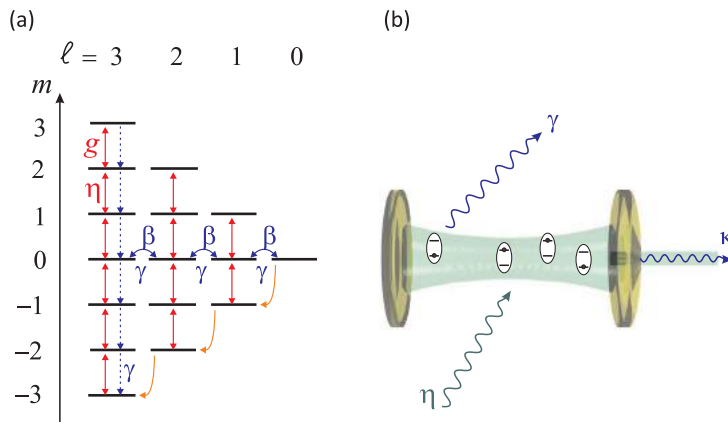


Figure 21.3: Illustration of the Dicke states for  $N = 6$ . Hamiltonian interactions are in depicted in red. Superradiant decay occurs through a cascade from state  $m = \ell$  to state  $m = -\ell$ . Spontaneous emission and phase noise leads to transitions along the blue arrows. The lowest states in each  $\ell$  subspace are dark and can only decay through a (subradiant) dark states cascade.

### 21.2.1.1 The open Dicke model

In the presence of spontaneous decay or dephasing, superradiant spin conservation is no longer guaranteed. Let us have a look at the master equation for a set of  $N$  atoms coupled with the strength  $g$  to the mode of a cavity and additionally pumped by a classical laser field  $\eta$  [396] (see (16.40)). After transformation into the rotating frame we have,

$$\begin{aligned} \dot{\hat{\rho}} &= \frac{i}{\hbar}[\hat{\rho}, \hat{H}_{Dicke}] + \sum_j \mathcal{L}_{\gamma_j, \hat{L}_j} \hat{\rho} \quad \text{or} \quad \dot{\hat{A}} = -\frac{i}{\hbar}[\hat{A}, \hat{H}_{Dicke}] + \sum_j \mathcal{L}_{\gamma_j, \hat{L}_j}^{\dagger} \hat{A} \\ \text{with } \hat{H}_{Dicke} &= -\hbar\Delta_c \hat{a}^{\dagger} \hat{a} - \hbar\Delta_a \hat{S}_z + 2\hbar g(\hat{a} + \hat{a}^{\dagger})(\hat{S}_+ + \hat{S}_-) + \hbar\eta(\hat{a} + \hat{a}^{\dagger}) \\ \text{and } \mathcal{L}_{\gamma, \hat{L}} \hat{\rho} &\equiv \gamma(2\hat{L}\hat{\rho}\hat{L}^{\dagger} - \hat{L}^{\dagger}\hat{L}\hat{\rho} - \hat{\rho}\hat{L}^{\dagger}\hat{L}) \\ \text{and } \mathcal{L}_{\gamma, \hat{L}}^{\dagger} \hat{A} &\equiv \gamma(2\hat{L}^{\dagger}\hat{A}\hat{L} - \hat{L}^{\dagger}\hat{L}\hat{A} - \hat{A}\hat{L}^{\dagger}\hat{L}) \end{aligned} \tag{21.42}$$

Here,  $\gamma_j$  are the rates of possible decay processes to which the degrees of freedom  $\hat{L}_j$  are subject. The most relevant decay processes are listed in the following table:

decay rate	dissipative operator	physical process
$\kappa$	$\hat{a}$	cavity decay
$\Gamma$	$\hat{S}_- = \sum_j \hat{s}_j^-$	collective atomic decay
$\gamma_1$	$\hat{s}_j^-$	cavity decay
$\beta$	$\hat{s}_j^z$	single-atom dephasing

$\Gamma$  and  $\kappa$  describe collective decay, while  $\gamma_1$  and  $\beta$  stand for spontaneous emission and phase fluctuation of individual atoms. The equations (21.42) describe the so-called *open Dicke model*. In Exc. 21.2.5.3 we derive the Heisenberg equations for the relevant degrees of freedom,

$$\begin{aligned} \dot{\hat{a}} &= (i\Delta_c - \kappa)\hat{a} - 4ig\hat{S}_x + \eta \\ \dot{\hat{S}}_- &= (i\Delta_a + 2\Gamma\hat{S}_z)\hat{S}_- + 4ig(\hat{a} + \hat{a}^{\dagger})\hat{S}_z \\ \dot{\hat{S}}_z &= -2\Gamma\hat{S}_+\hat{S}_- + 4g(\hat{a} + \hat{a}^{\dagger})\hat{S}_y \\ \dot{\hat{s}}_j^- &= (i\Delta_a - \beta)\hat{S}_- + \sum_j 2\gamma_1\hat{s}_j^z\hat{s}_j^- + 4ig(\hat{a} + \hat{a}^{\dagger})\hat{S}_z \\ \dot{\hat{s}}_j^z &= -2\gamma_1\sum_j \hat{s}_j^+\hat{s}_j^- + 4g(\hat{a} + \hat{a}^{\dagger})\hat{S}_y. \end{aligned} \tag{21.43}$$

In Exc. 21.2.5.4 we verify that these equations of motion do not change the spin  $\hat{\mathbf{S}}$ . The eqs. (21.43) can be rewritten in terms of observables as,

$$\dot{\hat{\mathbf{S}}} = \begin{pmatrix} 4g(\hat{a} + \hat{a}^{\dagger}) \\ 0 \\ -\Delta_a \end{pmatrix} \times \hat{\mathbf{S}} + \Gamma \begin{pmatrix} -\hat{S}_x + \hat{S}_x\hat{S}_z + \hat{S}_z\hat{S}_x \\ -\hat{S}_y + \hat{S}_y\hat{S}_z + \hat{S}_z\hat{S}_y \\ -2\hat{S}_z - 2\hat{S}_x^2 - 2\hat{S}_y^2 \end{pmatrix}. \tag{21.44}$$

Only the terms  $\mathcal{L}_{\gamma_1}$  and  $\mathcal{L}_{\beta}$  can change  $\hat{\mathbf{S}}^2$ . The  $\hat{\mathbf{S}}^2$  and  $\hat{S}_z$  eigenvalues determine the coupling strength of the many-atom (Dicke) state to the cavity mode and the

coherent, external drive. This coupling determines the rate of cavity photon generation as well as the pumping strength. The magnitude of the coupling strength distinguishes between superradiance and subradiance. For superradiant states the coupling strength scales superlinear in  $N$ , while for subradiant states the scaling is sublinear in  $N$ , and some subradiant states are dark. Dark means that the collective coupling to the cavity and the coherent, external drive of these states vanishes, meaning these states cannot decay via collective interactions e.g. by creating a cavity photon. However these states still decay into other states via the decay and dephasing processes  $\mathcal{L}_{\gamma_1}$  and  $\mathcal{L}_{\beta}$  acting individually on the emitters, see Fig. 21.3. Hence, spontaneous decay is an individualization process [261]. Generally, the spin preserving contributions in the master equation (21.49) generate quantum correlations leading to collective behavior (both super- and subradiance are collective effects) and the non-preserving terms destroy correlations leading to individualization (all properties scale exactly linear in  $N$ ). However only the spin non-preserving contributions introduce coupling between superradiant and subradiant states, thus in order to prepare subradiant states an interplay of collectivity and individualization is necessary. Based on these considerations, we may distinguish between collective versus individual behavior and superradiant versus subradiant behavior. The latter are special cases of collective behavior. This twofold distinction seems crucial when investigating super- and subradiance in the presence of dephasing and individual decay.

### 21.2.1.2 The open Tavis-Cummings model

Let us compare with *Tavis-Cummings model*, which is obtained from the Dicke Hamiltonian under the rotating wave approximation,

$$\boxed{\hat{H}_{TC} = -\hbar\Delta_c\hat{a}^\dagger\hat{a} - \hbar\Delta_a\hat{S}_z + 2\hbar g(\hat{a}\hat{S}_+ + \hat{S}_-\hat{a}^\dagger) + \hbar\eta(\hat{a} + \hat{a}^\dagger)}, \quad (21.45)$$

with the same dissipative terms as in (21.42). The Heisenberg-Liouville equations are now,

$$\begin{aligned} \dot{\hat{a}} &= (i\Delta_c - \kappa)\hat{a} - 2ig\hat{S}_- + \eta \\ \dot{\hat{S}}_- &= (i\Delta_a + 2\Gamma\hat{S}_z)\hat{S}_- + 4ig\hat{a}\hat{S}_z \\ \dot{\hat{S}}_z &= -2\Gamma\hat{S}_+\hat{S}_- - 2ig(\hat{a}\hat{S}_+ - \hat{S}_-\hat{a}^\dagger). \end{aligned} \quad (21.46)$$

The eqs. (21.46) can be rewritten in terms of observables as,

$$\dot{\hat{\mathbf{S}}} = \begin{pmatrix} 2g(\hat{a} + \hat{a}^\dagger) \\ 2ig(\hat{a} - \hat{a}^\dagger) \\ -\Delta_a \end{pmatrix} \times \hat{\mathbf{S}} + \Gamma \begin{pmatrix} -\hat{S}_x + \hat{S}_x\hat{S}_z + \hat{S}_z\hat{S}_x \\ -\hat{S}_y + \hat{S}_y\hat{S}_z + \hat{S}_z\hat{S}_y \\ -2\hat{S}_z - 2\hat{S}_x^2 - 2\hat{S}_y^2 \end{pmatrix}. \quad (21.47)$$

### 21.2.1.3 Symmetries of the Dicke and the Tavis-Cummings model

The total number of excitations,

$$\hat{N}_{ex} \equiv \hat{a}^\dagger\hat{a} + \hat{S}_z \quad (21.48)$$

is a constant of motion only for the Tavis-Cummings model and in the absence of pumping,  $\eta = 0$ ,

$$[\hat{H}_{Dicke}, \hat{N}_{ex}] = \eta(\hat{a} - \hat{a}^\dagger) + 4g(\hat{S}_- \hat{a} - \hat{S}_+ \hat{a}^\dagger) \quad (21.49)$$

$$[\hat{H}_{TC}, \hat{N}_{ex}] = \eta(\hat{a} - \hat{a}^\dagger) . \quad (21.50)$$

That is, the Hamiltonian preserves the excitation number, except for the counter-rotating terms, which can only change the excitation number by  $\pm 2$ .

The Dicke model has one global symmetry <sup>7</sup>,

$$\mathcal{P} : (\hat{a}, \hat{\sigma}^\pm) \rightarrow (-\hat{a}, -\hat{\sigma}^\pm) . \quad (21.51)$$

Because  $\mathcal{P}$  squares to unity, it has two eigenvalues, 1 and  $-1$ . This symmetry is associated with a conserved quantity: the parity of the total number of excitations,  $\mathcal{P} = (-1)^{N_{ex}}$ . This parity conservation is a consequence of the preserved excitation number. A state of the Dicke model is said to be normal when this symmetry is preserved, and superradiant when this symmetry is spontaneously broken.

## 21.2.2 Superradiant Dicke phase transition

### 21.2.2.1 Equilibrium Dicke phase transition

The Dicke model predicts a phase transition to a superradiant state, when the coupling strength  $g$  exceeds a certain critical value. To see this we simplify the Hamiltonian (21.5) by the mean-field approximation,

$$\hbar\omega_c \hat{a}^\dagger \hat{a} = \hbar\omega_c \alpha^2 , \quad (21.52)$$

where the field amplitude  $\alpha$  is a real number, and (as shown in Exc. 21.2.5.5) calculate the free energy as a function of  $\alpha$ ,

$$F(\alpha) \equiv -\frac{1}{\beta} \ln Z(\alpha) = \hbar\omega_c \alpha^2 - \frac{N}{\beta} \ln(2 \cosh \beta E) \quad (21.53)$$

$$\text{with } Z(\alpha) = \text{Tr } e^{-\beta \hat{H}}$$

$$\text{and } \langle \hat{h} \rangle = \pm E = \pm \sqrt{\left(\frac{\hbar\omega_a}{2}\right)^2 + (2\hbar g \alpha)^2} .$$

$Z(\alpha)$  is the partition function and  $\langle sm | \hat{h} | sm \rangle$  the single-atom energy eigenvalues. Below a critical coupling strength,

$$g_c \sqrt{N} = \frac{1}{2} \sqrt{\omega_c \omega_a \coth \frac{\beta \omega_a}{2}} , \quad (21.54)$$

the free energy minimizes for  $\alpha = 0$ , and beyond  $g_c$  it minimizes for  $\alpha > 0$ , as seen in Fig. 21.4 .

Note that the critical coupling smoothly evolves down to zero temperature ( $\beta \rightarrow 0$ ), where one obtains  $g_c = \sqrt{\omega_c \omega_a / 2N}$  <sup>8</sup>.

<sup>7</sup>For a Dicke picture of CARL see Exc. 22.5.7.1.

<sup>8</sup>Note, that in the thermodynamic limit,  $N \rightarrow \infty$ , the operators can be replaced by [396]:

$$\hat{S}_x \xrightarrow{N \rightarrow \infty} \frac{1}{2} \hat{N} \cos \hat{\varphi} \quad \text{and} \quad \hat{S}_y \xrightarrow{N \rightarrow \infty} \frac{1}{2} \hat{N} \sin \hat{\varphi} .$$

In this case, the operators commute  $[\hat{S}_x, \hat{S}_y] \rightarrow 0$ .



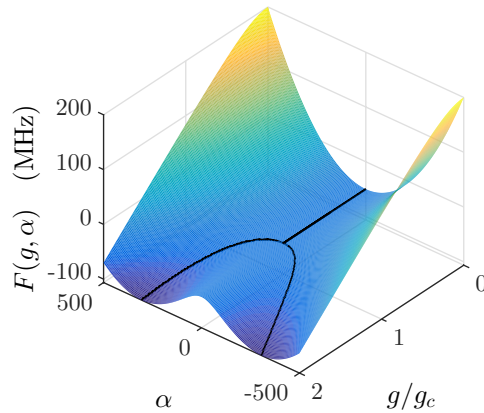


Figure 21.4: (code) Free energy as a function of coupling strength and photon number. Beyond the critical coupling strength  $g_c$  the minimum of the free energy splits opening the way for two possible equilibrium states of the mean-field phase.

### 21.2.2.2 Superradiant phase transition in the Holstein-Primakoff approximation

The superradiant phase transition was originally predicted by the Dicke model [196, 327]. It occurs when the strength of the interaction between the atoms and the field is greater than the energy of the non-interacting part of the system<sup>9</sup>. The collective Lamb shift, relating to the system of atoms interacting with the vacuum fluctuations, becomes comparable to the energies of atoms alone, and the vacuum fluctuations cause the spontaneous self-excitation of matter.

The transition can be readily understood by the use of the Holstein-Primakoff transformation applied to an ensemble of two-level atoms, as shown in Sec. 21.1.5, as a result of which the atoms become harmonic oscillators with frequencies equal to the difference between the energy levels. If the interaction between the atomic and the field oscillator is so strong that the system collapses in a ferroelectric-like phase transition. In Exc. 21.2.5.6 we will derive the Heisenberg equations for the open Dicke model in the Holstein-Primakoff approximation.

**Example 99** (*Dicke phase transition with a superfluid gas in an optical cavity*): [52]

### 21.2.3 Superradiant lasing in the Tavis-Cummings model

Cavity-mediated superradiance is described within the *Tavis-Cummings model* [120]. It represents an extension of the Jaynes-Cummings model for several atoms. We discussed such systems in Sec. 21.4.

<sup>9</sup>This is similar to the case of superconductivity in ferromagnetism, which leads to the dynamic interaction between ferromagnetic atoms and the spontaneous ordering of excitations below the critical temperature.

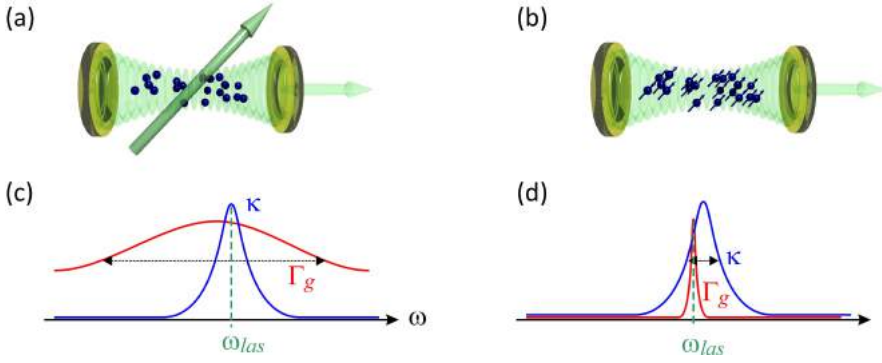


Figure 21.5: (a) Principle scheme of standard lasing. Here, the coherence is stored in the cavity field. The gain profile is much larger than the cavity width (good-cavity limit,  $\kappa \ll \Gamma_g$ ), as shown in (c). The laser frequency follows any (technical) cavity fluctuation:  $\omega_{las} = \omega_{cav} + \omega_g \frac{\kappa}{\Gamma_g}$ . (b) *Superradiant lasing*. Here, the coherence is stored in the gain. We are in the bad-cavity limit,  $\kappa \gg \Gamma_g$ , as shown in (d). The laser frequency is robust to cavity fluctuations:  $\omega_{las} = \omega_g + \omega_{cav} \frac{\Gamma_g}{\kappa}$ .

#### 21.2.4 Adiabatic elimination of the modes of a bad high-finesse cavity

We consider again the Heisenberg-Liouville equations for the open Dicke model (21.44) and the open Tavis-Cummings model Hamiltonian (21.47), restricting to many immobile atoms and a single cavity mode. In the bad cavity limit,  $\kappa \gg g$ , the cavity field is effectively slaved to the internal atomic dynamics. Hence, we may assume  $\dot{\hat{a}} \equiv 0$  and adiabatically eliminate the field,

$$g\hat{a} = \frac{-2ig^2}{\kappa - i\Delta_c} \hat{S}_- = -2i(\kappa_c + iU_c) \hat{S}_-. \quad (21.55)$$

where we additionally assumed  $\eta \equiv 0$  and introduced the abbreviations,

$$U_c \equiv \frac{g^2 \Delta_c}{\Delta_c^2 + \kappa^2} \quad \text{and} \quad \kappa_c \equiv \frac{g^2 \kappa}{\Delta_c^2 + \kappa^2}.$$

Inserting this into the above Heisenberg-Liouville equations of the Dicke model (21.44), we obtain neglecting  $\Gamma$ ,

$$\dot{\hat{\mathbf{S}}} = \begin{pmatrix} -16\kappa_c \hat{S}_y + 16U_c \hat{S}_x \\ 0 \\ -\Delta_a \end{pmatrix} \times \hat{\mathbf{S}}. \quad (21.56)$$

Inserting this into the above Heisenberg-Liouville equations of the Tavis-Cummings model (21.47), we obtain neglecting  $\Gamma$ ,

$$\dot{\hat{\mathbf{S}}} = \begin{pmatrix} -8\kappa_c \hat{S}_y + 8U_c \hat{S}_x \\ 8\kappa_c \hat{S}_x + 8U_c \hat{S}_y \\ -\Delta_a \end{pmatrix} \times \hat{\mathbf{S}}. \quad (21.57)$$

Alternatively, as studied in Exc 21.2.5.7, we may use the adiabatic elimination to simplify the Hamiltonians of the respective models and derive the Heisenberg-Liouville equations from these Hamiltonians [521]. E.g. for the Tavis-Cummings model, we get,

$$\hat{H}_{TC} = 4\hbar U_c \hat{S}_+ \hat{S}_- - \hbar \Delta_a \hat{S}_z. \quad (21.58)$$

This is the effective Hamiltonian of the *XX-Heisenberg model*.

**Example 100 (One-axis twisting in the XX-Heisenberg model):** The coupling strength  $\sqrt{N_+ N_-} \leq \frac{N}{2}$  between the cavity mode and the atoms depends on the inversion. Hence, this leads to an inversion-dependent frequency shift known as *one-axis twisting*<sup>10</sup>. In the mean field treatment we simply replace the operators by their expectation values. Setting  $\Delta_a = 0$  in the Heisenberg-Liouville equations (21.57) and neglecting terms  $\dot{\hat{S}}_z \propto \hat{S}_z$ , we get,

$$\dot{\hat{S}} \simeq 8 \begin{pmatrix} (\kappa_c \hat{S}_x + U_c \hat{S}_y) \hat{S}_z \\ (\kappa_c \hat{S}_y - U_c \hat{S}_x) \hat{S}_z \\ -\kappa_c (\hat{S}_x^2 + \hat{S}_y^2) \end{pmatrix}.$$

Starting from the initial condition,  $\vec{S} = (0, 0, N/2)$ , we see that the instantaneous collective dipole moment  $\hat{S}_x^2 + \hat{S}_y^2$  determines the decay of the inversion, while the inversion  $\hat{S}_z$  twists the dipole moment [471, 450, 523, 522, 521]. Collective decay occurs at a rate  $\hat{S}_- \sqrt{\kappa_c/2}$ .

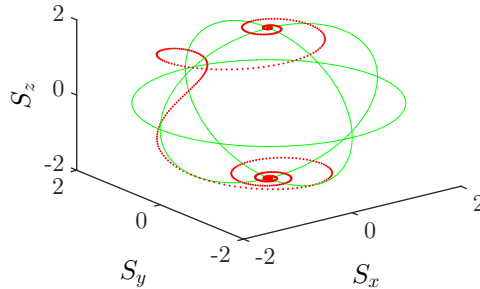


Figure 21.6: (code) One-axis twisting.

## 21.2.5 Exercises

### 21.2.5.1 Ex: Lindblad term for two atoms

Write down explicitly the master equation including the cooperative Lindblad term for two atoms.

### 21.2.5.2 Ex: Relationship between super- and subradiance and cooperativity

a. Discuss whether super- and subradiant states can be transformed into each other via unitary transformations.

<sup>10</sup>This is somewhat analogous to the photon number-dependent phase shift observed in dispersive interaction in the Jaynes-Cummings model.

b. Seek an interpretation of super- and subradiance as a modification of the structure factor by cooperativity.

### 21.2.5.3 Ex: Heisenberg equation for the open Dicke model

Derive the Heisenberg equation for the open Dicke model.

### 21.2.5.4 Ex: Spin conservation in the open Dicke and Tavis-Cummings model

- Show that the Dicke Hamiltonian (21.42) preserves the spin  $\hat{S}^2$ .
- Show that the Tavis-Cummings Hamiltonian (21.45) preserves the spin  $\hat{S}^2$ .
- Show that the dissipative terms of both models preserve the spin  $\hat{S}^2$ .

### 21.2.5.5 Ex: Equilibrium phase transition

- Calculate the free energy of the Hamiltonian (21.5) in the mean-field approximation.
- Minimize the free energy as a function of the field amplitude  $\alpha$  for various coupling strengths  $g$ . **Help:** Expand the expression for  $F'(\alpha)$  for small values of  $\alpha$ . Derive the expression for the critical coupling strength.

### 21.2.5.6 Ex: Heisenberg equation for the open Dicke model in the Holstein-Primakoff approximation

Derive the Heisenberg equations for the open Dicke model in the Holstein-Primakoff approximation.

### 21.2.5.7 Ex: Open system Hamiltonians after adiabatic elimination of the cavity mode

Use the adiabatic elimination of the cavity mode to simplify the Hamiltonians of the respective models and derive the Heisenberg-Liouville equations from these Hamiltonians.

## 21.3 Quantum correlations and entanglement

The concept of *entanglement* arose in quantum mechanics by Einstein, Podolski and Rosen's famous Gedankenexperiment, today called the *EPR paradox* [223]. In his Gedankenexperiment, Einstein tried to prove the necessity of hidden variables for quantum mechanics to be a complete theory. Consequently, we begin this chapter by introducing the notion of entangled particles and recapitulating the discussion of the EPR paradox.

Since Feynman discovered the utility of entangled states for quantum computation [540, 137], this area of research exploded with thousands of theoretical researchers, but very few experimentalists, due to the enormous technical difficulties of creating and controlling these states. On the other side, states of entangled photons already play

an important role in *quantum cryptography* [60]. And in the context of metrology, *spin-squeezed* correlated quantum states offer the possibility of quantum noise reduction in frequency standards [724].

Among the various systems proposed for the realization of entangled states and quantum computing gates we will only discuss one idea, which is based on the mutual coupling of atoms through a Jaynes-Cummings-like interaction mediated by an optical mode.

### 21.3.1 The EPR paradox and GHZ states

Let us imagine two maximally correlated particles produced by a suitable source, which fly freely without interaction in opposite directions along the  $z$ -axis toward two detectors  $a$  and  $b$ . The particles have an internal degree of freedom (spin)  $|\pm\rangle_{a,b}$ , which can be measured in various directions, for example,  $x$  or  $y$  by operators  $\hat{\sigma}_x^{a,b}$  or  $\hat{\sigma}_y^{a,b}$ . Since the particles are completely entangled, the result of a measurement on the first particle  $\hat{\sigma}_x^a$  allows the prediction of the result of another measurement  $\hat{\sigma}_x^b$  performed on the second particle, and similarly for  $\hat{\sigma}_y^a$  and  $\hat{\sigma}_y^b$ . Why is that?

The theory of *hidden variables* proposed by Einstein, Podolsky and Rosen [223] postulates, that the total state describing the two particles contains all information about the way, how the particles should behave at the detectors. The information was imprinted on each one of the two particle's when they were created in the source, i.e. the total state must be of the type,

$$|\psi\rangle = \begin{pmatrix} \pm_x^a & \pm_x^b \\ \pm_y^a & \pm_y^b \end{pmatrix}, \quad (21.59)$$

where the notation should be read as a decision table.

On the other hand, quantum mechanics postulates that the reduction of the wavepacket describing the particle at detector  $a$  decides *spontaneously* on the result of the measurement at detector  $b$ . This decision *has no physical cause*. If the particles move with the speed of light, this decision is not restricted by *local causality* [319]. The state can be given in the form,

$$|\psi\rangle = |+_a +_b\rangle - |-_a -_b\rangle. \quad (21.60)$$

**Example 101 (Bell's inequality):** Let us consider the EPR state (21.60). Particle 'a' is embarked with Alice on a starship, while particle 'b' flies with Bob in opposite direction. Quantum mechanics tells us that, before any measurement, the wavefunction is in a superposition of spin-up and spin-down states. After some time, Alice measures her spin in  $z$ -direction. Let us assume her measurement collapses the wavefunction in the spin-up state (for  $z$ -direction). Doing so, she instantaneously also collapses the wavefunction of Bob's spin in spin-up along the  $z$ -direction. Now, Bob tries to measure his spin in  $x$ -direction. If he succeeds and finds spin-up in the  $x$ -direction, Alice's wavefunction should collapse in spin-up along the  $x$ -direction, as well. But according to quantum mechanics, Alice should be unable to know the spin value in  $x$ -direction, since the spin operator components do not commute with each other,

$$[\hat{\sigma}_z^a, \hat{\sigma}_x^a] = i\hbar\hat{\sigma}_y^a, \quad [\hat{\sigma}_z^b, \hat{\sigma}_x^b] = i\hbar\hat{\sigma}_y^b. \quad (21.61)$$

That is, the direction of measurement in Alice’s experiment fixes the quantization axis for Bob’s experiment.

Two hypotheses have been put forward: The first one is that Alice’s experiment sends information to Bob’s experiment. Alice’s particle told Bob’s particle which spin state he should be in. But this hypothesis violates the locality requirement of special relativity claiming that information cannot travel faster than light. Einstein called it ‘spooky action at a distance’. The second hypothesis is to assume that quantum mechanics does not violate locality, but that the particles carry with them ‘local hidden variables’ (like a proper DNA) whose values would be set right from the moment of the separation of the particles and which would determine the outcomes of any future spin measurement. Then, quantum mechanics would not be a complete theory, because it has nothing to say about these hidden variables.

In 1964 John S. Bell suggested an experimental test for the EPR paradox. He proposed a theorem formulated as an inequality, the famous *Bell’s inequality*, stating that *if the hidden variables hypothesis proposed by Einstein is correct, then the inequality must be satisfied by experiment.*

There are many versions of Bell’s inequality, all of them are equivalent. Let us consider the Wigner-d’Espagnat version,

$$P(k+, n+) \leq P(k+, m+) + P(m+, n+) , \tag{21.62}$$

where  $P(k+, n+)$  is the joint probability for Alice to measure ‘spin-up’ in  $k$ -direction ( $\langle\sigma_k^a\rangle = +$ ) and Bob to measure ‘spin-up’ in  $n$ -direction ( $\langle\sigma_n^b\rangle = +$ ). Alice and Bob perform their experiments along the three possible directions  $\hat{\mathbf{e}}_k, \hat{\mathbf{e}}_m, \hat{\mathbf{e}}_n$  and they can get spin-up (+) or spin-down (–) in each direction. Furthermore, if Alice measures  $k+$ , Bob must also measure  $k+$ ,

$$\begin{pmatrix} \langle\sigma_k^a\rangle & \langle\sigma_k^b\rangle \\ \langle\sigma_m^a\rangle & \langle\sigma_m^b\rangle \\ \langle\sigma_n^a\rangle & \langle\sigma_n^b\rangle \end{pmatrix} = \tag{21.63}$$

$$\begin{pmatrix} + & + \\ + & + \\ + & + \end{pmatrix} \begin{pmatrix} + & + \\ + & + \\ - & - \end{pmatrix} \begin{pmatrix} + & + \\ - & - \\ + & + \end{pmatrix} \begin{pmatrix} - & - \\ + & + \\ + & + \end{pmatrix} \begin{pmatrix} + & + \\ - & - \\ - & - \end{pmatrix} \begin{pmatrix} - & - \\ + & + \\ - & - \end{pmatrix} \begin{pmatrix} - & - \\ - & - \\ + & + \end{pmatrix} \begin{pmatrix} - & - \\ - & - \\ - & - \end{pmatrix}$$

Firstly, let us suppose hidden variables really exist and calculate the joint probability between Alice’s and Bob’s readings,

$$\begin{aligned} P(k+, n+) &= \frac{N_1 + N_3}{N_{tot}} = \frac{2}{8} \\ P(k+, m+) &= \frac{N_1 + N_2}{N_{tot}} = \frac{2}{8} \\ P(m+, n+) &= \frac{N_1 + N_4}{N_{tot}} = \frac{2}{8} . \end{aligned} \tag{21.64}$$

It is easy to see that the inequality (21.62) is satisfied, and we conclude that the hidden variables hypothesis respects Bell’s inequality. In contrast, in quantum mechanics the probabilities depend on angles between the measurement axes,

$$\begin{aligned} P(k+, m+) &= P(k-, m-) = \sin^2 \frac{\theta_{km}}{2} \\ P(k+, m-) &= P(k-, m+) = \cos^2 \frac{\theta_{km}}{2} , \end{aligned} \tag{21.65}$$

and analogously for  $P(k+, n+)$  and  $P(m+, n+)$ . Then, the Bell inequality becomes,

$$\sin^2 \frac{\theta_{kn}}{2} \leq \sin^2 \frac{\theta_{km}}{2} + \sin^2 \frac{\theta_{mn}}{2} . \tag{21.66}$$

Suppose that the angles between each direction are  $\theta_{km} = \frac{\pi}{4}$ ,  $\theta_{mn} = \frac{\pi}{4}$ , and  $\theta_{kn} = \frac{\pi}{2}$ , so the inequality (21.66) results in  $0.5 \leq 0.146 + 0.146$ . Obviously, the inequality is violated.

Actually, the inequality (21.66) is violated for any angle between 0 and  $\pi/2$ , because the system is invariant under rotation. In conclusion, quantum mechanics violates Bell's inequality, such that an experimental test of the inequality must tell us, whether the hidden variables theory or quantum mechanics is correct.

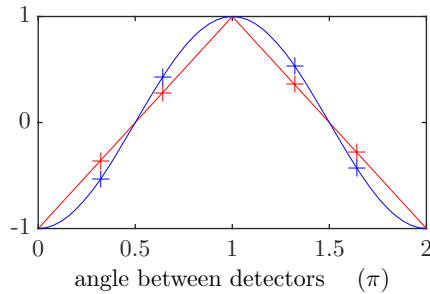


Figure 21.7: Correlations in hidden variables theory (red) and quantum mechanics (blue).

**Example 102 (GHZ states):** Here, we show a modified version of the EPR experiment proposed by Greenberger, Horne and Zeilinger (GHZ) based on the *GHZ state* [279]. They imagined a source creating three correlated non-interacting spin 1/2 particles flying toward three Stern-Gerlach type magnetic detectors, which measure the spins in  $x$  or in  $y$ -direction. The correct state is either quantum,  $|\psi\rangle = |+_a +_b +_c\rangle - |-_a -_b -_c\rangle$  or contains hidden variables  $|\psi\rangle = (\pm\pm\pm)$ . We know from quantum mechanics, that,

$$\hat{\sigma}_x |\pm\rangle_x = |\mp\rangle_x \quad \text{and} \quad i\hat{\sigma}_y |\pm\rangle_x = \mp |\mp\rangle_x . \tag{21.67}$$

From this follows,

$$\hat{\sigma}_x^a \hat{\sigma}_x^b \hat{\sigma}_x^c |\psi\rangle = -|\psi\rangle , \tag{21.68}$$

but also,

$$\hat{\sigma}_x^a \hat{\sigma}_y^b \hat{\sigma}_y^c |\psi\rangle = |\psi\rangle \quad , \quad \hat{\sigma}_y^a \hat{\sigma}_x^b \hat{\sigma}_y^c |\psi\rangle = |\psi\rangle \quad , \quad \hat{\sigma}_y^a \hat{\sigma}_y^b \hat{\sigma}_x^c |\psi\rangle = |\psi\rangle . \tag{21.69}$$

Hidden variables in a state  $|\psi\rangle$  that is *not a coherent superposition* should at least be able to predict how each particle will behave in its respective detector, when we measure each one of the two spin components. Eight combinations can satisfy the requirement (21.69):

$$\begin{aligned} & \begin{pmatrix} \langle \sigma_x^a \rangle & \langle \sigma_x^b \rangle & \langle \sigma_x^c \rangle \\ \langle \sigma_y^a \rangle & \langle \sigma_y^b \rangle & \langle \sigma_y^c \rangle \end{pmatrix} = & (21.70) \\ & \begin{pmatrix} +++ \\ +++ \end{pmatrix} \begin{pmatrix} +-- \\ +-- \end{pmatrix} \begin{pmatrix} -+- \\ -+- \end{pmatrix} \begin{pmatrix} -++ \\ -++ \end{pmatrix} \begin{pmatrix} +++ \\ --- \end{pmatrix} \begin{pmatrix} +-- \\ -++ \end{pmatrix} \begin{pmatrix} -+- \\ +-+ \end{pmatrix} \begin{pmatrix} --- \\ +++ \end{pmatrix} \end{aligned}$$

but none satisfies (21.68). Therefore, the EPR critique of quantum mechanics regarding *non-locality* and its incompleteness must be refuted <sup>11</sup>.

Which one of the two pictures is correct, the hidden variables assumption or quantum mechanics, can actually be tested by Wheeler’s *delayed choice* experiment. It consists of using pairs of correlated photons emitted in different directions, where they are expected by photodetectors. Polarizers located in front of the detectors fix the quantization axis to  $\hat{\mathbf{e}}_x$  or  $\hat{\mathbf{e}}_y$ , but the choice of the axis is made only after the photons were created by the source, in order to avoid possible backactions of the polarizers on the source <sup>12</sup>. Bell’s inequality condition [56] predicts a statistics for the results of repeated measurements where the orientation of the polarizers is randomly varied. The experiment run by Aspect [26, 25] showed that the assumption of hidden variables violates *local realism* and thus confirmed quantum mechanics as being a complete theory.

### 21.3.2 Information entropy

According to von Neumann, we can define the *von Neumann entropy*, also called quantum *information entropy* as,

$$S \equiv -\langle \log_2 \hat{\rho} \rangle = \text{Tr} (\hat{\rho} \log_2 \hat{\rho}) = - \sum_n \hat{\rho}_n \log_2 \hat{\rho}_n , \quad (21.71)$$

where  $\rho_n \equiv \langle n | \hat{\rho} | n \rangle$ . For statistically independent systems the density operator is  $\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2$  and the entropy is additive  $S = S_1 + S_2$ . The entropy is observable, that is, independent of the basis and invariant with respect to unitary transformations. Therefore,  $\hat{\rho}$  can be diagonalized and can be assumed diagonal in the following examples. For  $N$  independent qubits the density operator  $\hat{\rho}^{(N)}$  and the entropy  $S^{(N)}$  are:

$$\begin{aligned} \hat{\rho}^{(0)} &= |1\rangle\langle 1| & , & \quad S^{(0)} = 0 \text{ bit} & \quad (21.72) \\ \hat{\rho}^{(1)} &= \frac{1}{2}(|1\rangle\langle 1| + |2\rangle\langle 2|) & , & \quad S^{(1)} = 1 \text{ bits} \\ \hat{\rho}^{(2)} &= \frac{1}{4}(|11\rangle\langle 11| + |12\rangle\langle 12| + |21\rangle\langle 21| + |22\rangle\langle 22|) & , & \quad S^{(2)} = 2 \text{ bits} \\ \hat{\rho}^{(N)} &= \frac{1}{2^N}(|11\dots\rangle\langle 11\dots| + \dots) & , & \quad S^{(N)} = N \text{ bits} . \end{aligned}$$

The set is canonical and the entropy maximal. On the other hand, if the states are entangled, the entropy is always less than  $S^{(N)} = N$  bits. For the state of maximally entangled spins, we have,

$$\rho_{corr}^{(N)} = \frac{1}{2^N}(|11\dots 1\rangle\langle 11\dots 1| + |22\dots 2\rangle\langle 22\dots 2|) \quad , \quad S_{corr}^{(N)} = 1 \text{ bit} . \quad (21.73)$$

<sup>11</sup>Note that the coupling of different degrees of freedom *is not* an entanglement, but it is the *condition* for being able to generate entanglement.

<sup>12</sup>We note that first attempts to demonstrate wave-particle duality with single photons in dilute laser beams are not really conclusive, because the attenuation of a coherent state does NOT result in a single photon states (non-classical Fock state). Even if on average only less than one photon is in the interferometer, this may still be a Glauber state. Nonetheless, real single photon experiments involving the deexcitation of individual atoms by emission of two photons, produced the same result.



Entropy is a measure for the degree of entanglement of a system. For a Dicke state  $|J, M\rangle$  the entropy is,

$$S_{JM} = -\log_2 \binom{2J}{J+M}. \quad (21.74)$$

For beam splitters, the information entropy is calculated as follows: A Fock state  $|N\rangle = |1\rangle^N$  divided by a beam splitter is described by,

$$2^{-N/2} \cdot (|1\rangle + |2\rangle)^N = \frac{1}{2^{N/2}} \sum_{n=0}^N \binom{N}{n} |1\rangle^{N-n} |2\rangle^n \quad (21.75)$$

$$\rho_{split}^{(N)} = \frac{1}{2^N} \sum_{n,m=0}^N \binom{N}{n} \binom{N}{m} |1\rangle^{N-n} |2\rangle^n \langle 1|^{N-m} \langle 2|^m$$

$$\rho_{split}^{(N)} = \frac{1}{2^N} \sum_{n=0}^N \binom{N}{n} \binom{N}{n} |1\rangle^{N-n} |2\rangle^n \langle 1|^{N-n} \langle 2|^n.$$

For the information entropy, we obtain,

$$S_{split}^{(N)} = N + \frac{1}{2^N} \sum_{n=0}^N \binom{N}{n} \log_2 \binom{N}{n}. \quad (21.76)$$

The division of a beam is an incoherent process in the sense that it increases the entropy. The process is *irreversible*. The divided beams can not be recombined by a coherent process. For example, an interferometer always has two output ports. However, the phase is preserved.

The *quantum information content* is defined by the deviation from maximum entropy,

$$Q = S_{max} - S_{actual}. \quad (21.77)$$

If the system is in a mixed state, the entropy measures deviations from a pure state behavior [49].

### 21.3.3 Exercises

#### 21.3.3.1 Ex: Bell states

Show that the *Bell states* cannot be written as products of two states.

#### 21.3.3.2 Ex: Bell states

Calculate the reduced density matrix corresponding to a Bell state and the corresponding entropy (linear and von Neumann).

#### 21.3.3.3 Ex: Entanglement

Upon detecting the polarization of one photon in an entangled photon pair, the polarization of the other photon gets determined. Does this lead to a faster than light communication? Justify your answer. How would you demonstrate the no-cloning theorem from the assumption that relativistic causality should prevail.

**21.3.3.4 Ex: Entanglement**

Three photon are prepared in the state GHZ:

$$|\psi\rangle = \frac{1}{\sqrt{3}} (|h\rangle_1|h\rangle_2|h\rangle_3 + |h\rangle_1|h\rangle_2|h\rangle_3) .$$

Show that, when the components of polarization are measured along the axes that have an angle of  $45^\circ$  with respect to the original axes, corresponding to the states,

$$|h'\rangle = \frac{1}{\sqrt{2}}(|h\rangle + |v\rangle) \quad (x = 1) \quad \text{and} \quad |v'\rangle = \frac{1}{\sqrt{2}}(|h\rangle - |v\rangle) \quad (x = -1) ,$$

one gets necessarily an even number of photons with vertical polarization  $v'$ .

**21.3.3.5 Ex: NOON state**

A *NOON state* is a quantum-mechanical many-body entangled state:

$$|\psi_{\text{NOON}}\rangle = \frac{|N\rangle_a|0\rangle_b + e^{iN\theta}|0\rangle_a|N\rangle_b}{\sqrt{2}} , \quad (21.78)$$

which represents a superposition of  $N$  particles in mode  $a$  with zero particles in mode  $b$ , and vice versa. Usually, the particles are photons, but in principle any bosonic field can support NOON states.

Two-photon NOON states, where  $N = 2$ , can be created deterministically from two identical photons and a 50:50 beam splitter. This is called the Hong-Ou-Mandel effect in quantum optics. Three- and four-photon NOON states cannot be created deterministically from single-photon states, but they have been created probabilistically via post-selection using spontaneous parametric down-conversion.

## 21.4 Creation of quantum correlations

Since the experimental verification of *Bell's inequality* [27] numerous ideas were proposed for the creation and application of correlated states in distant particles. Realistic proposals on how to create such states are often based on a Jaynes-Cummings type coupling between states of atomic excitation and the degrees of freedom of a harmonic oscillator. The Jaynes-Cummings dynamics has been extensively studied in micromasers, where the non-resonant interaction of an atomic transition with the  $\text{TEM}_{00}$  mode of a stored radiation field generates quantum coherences. In very high finesse cavities, light field states with sub-Poissonian photon statistics can be generated and stored for macroscopic times, and schemes for the creation of Fock states and Schrödinger cat states were proposed and tested. Furthermore, the electronic excitation states of atoms successively traversing a micromaser can be correlated under suitable conditions. The availability of fundamental techniques motivated proposals for the investigation of phenomena such as EPR correlations, quantum teleportation, and quantum switching [208]. On the other hand, quantum coherences are very fragile to dissipation and rapidly decay when exposed to perturbations.

Jaynes-Cummings type dynamics can also be realized with a single ion stored in a Paul trap, where the interaction of its mechanical motion with an electronic transition [83] can induce very stable quantum coherences in the vibrational degrees

of freedom. Schrödinger cat states have already been demonstrated in this system [469], as well as fundamental parts of a quantum computer, the quantum *controlled not gate* [469] and the quantum *phase gate* [691]. A possible extension of these ideas is the collective Jaynes-Cummings interaction of a sample of ions with an optical field, where the vibrational degrees of freedom are coupled through Coulomb repulsion. Such scenarios are close to the currently most realistic ideas of quantum computers [137].

In order to correlate particles, they must be able to exchange information, that is, they must interact. One method used on ions trapped in a linear Paul trap, where they form a straight chain, and also on neutral atoms trapped in a dual optical lattice, consists in letting them undergo *controlled collisions* [362]. The proposed conditional quantum operation is based on a conditional collisional phase shift, the condition being that the atoms are in a particular state of excitation. In a suggestive notation for the Bloch vector of a particle subject to a resonant radiation pulse, the interaction is described by,

$$|\downarrow\rangle \xrightarrow{\pi/2} |\downarrow\rangle + \imath|\uparrow\rangle \xrightarrow{\pi/2} |\uparrow\rangle \xrightarrow{\pi/2} |\downarrow\rangle - \imath|\uparrow\rangle \xrightarrow{\pi/2} |\downarrow\rangle. \quad (21.79)$$

Jaksch demonstrated the following *phase gate*,

$$\begin{array}{ccc} \downarrow\downarrow & & \downarrow\downarrow \\ \uparrow\downarrow & \longrightarrow & -\downarrow\uparrow \\ \downarrow\uparrow & & \uparrow\downarrow \\ \uparrow\uparrow & & \uparrow\uparrow \end{array}. \quad (21.80)$$

This gate is equivalent to the *XOR* port for the qubits defined by  $\downarrow$  and  $\downarrow \pm \uparrow$ , since,

$$\begin{array}{ccc} \downarrow(\downarrow \pm \uparrow) & \longrightarrow & \downarrow(\downarrow \mp \uparrow) \\ \uparrow(\downarrow \pm \uparrow) & & \uparrow(\downarrow \pm \uparrow) \end{array}. \quad (21.81)$$

Alternative approaches to realizing quantum gates use dipole-dipole interactions [105], conditional Raman adiabatic passages by laser-induced excitation of interatomic dipole-dipole interactions [444], or interactions between permanent dipoles of atoms in Rydberg states [363]<sup>13</sup>

In Sec. 15.2 we showed already that the Jaynes-Cummings model is able to perform coherent operations on a two-level system –which from now on we will call *qubit*–, such as the *population inversion* (NOT-gate) and the controlled dephasing of an excited dipole moment (phase gate). These operations are fundamental for applications in quantum information, however, we still lack essential ingredients allowing us to entangle states of two, three or more qubits in order to perform a *quantum register* of *qubits*. Once these register are realized, we must define coherent quantum operations called *quantum gates*.

### 21.4.1 Jaynes-Cummings model for 1 atom and 2 radiation modes

The Hamiltonian for a single motionless atom interacting with two cavity modes  $|+\rangle$  and  $|-\rangle$  (we may, for instance, consider the counterpropagating modes of a ring cavity)

<sup>13</sup>A system to create quantum correlations is the *optical parametric oscillator* (OPO).





The observables of interest are the atomic Bloch vector (14.74), whose components are obtained from,

$$\begin{aligned} \rho_{ij} &= \langle i | \text{Tr}_{n_+, n_-} \hat{\rho} | j \rangle = \sum_{n_+, n_-} \langle i, n_+, n_- | \psi \rangle \langle \psi | j, n_+, n_- \rangle \\ &= \sum_{n_+, n_-} c_{i, n_+, n_-}^* c_{j, n_+, n_-} = \sum_{n_+, n_-} \tilde{c}_{n_+ + n_- + i, n_+ - n_-}^* \tilde{c}_{n_+ + n_- + j, n_+ - n_-} , \end{aligned} \quad (21.92)$$

the photon statistics in each mode,

$$\begin{aligned} p_{n_+} &= \langle n_+ | \text{Tr}_{i, n_-} \hat{\rho} | n_+ \rangle = \sum_{j, n_-} \langle j, n_+, n_- | \psi \rangle \langle \psi | j, n_+, n_- \rangle \\ &= \sum_{j, n_-} |c_{j, n_+, n_-}|^2 = \sum_{j, n_-} |\tilde{c}_{n_+ + n_- + j, n_+ - n_-}|^2 , \end{aligned} \quad (21.93)$$

and analogously for  $p_{n_-}$ , and the field distribution functions, such as the Husimi function,

$$\begin{aligned} \pi Q_+(\alpha) &\equiv \langle \alpha_+ | \text{Tr}_{i, n_-} \hat{\rho} | \alpha_+ \rangle \\ &= e^{-|\alpha_+|^2} \sum_{n_-} \left( \left| \sum_{n_+} c_{1, n_+, n_-} \frac{\alpha^{n_+}}{\sqrt{n_+!}} \right|^2 + \left| \sum_{n_+} c_{2, n_+, n_-} \frac{\alpha^{n_+}}{\sqrt{n_+!}} \right|^2 \right) , \end{aligned} \quad (21.94)$$

and analogously for  $Q_-(\alpha)$ , or the Wigner functions  $W_{\pm}(\alpha)$  from the coefficients  $\tilde{c}_{j, n_+, n_-}$ , respectively,  $\tilde{c}_{N, \delta}$ , as shown in Secs. 3.7.3 and 15.2.2.

### 21.4.2 Jaynes-Cummings model for 2 atoms and 1 light mode

In Sec. 15.2 we showed, how a Jaynes-Cummings interaction between an atom and a radiation field can exchange quantum correlations. It is reasonable to expect that, when we have two (or more) atoms interacting with the same radiation field, we can exchange correlations between atoms via the field. This would allow the implementation of entanglement protocols and quantum gates. We will disregard spontaneous processes, such that all couplings are then coherent and the processes reversible.

In Sec. 2.3.8 we learned, how to span a Hilbert space of various particles. We will now apply these notions in the scope of generalizing the Jaynes-Cummings model to *two atoms interacting with the same optical mode*, without spontaneous decay processes considered. The system is often referred to as the *Tavis-Cummings model*. The Hamiltonian of the system, which consists of two non-interacting atoms, both coupled in the same optical mode, is,

$$\hat{H} = \omega \hat{a}^\dagger \hat{a} + \sum_{i=1,2} \omega_{0i} (\hat{\sigma}_i^+ \hat{\sigma}_i^- - \frac{1}{2}) + \sum_{i=1,2} \frac{1}{2} \Omega_i(t) (\hat{a} \hat{\sigma}_i^+ + \hat{a}^\dagger \hat{\sigma}_i^-) . \quad (21.95)$$

The suffix denotes the individual atoms. Note that the coupling constant  $\frac{1}{2} \Omega_i(t)$  can be considered as time dependent, which may be useful for modeling radiation pulse

envelopes. In matrix representation the Hamiltonian acting on the subspace of  $n$  photons is,

$$|\psi\rangle = \sum_n \begin{pmatrix} c_{22} & n-1 \\ c_{21} & n \\ c_{12} & n \\ c_{11} & n+1 \end{pmatrix} |n\rangle \quad \text{where} \quad c_{ij} \equiv_{A2} \langle j|_{A1} \langle i| \langle n|\psi\rangle \quad (21.96)$$

for example,

$$|n\rangle|2\rangle_{A1}|2\rangle_{A2} = |n\rangle \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |n\rangle|2\rangle_{A1}|1\rangle_{A2} = |n\rangle \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{etc. .}$$

The atomic transition operators are generalized to,

$$\hat{\sigma}_{A1}^+ = \sum_n |n\rangle \hat{\sigma}^+ \otimes \mathbb{I} \langle n| = \sum_n |n\rangle \begin{pmatrix} & & 1 \\ & & \\ 0 & & 1 \\ & 0 & & \end{pmatrix} \langle n| \quad (21.97)$$

$$\hat{\sigma}_{A2}^+ = \sum_n |n\rangle \mathbb{I} \otimes \hat{\sigma}^+ \langle n| = \sum_n |n\rangle \begin{pmatrix} & & & \\ & & 1 & \\ 0 & & & \\ & 0 & & 1 \end{pmatrix} \langle n| \quad \text{etc. .}$$

The Hamiltonian is, on this basis,

$$\hat{H} = \sum_n |n\rangle \begin{pmatrix} n\omega - \frac{\omega_{01}}{2} - \frac{\omega_{02}}{2} & & & \\ & n\omega - \frac{\omega_{01}}{2} + \frac{\omega_{02}}{2} & & \\ & & n\omega + \frac{\omega_{01}}{2} - \frac{\omega_{02}}{2} & \\ & & & n\omega + \frac{\omega_{01}}{2} + \frac{\omega_{02}}{2} \end{pmatrix} \langle n|$$

$$+ \sum_n |n-1\rangle \sqrt{n} \begin{pmatrix} 0 & & & \\ \frac{\Omega_2}{2} & & & \\ \frac{\Omega_1}{2} & & & \\ 0 & \frac{\Omega_1}{2} & \frac{\Omega_2}{2} & 0 \end{pmatrix} \langle n| + \sum_n |n+1\rangle \sqrt{n+1} \begin{pmatrix} 0 & \frac{\Omega_2}{2} & \frac{1}{2}\Omega_1 & 0 \\ & & & \frac{\Omega_1}{2} \\ & & & \frac{\Omega_2}{2} \\ & & & 0 \end{pmatrix} \langle n|. \quad (21.98)$$

Now, we can rearrange the subspaces and finally get,

$$\hat{H} = \sum_n |n\rangle \begin{pmatrix} (n-1)\omega + \frac{\omega_{01}}{2} + \frac{\omega_{02}}{2} & \frac{\Omega_1}{2}\sqrt{n} & \frac{\Omega_2}{2}\sqrt{n} & \\ \frac{\Omega_1}{2}\sqrt{n} & n\omega - \frac{\omega_{01}}{2} + \frac{\omega_{02}}{2} & & \frac{\Omega_2}{2}\sqrt{n+1} \\ \frac{\Omega_2}{2}\sqrt{n} & & n\omega + \frac{\omega_{01}}{2} - \frac{\omega_{02}}{2} & \frac{\Omega_1}{2}\sqrt{n+1} \\ \frac{\Omega_2}{2}\sqrt{n+1} & \frac{\Omega_1}{2}\sqrt{n+1} & (n+1)\omega - \frac{\omega_{01}}{2} - \frac{\omega_{02}}{2} & \end{pmatrix} \langle n|. \quad (21.99)$$

The density operator for the subspace is,

$$\hat{\rho} = \begin{pmatrix} |n-1\rangle|2\rangle_{A1}|2\rangle_{A2}\langle 2|_{A1}\langle 2|\langle n-1| & |n-1\rangle|2\rangle_{A1}|2\rangle_{A2}\langle 2|_{A1}\langle 1|\langle n| & \dots \\ |n\rangle|1\rangle_{A1}|2\rangle_{A2}\langle 2|_{A1}\langle 2|\langle n-1| & \dots & \dots \\ |n\rangle|2\rangle_{A1}|1\rangle_{A2}\langle 2|_{A1}\langle 2|\langle n-1| & \dots & \dots \\ |n+1\rangle|1\rangle_{A1}|1\rangle_{A2}\langle 2|_{A1}\langle 2|\langle n-1| & \dots & \dots \end{pmatrix}, \quad (21.100)$$

if the basis is again defined by equation (21.97).

### 21.4.2.1 Resonant excitation

To discuss the case of resonant excitation,  $\Delta_1 = \Delta_2 = 0$ , let us assume identical atoms,  $\omega_{01} = \omega_{02} \equiv \omega_0$ , and equal Rabi frequencies,  $\Omega_1 = \Omega_2 \equiv \Omega$ . Assuming dipolarly forbidden strongly saturated transition,  $n = \alpha^2$  for all  $n$ , the Hamiltonian simplifies considerably,

$$\hat{H}_n = \begin{pmatrix} n\omega & \frac{1}{2}\sqrt{n}\Omega & \frac{1}{2}\sqrt{n}\Omega & \\ \frac{1}{2}\sqrt{n}\Omega & n\omega & & \frac{1}{2}\sqrt{n}\Omega \\ \frac{1}{2}\sqrt{n}\Omega & & n\omega & \frac{1}{2}\sqrt{n}\Omega \\ \frac{1}{2}\sqrt{n}\Omega & \frac{1}{2}\sqrt{n}\Omega & \frac{1}{2}\sqrt{n}\Omega & n\omega \end{pmatrix},$$

the eigenvalues can be calculated and the time evolution matrix becomes, using the abbreviation  $\varphi \equiv \sqrt{n}\Omega t/2$ ,

$$e^{-i\hat{H}_n t} = e^{-i\hat{H}_n^{A1} t} e^{-i\hat{H}_n^{A2} t} = \begin{pmatrix} \cos^2 \varphi & i \sin \varphi \cos \varphi & i \sin \varphi \cos \varphi & -\sin^2 \varphi \\ i \sin \varphi \cos \varphi & \cos^2 \varphi & -\sin^2 \varphi & i \sin \varphi \cos \varphi \\ i \sin \varphi \cos \varphi & -\sin^2 \varphi & \cos^2 \varphi & i \sin \varphi \cos \varphi \\ -\sin^2 \varphi & i \sin \varphi \cos \varphi & i \sin \varphi \cos \varphi & \cos^2 \varphi \end{pmatrix}. \quad (21.101)$$

For a  $\pi$ -pulse, we get,

$$e^{-i\hat{H}_n t} \xrightarrow{\pi/2} \frac{1}{2} \begin{pmatrix} 1 & i & i & -1 \\ i & 1 & -1 & i \\ i & -1 & 1 & i \\ -1 & i & i & 1 \end{pmatrix}. \quad (21.102)$$

It is interesting to note that some superposition states completely separate from the optical mode,

$$e^{-i\hat{H}_n t} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \quad \text{and} \quad e^{-i\hat{H}_n t} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}. \quad (21.103)$$

### 21.4.2.2 Dispersive excitation

In the dispersive limit,  $\Delta_i \gg n^{1/2}\Omega_i$ , the dynamic evolution can be evaluated from a first order perturbative approach, analogous to the one already made for the standard



JCM model. In this approach, the off-diagonal matrix elements (21.99) generate a light-shift of the energy levels appearing on the diagonal of the approximated matrix. Using the abbreviation  $\Lambda_i \equiv \Omega_i^2/4\Delta_i$ , the temporal evolution matrix  $e^{-i\hat{H}_n t}$  can now be evaluated from,

$$\hat{H}_n = -\frac{\Delta_1 + \Delta_2}{2} \mathbb{I}_4 \quad (21.104)$$

$$+ \begin{pmatrix} n\Lambda_1 + n\Lambda_2 & & & \\ & -n\Lambda_1 + (n+1)\Lambda_2 & & \\ & & (n+1)\Lambda_1 - n\Lambda_2 & \\ & & & -(n+1)\Lambda_1 - (n+1)\Lambda_2 \end{pmatrix}.$$

We now assume that the light field only interacts with the upper level, as in the case of the dual resonance configuration studied in Exc. 15.2.4.4. This can be taken into account, neglecting those terms in the matrix (21.103) rotating with a positive Rabi frequency. Letting, moreover,  $\Delta_1 = \Delta_2$  and  $\Omega_1 = \Omega_2$ , we obtain,

$$\hat{H}_n^{(1)} = \begin{pmatrix} 0 & & & \\ & -n\Lambda & & \\ & & -n\Lambda & \\ & & & -2(n+1)\Lambda \end{pmatrix}. \quad (21.105)$$

Thus, the temporal evolution is,

$$e^{-i\hat{H}_n t} = \begin{pmatrix} 1 & & & \\ & e^{-n\Lambda} & & \\ & & e^{-n\Lambda} & \\ & & & e^{-2(n+1)\Lambda} \end{pmatrix}. \quad (21.106)$$

For  $\Lambda = \pi$ ,

$$e^{-i\hat{H}_n t} \xrightarrow{\pi} \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}. \quad (21.107)$$

### 21.4.3 Bloch vector and the $Q$ -function in the JC model with 2 atoms

Despite the more complex structure of the Hilbert space, the Bloch vectors of the individual atoms and the  $Q$ -function can be evaluated in analogy to Sec. 15.2.1. The Bloch vector is,

$$\vec{\rho}_{A1} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2}\text{Re } \rho_{12(A1)} \\ \sqrt{2}\text{Im } \rho_{12(A1)} \\ \rho_{22(A1)} - \rho_{11(A1)} \end{pmatrix} \quad \text{where} \quad \rho_{ij(A1)} = \text{Tr } |i\rangle_1 \langle j|\psi\rangle\langle\psi|. \quad (21.108)$$

In particular we have,

$$\begin{aligned}
 \rho_{22(A1)} &= \sum_{i,j,n} {}_2\langle j|_1\langle i|\langle n|1\rangle_1\langle 2|\psi\rangle\langle\psi|n\rangle|i\rangle_1|j\rangle_2 \quad (21.109) \\
 &= \sum_{j,n} {}_2\langle j|_1\langle 2|\langle n|\psi\rangle\langle\psi|n\rangle|1\rangle_1|j\rangle_2 \\
 &= \sum_{n,m,m'} \langle n| (c_{2,1,m}|m\rangle\langle m'+1|c_{1,1,m'+1}^* + c_{2,2,m}|m'-1\rangle\langle m'|c_{1,2,m'}^*) |n\rangle \\
 &= \sum_n (c_{1,1,n}^*c_{2,1,n} + c_{1,2,n}^*c_{2,2,n}) .
 \end{aligned}$$

Summarizing,

$$\begin{aligned}
 \rho_{12(Ai \neq Aj)} &= \sum_n (c_{1,1,n}^*c_{j,i,n} + c_{i,j,n}^*c_{2,2,n}) \\
 \rho_{11(Ai \neq Aj)} &= \sum_n (|c_{1,1,n}|^2 + |c_{i,j,n}|^2) \\
 \rho_{22(Ai \neq Aj)} &= \sum_n (|c_{j,i,n}|^2 + |c_{2,2,n}|^2)
 \end{aligned} \quad . \quad (21.110)$$

The function  $Q(\alpha)$  for the JC dynamics of 2 atoms is,

$$\begin{aligned}
 Q(\alpha) &= \frac{1}{\pi} \langle \alpha | \hat{\rho}_{field} | \alpha \rangle \quad (21.111) \\
 &= \frac{1}{\pi} \langle \alpha | \sum_{i,j} {}_2\langle j|_1\langle i|\psi\rangle\langle\psi|i\rangle_1|j\rangle_2 | \alpha \rangle \\
 &= \frac{1}{\pi} \langle \alpha | \sum_{m,n} (c_{2,2,m-1}^*c_{2,2,n-1}|n-1\rangle\langle m-1| + c_{1,2,m}^*c_{1,2,n}|n\rangle\langle m| \\
 &\quad + c_{2,1,m}^*c_{2,1,n}|n\rangle\langle m| + c_{1,1,m+1}^*c_{1,1,n+1}|n+1\rangle\langle m+1|) | \alpha \rangle \\
 &= e^{-|\alpha|^2} \left[ \left| \sum_n c_{2,2,n-1} \frac{\alpha^n}{\sqrt{n!}} \right|^2 + \left| \sum_n c_{1,2,n} \frac{\alpha^n}{\sqrt{n!}} \right|^2 + \left| \sum_n c_{2,1,n} \frac{\alpha^n}{\sqrt{n!}} \right|^2 + \left| \sum_n c_{2,2,n+1} \frac{\alpha^n}{\sqrt{n!}} \right|^2 \right] .
 \end{aligned}$$

#### 21.4.4 Correlating atoms in the JCM model

The investigations of the last section can be applied to describe the transfer of quantum coherence from one atom to another. The size of our system is now increased by the additional degrees of freedom, provided by internal states of the second atom. A suitable basis was defined in equation (2.110). Now, we imagine the following Gedankenexperiment: Starting from the initial condition that two adjacent atoms are in their respective electronic ground states, we assume a microwave  $\pi/2$ -pulse to create *simultaneously, but independently* on both atoms, a superposition of the HFS levels. Then, a non-resonant optical  $\pi$ -pulse interacts with the upper HFS level of the first atom  $|1\rangle_{A1}$ , and afterward the second atom  $|2\rangle_{A2}$ . Instead of reducing the atomic states and preparing a Schrödinger cat state in the optical field, (as we did in Sec. 15.2), we now project the field state onto the coherent state  $|\beta\rangle$  and leave the atoms in a correlated state. The total procedure can be resumed by tracing the

evolution of the whole state in the following suggestive way [31]:

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ |\beta\rangle \end{pmatrix} \xrightarrow{\pi/2 \text{ microwave}} \frac{1}{4} \begin{pmatrix} -1 \\ i \\ i \\ 1 \end{pmatrix} |\beta\rangle \xrightarrow{\pi \text{ opt+atom1}} \frac{1}{4} \begin{pmatrix} |-\beta\rangle \\ i|\beta\rangle \\ -i|-\beta\rangle \\ |\beta\rangle \end{pmatrix} \xrightarrow{\pi \text{ opt+atom2}} \frac{1}{4} \begin{pmatrix} -|\beta\rangle \\ -i|-\beta\rangle \\ -i|-\beta\rangle \\ |\beta\rangle \end{pmatrix} \quad (21.112)$$

$$\xrightarrow{\pi/2 \text{ microwave}} \frac{1}{4} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} |\beta\rangle + \frac{1}{4} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} |-\beta\rangle \xrightarrow{\text{reduction}} \frac{1}{2} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} |\beta\rangle .$$

If this procedure is extended to an arbitrary number of atoms, obviously all atoms being excited by the same optical mode before its projection in a coherent state  $|\beta\rangle$  are included in the entangled state,

$$|\psi\rangle = \frac{1}{4} \begin{pmatrix} 1 \\ : \\ 1 \end{pmatrix} |\beta\rangle + \frac{1}{4} \begin{pmatrix} -1 \\ : \\ 1 \end{pmatrix} |-\beta\rangle . \quad (21.113)$$

Finally, the correlation of the spin orientation of the atoms must be probed with additional laser light fields, which are selectively irradiated onto the atoms and resonantly tuned to a rapidly decaying optical transition. The states correlated in this way show a relatively low order entanglement, the von Neumann information entropy only being  $S' = -\langle \log_2 \rho \rangle = N - 1$ .

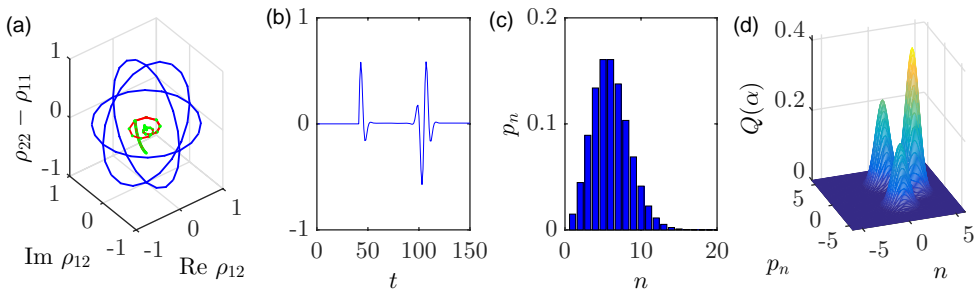


Figure 21.9: (code) Evolution of the state during a Jaynes-Cummings interaction with 2 atoms: (a) Bloch vector for the two atoms, (b) time evolution of the coherence  $\rho_{12}$  showing the phenomenon of collapse and revival, (c) distribution of photons, and (d)  $Q(\alpha)$ -function.

#### 21.4.4.1 The XOR gate, treating the field phase as degree of freedom

We define the state,

$$|\psi\rangle = (c_{+\alpha 11} \quad c_{+\alpha 11} \quad c_{+\alpha 12} \quad c_{+\alpha 12} \quad c_{-\alpha 21} \quad c_{-\alpha 21} \quad c_{-\alpha 22} \quad c_{-\alpha 22}) . \quad (21.114)$$

A dispersive  $\pi$ -pulse does,

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \\ 0 \\ -i \\ -i \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & & & & & & & \\ & & & -1 & & & & \\ & & & & & -1 & & \\ & & 1 & & & & & \\ & & & 1 & & & & \\ -1 & & & & & & & \\ & -1 & & & & & & \\ & & -1 & & & & & \\ & & & & & & & 1 \end{pmatrix} \begin{pmatrix} 1 \\ i \\ i \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (21.115)$$

A resonant  $\pi/2$ -pulse acting on the first atom only does,

$$\begin{pmatrix} 1 \\ -i \\ i \\ -1 \\ 1 \\ -i \\ -i \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & & i & & & & & \\ & 1 & & i & & & & \\ & i & & 1 & & & & \\ & & i & & 1 & & & \\ & & & & & 1 & & i \\ & & & & & & i & \\ & & & & & & & 1 \\ & & & & & & & & i & & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \\ 0 \\ -i \\ -i \\ 0 \end{pmatrix}. \quad (21.116)$$

By reducing the Glauber state  $|\alpha\rangle$  we obtain, a posteriori, the unitary XOR gate,

$$\begin{pmatrix} 1 \\ -i \\ i \\ -1 \end{pmatrix} = \begin{pmatrix} 1 & & i \\ & 1 & i \\ & i & 1 \\ & & & 1 \end{pmatrix} \begin{pmatrix} 0 \\ -1 \\ -i \\ 0 \end{pmatrix}. \quad (21.117)$$

### 21.4.5 Dicke states in the Jaynes-Cummings model

The Jaynes-Cummings Hamiltonian for two atoms in the limit  $\Delta_1 = \Delta_2$  and  $\Omega_1 = \Omega_2$  (both atoms are inside the mode volume of the field and are indistinguishable) is given by (21.101). This matrix shows two identical and non-shifted eigenvalues at  $\lambda = n\omega$ ,

$$\det(\hat{H}_n - \lambda\mathbb{I}) = (n\omega - \lambda)^2[(n\omega - \lambda)^2 - \Delta^2 - n\Omega^2] = 0. \quad (21.118)$$

The description of the dynamics can be simplified by reducing the order of the matrix by calculating the average of the lines 2 and 3,

$$\hat{H}_n = \begin{pmatrix} n\omega - \Delta & \frac{1}{2}\sqrt{2n}\Omega & \\ \frac{1}{2}\sqrt{2n}\Omega & n\omega & \frac{1}{2}\sqrt{2n(n+1)}\Omega \\ & \frac{1}{2}\sqrt{2(n+1)}\Omega & n\omega + \Delta \end{pmatrix},$$

since  $c_{01\ n} = c_{10\ n}$ , and opting for a new base defined by,

$$|\psi\rangle = \sum_n \begin{pmatrix} c_{11\ n-1} \\ c_{01\ n} \\ c_{00\ n+1} \end{pmatrix} |n\rangle. \quad (21.119)$$

The new Hamiltonian has the same eigenvalues  $\lambda = n\omega, n\omega \pm \varpi_n$ , but without degeneracies. If we assume furthermore that the excitation is resonant,  $\Delta = 0$ , with high intensity,  $n = \beta^2$  for all  $n$ , our matrix becomes,

$$\hat{H}_n \approx \begin{pmatrix} \beta^2\omega & \frac{1}{\sqrt{2}}\beta\Omega \\ \frac{1}{\sqrt{2}}\beta\Omega & \beta^2\omega & \frac{1}{\sqrt{2}}\beta\Omega \\ & \frac{1}{\sqrt{2}}\beta\Omega & \beta^2\omega \end{pmatrix}, \quad (21.120)$$

with the eigenvalue matrix,

$$E_n = U_n^\dagger \hat{H}_n U_n \approx \begin{pmatrix} \beta^2\omega - \beta\Omega & & \\ & \beta^2\omega & \\ & & \beta^2\omega + \beta\Omega \end{pmatrix}, \quad (21.121)$$

where

$$U_n \simeq \frac{1}{2} \begin{pmatrix} -1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & -1 \end{pmatrix}. \quad (21.122)$$

With this we can derive the propagator,

$$e^{-i\hat{H}_n t} = \frac{1}{2} e^{-i\beta^2\omega t} \begin{pmatrix} 1 + \cos \beta\Omega t & -\sqrt{2}i \sin \beta\Omega t & -1 + \cos \beta\Omega t \\ -\sqrt{2}i \sin \beta\Omega t & 2 \cos \beta\Omega t & -\sqrt{2}i \sin \beta\Omega t \\ -1 + \cos \beta\Omega t & -\sqrt{2}i \sin \beta\Omega t & 1 + \cos \beta\Omega t \end{pmatrix} \\ \xrightarrow{\beta\Omega t = \pi/2} \frac{1}{2} e^{-i\pi/2 \cdot \beta\omega/\Omega} \begin{pmatrix} 1 & -\sqrt{2}i & -1 \\ -\sqrt{2}i & 0 & -\sqrt{2}i \\ -1 & -\sqrt{2}i & 1 \end{pmatrix}.$$

The generalization to three atoms,

$$\hat{H}_n \simeq \begin{pmatrix} (n + \frac{1}{2})\omega - \frac{3}{2}\Delta & \frac{1}{2}\sqrt{3n}\Omega & & \\ \frac{1}{2}\sqrt{3n}\Omega & (n + \frac{1}{2})\omega - \frac{1}{2}\Delta & \frac{1}{2}\sqrt{4(n+1)}\Omega & \\ & \frac{1}{2}\sqrt{4(n+1)}\Omega & (n + \frac{1}{2})\omega + \frac{1}{2}\Delta & \frac{1}{2}\sqrt{3(n+2)}\Omega \\ & & \frac{1}{2}\sqrt{3(n+2)}\Omega & (n + \frac{1}{2})\omega + \frac{3}{2}\Delta \end{pmatrix},$$

or  $N$  atoms is easy. We define  $2S$  as the number of atoms,  $M$  as the collective atomic spin,  $n$  as the number of photons in the optical mode, and  $\hat{S}^\pm \equiv \sum_i \hat{\sigma}_i^\pm$ . The so-called *Dicke state*  $|S, M, n\rangle$  basically consists of a set of  $N$  indistinguishable spin-1/2 states ( $\hbar \equiv 1$ ). We introduce a basis by,

$$|\psi\rangle = \sum_n \begin{pmatrix} |S, S, n\rangle \\ \vdots \\ |S, -S, n + 2S\rangle \end{pmatrix}. \quad (21.123)$$

Obviously, we have [196],

$$\langle S, M - 1, n + 1 | \frac{1}{2}\Omega \hat{a}^\dagger \hat{\sigma}^- | S, M, n \rangle = \frac{1}{2}\Omega \sqrt{n+1} \sqrt{S(S+1) - M(M+1)}. \quad (21.124)$$

The Dicke states  $|SM\rangle$  follow the  $SU(2)$  algebra explained in Sec. 4.3.2. The Dicke state model has been discussed extensively in Sec. 21.1.

## 21.5 Quantum gates

In *quantum information* we use the notions introduced in the preceding sections and formalize the calculation. In this section, we present a brief formal introduction to the field of *quantum computation with qubit matrices*. The formalism is abstract, but we may keep in mind a chain of entangled ions confined in a linear Paul trap. We will show how the electronic states of the ions are correlated to form a single collective state, and how quantum gates can be realized on such correlated particles. With three ions, an arbitrary quantum gate can be implemented, which includes and generalizes the three-bit Toffoli gate.

To construct a quantum gate, we need at least two qubits spanning a 4-dimensional Hilbert space, since  $\mathcal{H}^2 \otimes \mathcal{H}^2$  and  $\mathcal{H}^1 \otimes \mathcal{H}^4$  are isomorph, that is,

$$\begin{aligned}
 |\varepsilon\rangle_1|\mu\rangle_2 &= (|1\rangle_1 + \imath|2\rangle_1)(|1\rangle_2 + \imath|2\rangle_2) = \begin{pmatrix} |1\rangle_1|1\rangle_2 \\ \imath|1\rangle_1|2\rangle_2 \\ \imath|2\rangle_1|1\rangle_2 \\ -|2\rangle_1|2\rangle_2 \end{pmatrix} \\
 \triangleq |0\rangle_1|\varepsilon\mu\rangle_2 &= |11\rangle_2 + \imath|12\rangle_2 + \imath|21\rangle_2 - |22\rangle_2 = \begin{pmatrix} |11\rangle_2 \\ \imath|12\rangle_2 \\ \imath|21\rangle_2 \\ -|22\rangle_2 \end{pmatrix}.
 \end{aligned} \tag{21.125}$$

A presentation on the subject is available at [\(watch talk\)](#).

### 21.5.1 The qubit

As we have seen above, the two principle ways a light mode acts on a two-level system are the resonant interaction and the dispersive interaction. From the Jaynes-Cummings model (15.37) and (15.44),

$$\begin{aligned}
 R(\tau) &\equiv \begin{pmatrix} \cos \frac{\pi}{2}\tau & \imath \sin \frac{\pi}{2}\tau \\ \imath \sin \frac{\pi}{2}\tau & \cos \frac{\pi}{2}\tau \end{pmatrix} \xrightarrow{\tau \rightarrow 1} \begin{pmatrix} & \imath \\ \imath & \end{pmatrix} \equiv \hat{R}, \\
 D(\tau) &\equiv \begin{pmatrix} e^{\imath\pi\tau} & 0 \\ 0 & 1 \end{pmatrix} \xrightarrow{\tau \rightarrow 1} \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} \equiv \hat{D}.
 \end{aligned} \tag{21.126}$$

For example, a resonant  $\pi$ -pulse corresponds to a *negation* in the Hilbert  $\mathcal{H}^2$ ,

$$\boxed{U = |\bar{A}\rangle\langle A| = \hat{R}}. \tag{21.127}$$

A qubit in the Hilbert space  $\mathcal{H}^2$  can be understood as a quantum superposition,

$$|\varepsilon\rangle = \alpha|0\rangle + \imath\beta|1\rangle = \begin{pmatrix} \alpha \\ \imath\beta \end{pmatrix}, \tag{21.128}$$

or represented by a classical truth table,

$$\begin{matrix} |A\rangle \\ |0\rangle \\ |1\rangle \end{matrix}, \text{ for example } |01\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{21.129}$$

The only difference is, that now the possible values are not restricted to the binaries 0 or 1, but can be anything between 0 and 1, provide the total wavefunction stays normalized.

### 21.5.2 Quantum gates of 2 qubits, the 'controlled NOT' gate

We can generalize the single-qubit algebra to arbitrary registers using the *direct sum* and the *external product* defined in (2.110) and (2.112),

$$\begin{matrix} |A & B\rangle \\ |0 & 0\rangle \\ |0 & 1\rangle \\ |1 & 0\rangle \\ |1 & 1\rangle \end{matrix}, \text{ for example } |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}. \quad (21.130)$$

The most interesting two-qubit quantum gate is the 'controlled NOT' gate, which we will now discuss in detail. This gate is originally defined on  $\mathcal{H}^2 \otimes \mathcal{H}^2$ . The quantum operation is implemented by first going to the Hilbert space  $\mathcal{H}^1 \otimes \mathcal{H}^4$ , applying the unitary transform,

$$\hat{N} = \begin{pmatrix} \mathbb{I}_2 & \\ & \hat{R} \end{pmatrix}, \quad (21.131)$$

where  $\hat{R}$  has been defined in Eq. (21.126), and finally returning to  $\mathcal{H}^2 \otimes \mathcal{H}^2$ :

$$\begin{aligned} |\varepsilon\rangle_1 |\mu\rangle_2 &\triangleq |0\rangle_1 |\varepsilon\mu\rangle_2 \xrightarrow{\hat{N}} \delta_{\varepsilon=1} |\varepsilon\rangle_1 |\mu\rangle_2 + \delta_{\varepsilon=2} |\varepsilon\rangle_1 \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} |\mu\rangle_2 \triangleq |\varepsilon\rangle_1 |\varepsilon \oplus \mu\rangle_2 \\ \begin{pmatrix} |1\rangle_1 |1\rangle_2 \\ i|1\rangle_1 |2\rangle_2 \\ i|2\rangle_1 |1\rangle_2 \\ -|2\rangle_1 |2\rangle_2 \end{pmatrix} &\triangleq \begin{pmatrix} |11\rangle_2 \\ i|12\rangle_2 \\ i|21\rangle_2 \\ -|22\rangle_2 \end{pmatrix} \xrightarrow{\hat{N}} \begin{pmatrix} |11\rangle_2 \\ i|12\rangle_2 \\ i|22\rangle_2 \\ -|21\rangle_2 \end{pmatrix} \triangleq \begin{pmatrix} |1\rangle_1 |1\rangle_2 \\ i|1\rangle_1 |2\rangle_2 \\ i|2\rangle_1 |2\rangle_2 \\ -|2\rangle_1 |1\rangle_2 \end{pmatrix}. \end{aligned} \quad (21.132)$$

Or, using a short hand notation we can express the *negation* in  $\mathcal{H}^4$  by,

$$\boxed{\begin{matrix} U = |A, \bar{B}\rangle \langle A, B| = \mathbb{I} \otimes \hat{R} \\ U = |\bar{A}, B\rangle \langle A, B| = \hat{R} \otimes \mathbb{I} \end{matrix}}. \quad (21.133)$$

Another operation is the *antivalence* in  $\mathcal{H}^4$

$$\boxed{\begin{matrix} |A, A \oplus B\rangle \langle A, B| = \mathbb{I} \oplus \hat{R}, \\ U = |B \oplus A, B\rangle \langle A, B| = \hat{S}(\mathbb{I} \oplus \hat{R})\hat{S} \end{matrix}}. \quad (21.134)$$

### 21.5.3 Quantum gates of 3 qubits

We now consider three qubits in  $\mathcal{H}^8 \equiv \mathcal{H}^2 \otimes \mathcal{H}^2 \otimes \mathcal{H}^2$ . The *truth table* has the shape,

$$\begin{array}{l}
 |A \ B \ C\rangle \\
 |0 \ 0 \ 0\rangle \\
 |0 \ 0 \ 1\rangle \\
 |0 \ 1 \ 0\rangle \\
 |0 \ 1 \ 1\rangle \\
 |1 \ 0 \ 0\rangle \\
 |1 \ 0 \ 1\rangle \\
 |1 \ 1 \ 0\rangle \\
 |1 \ 1 \ 1\rangle
 \end{array}
 , \text{ for example } |010\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} . \tag{21.135}$$

We choose  $\hat{1}_8$  as the basis of  $\mathcal{H}^8$ . It is possible to show that all quantum logic gates can be reduced to a gate called *Toffoli gate*,

$$\boxed{
 \begin{array}{l}
 \mathcal{H}^8 \xrightarrow{U} \mathcal{H}^8 \\
 |A, B, C\rangle \xrightarrow{U} |A, B, (A \cdot B) \oplus C\rangle \\
 \hat{1}_8 \xrightarrow{U} U .
 \end{array}
 } \tag{21.136}$$

The unitary transform implemented by a quantum gate can be understood as a permutation of the basis vectors in the truth table. We can generalize the permutation rules (2.116) to 3D Hilbert spaces  $\mathcal{H}^2 \otimes \mathcal{H}^2 \otimes \mathcal{H}^2$ , where  $M \otimes N \otimes R = S_{12}(N \otimes M \otimes R)S_{12} = S_{23}(M \otimes R \otimes N)S_{23} = S_{13}(R \otimes N \otimes M)S_{13}$ , with

$$S_{ij} = \mathbb{I}(k_{ij}, k_{ij}) \quad , \quad \begin{cases} k_{12} = [1, 2, 5, 6, 3, 4, 7, 8] \\ k_{23} = [1, 3, 2, 4, 5, 7, 6, 8] \\ k_{13} = [1, 3, 5, 7, 2, 4, 6, 8] \end{cases} . \tag{21.137}$$

We can also generate the transformation matrices  $S_{23} = \mathbb{I} \otimes S$ ,  $S_{13} = S \otimes \mathbb{I}$  and  $S_{12} = S_{13}S_{23}$ .

#### 21.5.3.1 Fundamental quantum gates

Examples of fundamental three-qubits gates are, in short notation, the *negation* in  $\mathcal{H}^8$ ,

$$\begin{aligned}
 U &= |A, B, \bar{C}\rangle\langle A, B, C| = \mathbb{I} \otimes \mathbb{I} \otimes R, \\
 U &= |A, \bar{B}, C\rangle\langle A, B, C| = \mathbb{I} \otimes R \otimes \mathbb{I} , \\
 U &= |\bar{A}, B, C\rangle\langle A, B, C| = R \otimes \mathbb{I} \otimes \mathbb{I} ,
 \end{aligned} \tag{21.138}$$





### 21.5.4 The quantum composer representation

See [IBM Circuit Composer](#).

#### 21.5.4.1 One qubit Hilbert space

The most fundamental gate can be written as,

$$U_3(\theta, \phi, \lambda) = \begin{pmatrix} \cos \frac{\theta}{2} & -e^{i\lambda} \sin \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} & e^{i\lambda+i\phi} \cos \frac{\theta}{2} \end{pmatrix}. \tag{21.143}$$

Special cases are the *Hadamard gate*,

$$H = U_3\left(\frac{\pi}{2}, 0, \pi\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{21.144}$$

and the *phase gate*,

$$U_1(\phi) = U_3(0, \phi, 0) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}. \tag{21.145}$$

Phase rotations about particular angles are named  $Z = U_1(\pi)$ ,  $S = U_1\left(\frac{\pi}{2}\right)$ ,  $T = U_1\left(\frac{\pi}{4}\right)$ .

#### 21.5.4.2 Two qubit Hilbert space

Obviously, to perform quantum calculations, we need at least two qubits and operations acting simultaneous on both.

### 21.5.5 The field of quantum information

The possibility to experimentally control, manipulate and read out individual qubits and gave birth to a new field of physics in the past two decades now called *quantum information*. This fields includes the more specific areas of *quantum processing* (which itself splits into the subareas of quantum computing and quantum simulation), *quantum communication*, and *quantum sensing* (see Sec. 16.5).

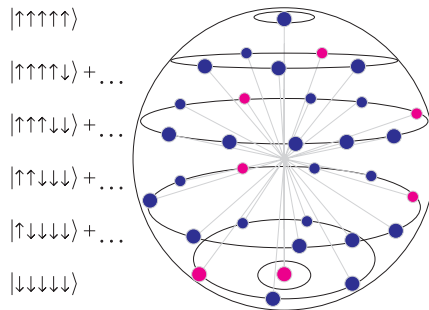


Figure 21.10: Illustration of the possible states of a 5-qubit system.

### 21.5.5.1 Quantum Fourier transform

The *quantum Fourier transform* (QFT) is a linear transformation on qubits and the quantum analogue of the inverse discrete Fourier transform. The quantum Fourier transform is a part of many quantum algorithms, notably Shor's algorithm for factoring and computing the discrete logarithm or the quantum phase estimation algorithm for estimating the eigenvalues of a unitary operator.

The quantum Fourier transform can be performed efficiently on a quantum computer, with a particular decomposition into a product of simpler unitary matrices. Using a simple decomposition, the discrete Fourier transform on  $2^n$  amplitudes can be implemented as a quantum circuit consisting of only  $O(n^2)$  Hadamard gates and controlled phase shift gates, where  $n$  is the number of qubits. This can be compared with the classical discrete Fourier transform, which takes  $O(2^n)$  gates, which is exponentially more than in the classical case. However, the quantum Fourier transform acts on a quantum state, whereas the classical Fourier transform acts on a vector, so not every task that uses the classical Fourier transform can take advantage of this exponential speedup.

The quantum Fourier transform is the classical discrete Fourier transform applied to the vector of amplitudes of a quantum state, where we usually consider vectors of length  $N = 2^n$ . The classical Fourier transform acts on a vector  $(x_0, x_1, \dots, x_{N-1}) \in \mathbb{C}^N$  and maps it to the vector  $(y_0, y_1, \dots, y_{N-1}) \in \mathbb{C}^N$  according to the formula:

$$y_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} x_n \omega_N^{\mp kn}, \quad (21.146)$$

where  $k = 0, 1, \dots, N-1$  and  $\omega_N = e^{2\pi i/N}$  and  $\omega_N^n$  is an  $N^{\text{th}}$  root of unity. The lower sign holds for the *inverse* FT.

Similarly, the quantum Fourier transform acts on a quantum state  $|x\rangle = \sum_{i=0}^{N-1} x_i |i\rangle$  and maps it to a quantum state  $\sum_{i=0}^{N-1} y_i |i\rangle$  according to the same formula (21.146). In case that  $|x\rangle$  is a basis state, the quantum Fourier Transform can also be expressed as the map,

$$|x\rangle \mapsto \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \omega_n^{xk} |k\rangle. \quad (21.147)$$

Equivalently, the quantum Fourier transform can be viewed as a unitary matrix (or a quantum gate, similar to a Boolean logic gate for classical computers) acting on quantum state vectors, where the unitary matrix is given by,

$$F_N = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \dots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \dots & \omega^{2(N-1)} \\ 1 & \omega^3 & \omega^6 & \omega^9 & \dots & \omega^{3(N-1)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \omega^{3(N-1)} & \dots & \omega^{(N-1)(N-1)} \end{pmatrix} \quad (21.148)$$

where  $\omega = \omega_N$ . Do the Exc. 21.5.6.5.

The QFT is unitary,

$$FF^\dagger = \mathbb{I}, \tag{21.149}$$

and can be efficiently performed on a quantum computer. The quantum gates used in the circuit are the Hadamard gate and the controlled phase gate  $R_m$ ,

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad \text{and} \quad R_m = \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i/2^m} \end{pmatrix}, \tag{21.150}$$

with  $e^{2\pi i/2^m} = \omega_{(2^m)}$  the primitive  $2^m$ -th root of unity. The circuit is composed of  $H$  gates and the controlled version of  $R_m$ .

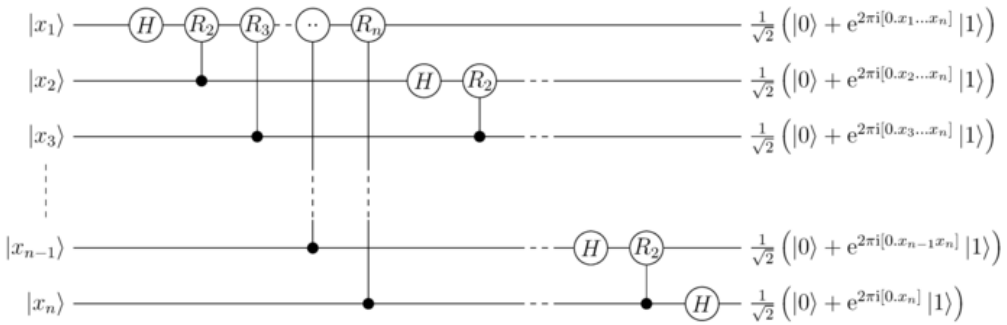


Figure 21.11: Quantum circuit for QFT with  $n$  qubits (without rearranging the order of output states).

All quantum operations must be linear, so it suffices to describe the function on each one of the basis states and let the mixed states be defined by linearity. This is in contrast to how Fourier transforms are usually described. We normally describe Fourier transforms in terms of how the components of the results are calculated on an arbitrary input. This is how you would calculate the path integral or show BQP is in PP. But it is much simpler here (and in many cases) to just explain what happens to a specific arbitrary basis state, and the total result can be found by linearity.

The quantum Fourier transform can be approximately implemented for any  $N$ ; however, the implementation for the case where  $N$  is a power of 2 is much simpler. As already stated, we assume  $N = 2^n$ . We have the orthonormal basis consisting of the vectors  $|0\rangle, \dots, |2^n - 1\rangle$ . The basis states enumerate all the possible states of the qubits,  $|x\rangle = |x_1 x_2 \dots x_n\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \dots \otimes |x_n\rangle$ , where  $|x_j\rangle$  indicates that qubit  $j$  is in state  $x_j$ , with  $x_j$  either 0 or 1. By convention, the basis state index  $x$  orders the possible states of the qubits lexicographically, i.e. by converting from binary to decimal in this way:

$$x = x_1 2^{n-1} + x_2 2^{n-2} + \dots + x_n 2^0. \tag{21.151}$$

It is also useful to borrow fractional binary notation:

$$[0.x_1 \dots x_m] = \sum_{k=1}^m x_k 2^{-k}. \tag{21.152}$$

For instance,  $[0.x_1] = \frac{x_1}{2}$  and  $[0.x_1x_2] = \frac{x_1}{2} + \frac{x_2}{2^2}$ . With this notation, the action of the quantum Fourier transform can be expressed in a compact manner:

$$\begin{aligned} \text{QFT}(|x_1x_2\dots x_n\rangle) &= \frac{1}{\sqrt{N}} \left( |0\rangle + e^{2\pi i [0.x_n]} |1\rangle \right) \otimes \left( |0\rangle + e^{2\pi i [0.x_{n-1}x_n]} |1\rangle \right) \otimes \dots \\ &\otimes \left( |0\rangle + e^{2\pi i [0.x_1x_2\dots x_n]} |1\rangle \right), \end{aligned} \quad (21.153)$$

where we have used  $[0.x_1x_2\dots x_m] = [x_1x_2\dots x_m]/2^m$ . This can be seen by rewriting the formula for the Fourier transform in the binary expansion:

$$\text{QFT}(|x\rangle) = \frac{1}{\sqrt{N}} \sum_{k=0}^{2^n-1} \omega_n^{xk} |k\rangle = \dots = \frac{1}{\sqrt{N}} \bigotimes_{j=1}^n \left( |0\rangle + \omega_n^{x2^{n-j}} |1\rangle \right). \quad (21.154)$$

Now, we have  $\omega_n^{x2^{n-j}} = e^{\frac{2\pi i}{2^n} x 2^{n-j}} = e^{2\pi i (x 2^{-j})}$ . Let,

$$\begin{aligned} f(j) = x 2^{-j} &= 2^{-j} \sum_{r=1}^n x_r 2^{n-r} = \sum_{r=1}^n x_r 2^{n-j-r} \\ &= \sum_{r=1}^{n-j} x_r 2^{n-j-r} + \sum_{r=n-j+1}^n x_r 2^{n-j-r} = a(j) + b(j). \end{aligned} \quad (21.155)$$

then  $a(j) \in \mathbb{N}_0$ , because  $2^{n-j-r} \geq 0$ , for  $n-j-r \geq 0$ , and  $b(j) = 0.x_{n-j+1}x_{n-j+2}\dots x_n$ , thus the (2) becomes:

$$e^{2\pi i f(j)} = e^{2\pi i (a(j)+b(j))} = e^{2\pi i a(j)} \cdot e^{2\pi i b(j)} = e^{2\pi i [0.x_{n-j+1}x_{n-j+2}\dots x_n]}, \quad (21.156)$$

since  $e^{2\pi i a(j)} = 1$  for all  $j$ . Then we can write:

$$\begin{aligned} \text{QFT}(|x_1x_2\dots x_n\rangle) &= \frac{1}{\sqrt{N}} \bigotimes_{j=1}^n \left( |0\rangle + \omega_n^{x 2^{n-j}} |1\rangle \right) \\ &= \frac{1}{\sqrt{N}} \bigotimes_{j=1}^n \left( |0\rangle + e^{2\pi i [0.x_{n-j+1}x_{n-j+2}\dots x_n]} |1\rangle \right) \\ &= \frac{1}{\sqrt{N}} \left( |0\rangle + e^{2\pi i [0.x_n]} |1\rangle \right) \otimes \left( |0\rangle + e^{2\pi i [0.x_{n-1}x_n]} |1\rangle \right) \otimes \dots \otimes \left( |0\rangle + e^{2\pi i [0.x_1x_2\dots x_n]} |1\rangle \right). \end{aligned} \quad (21.157)$$

To obtain this state from the circuit depicted above, a swap operations of the qubits must be performed to reverse their order. After the reversal, the  $n$ -th output qubit will be in a superposition state of  $|0\rangle$  and  $e^{2\pi i [0.x_1\dots x_n]} |1\rangle$ , and similarly the other qubits before that (take a second look at the sketch of the circuit above).

In other words, the discrete Fourier transform, an operation on  $n$  qubits, can be factored into the tensor product of  $n$  single-qubit operations, suggesting it is easily represented as a quantum circuit (up to an order reversal of the output). In fact, each of those single-qubit operations can be implemented efficiently using a Hadamard gate and controlled phase gates. The first term requires one Hadamard gate and  $(n-1)$  controlled phase gates, the next one requires a Hadamard gate and  $(n-2)$  controlled phase gate, and each following term requires one fewer controlled phase

gate. Summing up the number of gates, excluding the ones needed for the output reversal, gives  $n + (n - 1) + \dots + 1 = n(n + 1)/2 = O(n^2)$  gates, which is quadratic polynomial in the number of qubits.

The QFT is useful in the simulation of Hamiltonian evolution governed by conjugate variables,

$$e^{-\hat{H}t/\hbar} \quad \text{where} \quad \hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2 \hat{x}^2, \quad (21.158)$$

where, similar to the *time-splitting spectral algorithm*, we may replace differential operators,

$$\hat{p} = F^{-1} \hat{x} F. \quad (21.159)$$

### 21.5.6 Exercises

#### 21.5.6.1 Ex: Quantum composer

Show that:

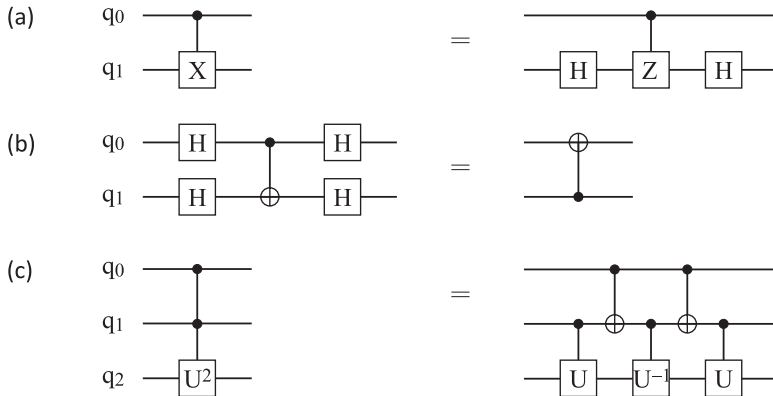


Figure 21.12:

#### 21.5.6.2 Ex: Beam splitter

Calculate the negativity corresponding to the entangled state that evolves from the initial two-atoms state  $\alpha|gg\rangle + \beta|ee\rangle$ , where  $r$  and  $e$  are the ground and excited state of each atom, respectively, and the evolution law for each atom is,

$$\begin{aligned} |g\rangle_S \otimes |0\rangle_E &\longrightarrow |g\rangle_S \otimes |0\rangle_E \\ |e\rangle_S \otimes |0\rangle_E &\longrightarrow \sqrt{1-p}|e\rangle_S \otimes |0\rangle_E + \sqrt{p}|g\rangle_S \otimes |1\rangle_E \end{aligned}$$

with  $p = 1 - e^{-\Gamma t}$ . Show that, if  $|\beta| > |\alpha|$ , entanglement vanishes for a finite time.

#### 21.5.6.3 Ex: Classical addition of two qubits

Design a quantum algorithm for the classical addition of up to 8 qubits.

**21.5.6.4 Ex: CARL simulation on a quantum computer**

Try to recast the so-called CARL Hamiltonian,

$$\hat{H} = U_0(\hat{a}_+^\dagger \hat{a}_- e^{-ik\hat{r}} + \hat{a}_+ \hat{a}_-^\dagger e^{ik\hat{r}})$$

such that it can be simulated by a sequence of quantum gates.

**21.5.6.5 Ex: CARL simulation on a quantum computer**

Write down the QF transformation matrix for the case of  $N = 4 = 2^2$  and phase  $\omega = \nu$ .

**21.6 Further reading****21.6.1 on spin squeezing**

R.H. Dicke, *Coherence in Spontaneous Radiation Processes* [DOI]

M. Kitagawa et al., *Spin-squeezed states* [DOI]

D.J. Wineland et al., *Squeezed atomic states and projection noise in spectroscopy* [DOI]

Ph. Bouyer et al., *Heisenberg-Limited Spectroscopy with Degenerate Bose-Einstein Gases* [DOI]

K. Baumann et al., *Dicke quantum phase transition with a superfluid gas in an optical cavity* [DOI]

L. Salvi et al., *Squeezing on Momentum States for Atom Interferometry* [DOI]

M. Gegg et al., *Superradiant to subradiant phase transition in the open system Dicke model: dark state cascades* [DOI]

P. Kirton et al., *Introduction to the Dicke Model: From Equilibrium to Nonequilibrium, and Vice Versa* [DOI]

J.G. Bohnet et al., *Reduced spin measurement back-action for a phase sensitivity ten times beyond the standard quantum limit* [DOI]

K. Cox et al., *Deterministic Squeezed States with Collective Measurements and Feedback* [DOI]

**21.6.2 on superradiant lasing**

D. Meiser et al., *Prospects for a Millihertz-Linewidth Laser* [DOI]

Th. Maier et al., *A superradiant clock laser on a magic wavelength optical lattice* [DOI]

M.A. Norcia et al., *Superradiance on the millihertz linewidth strontium clock transition* [DOI]

M.A. Norcia et al., *Cold-Strontium Laser in the Superradiant Crossover Regime* [\[DOI\]](#)

M.A. Norcia et al., *Cavity-mediated collective spin-exchange interactions in a strontium superradiant laser* [\[DOI\]](#)

A. Bychek et al., *Superradiant lasing in inhomogeneously broadened ensembles with spatially varying coupling* [\[DOI\]](#)

### 21.6.3 on entanglement

A. Einstein et al., *Can quantum-mechanical description of physical reality be considered complete* [\[DOI\]](#)

J.S. Bell et al., *On the Einstein-Podolsky-Rosen paradox* [\[DOI\]](#)

A. Aspect, *Experimental Test of Bell's Inequality Using Time-Varying Analyzers* [\[DOI\]](#)

S.J. van Enk, *Single-particle entanglement* [\[DOI\]](#)

### 21.6.4 on quantum information

S. Aaronson et al., *The computational complexity of linear optics* [\[DOI\]](#)

H. Azuma, *Quantum computation with the Jaynes-Cummings model* [\[DOI\]](#)

S.D. Bartlett et al., *Efficient Classical Simulation of Continuous Variable Quantum Information Processes* [\[DOI\]](#)

M. Bindhani et al., *Quantum simulation of Jaynes-Cummings model on IBM Q-system* [\[DOI\]](#)

V.K. Jain et al., *Quantum Simulation of Discretized Harmonic Oscillator on IBM Quantum Computer* [\[DOI\]](#)

S. Sefi et al., *How to Decompose Arbitrary Continuous-Variable Quantum Operations* [\[DOI\]](#)

P. Sundsoy et al., *Quantum Computing, Linear optics implementations* [\[DOI\]](#)

IBM, *Quantum computing* [\[http\]](#)

Wikipedia, *Quantum Fourier transform* [\[http\]](#)

C.S. Hamilton et al., *Gaussian boson sampling* [\[DOI\]](#)

N. Quesada et al., *Gaussian boson sampling using threshold detectors* [\[DOI\]](#)

Han-Sen Zhong et al., *Quantum computational advantage using photons* [\[DOI\]](#)





## Chapter 22

# Atomic motion in optical cavities

In the preceding chapter we concentrated on the dynamics of the field modes of laser-pumped cavities. We devoted a particular attention to the role of scatterers, e.g. atoms, located in the mode volume and coupling the dynamics of counterpropagating modes. We assumed the atoms to be fixed in space, or at most subject to an external force constraining their motion. We have also seen that the coupling of counterpropagating modes critically depends on the position of the atom. Now, the cavity fields are expected to exert light forces on the atoms eventually leading to their displacement. As we will see in the following, this fact can have enormous impact on the coupling dynamics and even induce macroscopic instabilities.

We devote Sec. 22.1 to the derivation of the complete equations of motion for the case of a single atom, allowing for all degrees of freedom to be treated as quantized: the atomic excitation, the motion of its center of mass, and the radiation field in the cavity. We will provide a simple recipe for finding the suitable equations of motion depending on which degree of freedom  $s$  to be treated as quantized and which dissipation process to be taken into account. We will also show how and under which circumstances the atomic excitation may be adiabatically eliminated.

In Sec. 22.2 we generalize the equations of motion of many atoms, but treating all degrees of freedom as classical. This leads us to the paradigmatic Collective Atomic Recoil Laser (CARL), a self-organization phenomenon whose relationship to other such instabilities will be discussed in Sec. 22.3.

Finally, in Secs. 22.4 and 22.5 we will treat the light field, respectively, the atomic motion quantum mechanically and show in which sense the obtained dynamics are different.

### 22.1 Cavity interacting with a single atom

Here, we consider atoms interacting with the modes of an optical cavity pumped by lasers. As we saw in the previous chapter, the density of the modes in a cavity is concentrated around the optical axis, such that a scatterer located within the mode emits preferentially within the cavity, where the light is recycled. Therefore, we can in many situations treat the system as one-dimensional.

In free space, as discussed in Chp. 18.4, the force of light has two components: the radiation pressure, which scatters photons isotropically into space, and the dipole

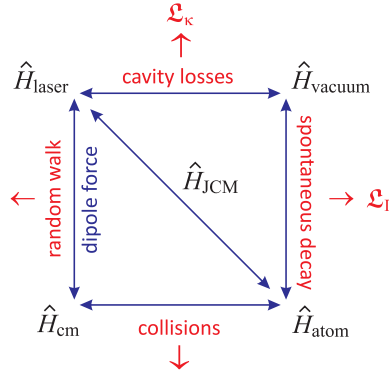


Figure 22.1: Hamiltonian in quantum optics.

force, which can be interpreted in terms of a redistribution of photons between light modes. In cavities, where the isotropic scattering is much reduced, radiative pressure can often be neglected. In contrast, if light is tuned away from atomic resonances, the atom will feel a dipole force originating from the backscattering of photons between counterpropagating modes.

### 22.1.1 Linear and ring cavities

We must distinguish two types of cavities with very different behaviors: The linear cavity or (*Fabry-Pérot etalon*), where counterpropagating modes form a single mode, and the ring cavity, where counterpropagating modes have independent photon budgets.

For a *linear cavity*, boundary conditions imposed by the surfaces of the cavity mirrors determine the possible spatial mode functions, which are necessarily standing waves. The amplitudes of the electric field are in second quantization (15.8),

$$\begin{aligned} \hat{E}(z, t) &= \hat{E}^+(z, t)e^{-i\omega t} + \hat{E}^-(z, t)e^{i\omega t} \\ \text{with } \hat{E}^+(z, t) &= E_1 \hat{a}(t)e^{ikz} = (\hat{E}^-(z, t))^\dagger. \end{aligned} \quad (22.1)$$

with  $[\hat{a}, \hat{a}^\dagger] = 1$ . With this we obtain, for a single atom coupled to the mode of the cavity pumped by a laser, within the dipolar approximation and the RWA<sup>1</sup>, the following relevant contributions to the Hamiltonian ( $\hbar = 1$ ),

$$\begin{aligned} \hat{H}_{atom} &= -\Delta_a \hat{\sigma}^+ \hat{\sigma}^- + \frac{\hat{p}^2}{2m} \\ \hat{H}_{cav} &= -\Delta_c \hat{a}^\dagger \hat{a} \\ \hat{H}_{atom:cav} &= g \hat{a}^\dagger \hat{\sigma}^- e^{-ikz} + h.c. \\ \hat{H}_{laser:cav} &= \eta \hat{a}^\dagger + h.c., \end{aligned} \quad (22.2)$$

neglecting the dynamics of the pump field, which is supposed to be classical,  $\eta = \delta_{fsr} \langle \hat{a}_{in}^\dagger \rangle$ . Note that the propagator  $e^{-i\hat{H}_{laser:cav} t}$  corresponds to a coherent state

<sup>1</sup>For the transformation into the rotating frame see the derivation of Sec. 14.2.2.

*displacement operator.*  $\Delta_a$  is the detuning between the light and the atomic resonance,  $\Delta_c$  between the light and cavity resonance and  $g$  is the light-atom coupling force, also called the single-photon Rabi frequency. Neglecting the kinetic energy term  $\hat{p}^2/2m$ , the photonic recoil  $e^{-ikv\hat{z}}$ , and the pumping  $\eta$  we recover the *Jaynes-Cummings model*. Do the Excs. 22.1.7.1 and 22.1.7.2.

For a *ring cavity*, we must distinguish the counterpropagating modes  $\hat{a}_\pm$ ,

$$\hat{E}^+(z, t) = E_1 \hat{a}_+(t) e^{ikz} + E_1 \hat{a}_-(t) e^{-ikz} = (\hat{E}^-(z, t))^\dagger. \quad (22.3)$$

such that the total Hamiltonian  $\hat{H}$  consists of the following parts <sup>2</sup>,

$$\begin{aligned} \hat{H}_{atom} &= \hat{H}_{electron} + \hat{H}_{motion} = -\Delta_a \hat{\sigma}^+ \hat{\sigma}^- + \frac{\hat{p}^2}{2m} \\ \hat{H}_{cav} &= -\Delta_c \hat{a}_+^\dagger \hat{a}_+ - \Delta_c \hat{a}_-^\dagger \hat{a}_- \\ \hat{H}_{atom:cav} &= g \hat{a}_+^\dagger \hat{\sigma}^- e^{-ik\hat{z}} + h.c. + g \hat{a}_-^\dagger \hat{\sigma}^- e^{ik\hat{z}} + h.c. \\ \hat{H}_{laser:cav} &= -\eta_+(\hat{a}_+ - \hat{a}_+^\dagger) - \eta_-(\hat{a}_- - \hat{a}_-^\dagger) \end{aligned} \quad (22.4)$$

We identify the degrees of freedom of the system through the quantum observables appearing in the Hamiltonian: the counterpropagating modes of light with the amplitudes ( $\hat{a}_\pm$ ), the internal degrees of freedom ( $\hat{\sigma}^z, \hat{\sigma}^\pm$ ), and the spatial coordinates of the atom ( $\hat{z}, \hat{p}$ ).

In contrast to linear cavities, ring cavities have the following particularities: 1. The phase of the standing wave is free to move; 2. the counterpropagating modes of the cavity have independent photon budgets, each backscattering event conserves momentum; 3. the backscattering acts on the phase of the standing wave. Atoms can be trapped by the dipole force within the cavity mode volume. The dipole force corresponds to a backscattering of photons between modes.

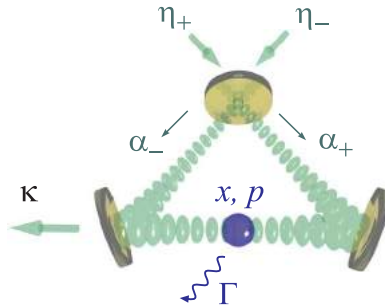


Figure 22.2: Scheme of an atom interacting with a ring cavity showing the relevant degrees of freedom ( $\hat{x}, \hat{p}, \hat{a}_\pm$ ) and the possible decay processes ( $\kappa, \Gamma$ ) for the derivation of the field equations.

<sup>2</sup>Throughout this chapter we will sometimes emphasize the motional degree of freedom in green color, photonic states in blue, electronic excitation states in pink.

### 22.1.2 Eliminating spontaneous emission and cavity decay

In fact, there are more degrees of freedom involved in the dynamics of atoms moving in a laser-pumped ring cavity, because of the atoms may scatter light into directions other than the cavity modes by spontaneous emission, and the cavity modes may decay by transmission through the mirrors. Therefore, we need to treat the respective vacuum field modes receiving the photons,  $\hat{a}_{\mathbf{k}}$  and  $\hat{a}_{\omega}$ , quantum mechanically and include the respective Hamiltonians,

$$\begin{aligned}\hat{H}_{atom:vacuum} &= \sum_{\mathbf{k}} g_{atom:vacuum} \hat{a}_{\mathbf{k}}^{\dagger} \hat{\sigma}^{-} e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}} + h.c. \\ \hat{H}_{cav:bath} &= \sum_{\omega} g_{cav:bath} \hat{a}_{\omega}^{\dagger} \hat{a}_{+} + g_{cav:bath} \hat{a}_{\omega}^{\dagger} \hat{a}_{-} + h.c. ,\end{aligned}\quad (22.5)$$

in the description of the coupled dynamics. Here,  $g_{atom:vacuum}$  denotes the vacuum Rabi frequency, that is, the coupling strength between the atomic dipole and the electromagnetic vacuum into which spontaneously emitted photons may escape. On the other hand,  $g_{cav:bath}$  denotes the coupling strength between the cavity mode and the spectrum of electromagnetic modes into which cavity photons can escape and which we will from now on call *heat bath* to facilitate its semantic distinction from the spontaneous vacuum. The total density operator, the Hamiltonian and the equation of motion are, consequently,

$$\begin{aligned}\bar{\rho} &= \hat{\rho}_{atom} \otimes \hat{\rho}_{electron} \otimes \hat{\rho}_{cav} \otimes \hat{\rho}_{vacuum} \otimes \hat{\rho}_{bath} \\ \bar{H} &= \hat{H}_{motion} + \hat{H}_{electron} + \hat{H}_{cav} + \hat{H}_{atom:cav} + \hat{H}_{laser:cav} + \hat{H}_{atom:vacuum} + \hat{H}_{cav:bath} \\ \dot{\rho} &= -i[\bar{H}, \bar{\rho}] .\end{aligned}\quad (22.6)$$

With the inclusion of the vacuum field modes  $\hat{a}_{\omega}$  and  $\hat{a}_{\mathbf{k}}$  the number of degrees of freedom to be treated literally explodes, and we have to find a way to eliminate them from the equation of motion. We do this by partially tracing the density operator over the vacuum field modes using the Weisskopf-Wigner theory,

$$\tilde{\rho} \equiv \text{Tr}_{vacuum} \text{Tr}_{bath} \bar{\rho} = \hat{\rho}_{atom} \otimes \hat{\rho}_{electron} \otimes \hat{\rho}_{cav} . \quad (22.7)$$

This allows us to reduce the Hamiltonian  $\hat{H} = \bar{H} - \hat{H}_{atom:vacuum} - \hat{H}_{cav:bath}$ . The price to pay is, that the equation of motion for this receives dissipative terms: The Liouville equation turns into a *master equation* with the following form,

$$\begin{aligned}\dot{\hat{\rho}} &= -i[\hat{H}, \hat{\rho}] + \mathcal{L}_{atom:vacuum} + \mathcal{L}_{cav:vacuum,+} + \mathcal{L}_{cav:vacuum,-} \\ \mathcal{L}_{atom:vacuum} \hat{\rho}(t) &= -\gamma \{ \hat{\sigma}^{+} \hat{\sigma}^{-} \hat{\rho}(t) - 2\hat{\sigma}^{-} \hat{\rho}(t) \hat{\sigma}^{+} + \hat{\rho}(t) \hat{\sigma}^{+} \hat{\sigma}^{-} \} \\ \mathcal{L}_{cav:bath,\pm} \hat{\rho}(t) &= -\kappa \{ \hat{a}_{\pm}^{\dagger} \hat{a}_{\pm} \hat{\rho}(t) - 2\hat{a}_{\pm} \hat{\rho}(t) \hat{a}_{\pm}^{\dagger} + \hat{\rho}(t) \hat{a}_{\pm}^{\dagger} \hat{a}_{\pm} \}\end{aligned}, \quad (22.8)$$

where  $\hat{H}$  is the Hamiltonian from (22.4). We see that each degree of freedom has its own loss mechanism.  $\kappa$  for the finite transmission of the resonator mirrors [147, 258]<sup>3</sup>,  $\Gamma$  for the spontaneous emission, and  $\gamma_{frc}$ , when we exert a frictional force on the atoms.

<sup>3</sup>Here, we only consider cavity decay into a zero temperature reservoir without quantum phase fluctuations.

### 22.1.2.1 The problem with spontaneous emission in cavities

The above treatment still is incomplete, if we regard  $\hat{\rho}$  as the atomic Bloch vector. The reason is that we know what the dissipative Lindblad terms  $\mathcal{L}_{vacuum}\hat{\rho}$  generated by spontaneous emission look like for the atomic excitation  $\hat{\rho}_{atom}$ , but the Hamiltonian  $\hat{H}_{atom:vacuum}$  also contains the motional degree of freedom  $e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}$ , which is intrinsically three-dimensional. That is, the dissipative terms also need to describe, how the motion diffuses in momentum space.

The inclusion of dissipative terms, however, is difficult, because unavoidable photonic recoil violates the supposed one-dimensionality of the atomic motion along the optical axis. Omnidirectional photonic recoil is also incompatible with the assumption that the momentum is quantized in multiples of  $2\hbar k$  in the direction of the optical axis. And finally, if we consider degenerate matter waves, photonic recoil will eject atoms from a BEC. Even if, neglecting the emission process, we only consider absorption, we would need a quantization in multiples of  $1\hbar k$  instead of  $2\hbar k$ . In the following, in order to keep the problem 1D, we will neglect momentum diffusion, i.e. we consider the simplified Hamiltonian  $\tilde{H}$  and discard motional terms from the term  $\mathcal{L}_{vacuum}\hat{\rho}$ .

### 22.1.2.2 Quantum derivation of the CARL equations

To obtain the equations of motion we insert the Hamiltonian (22.4) into the equations for the field operators, for which the following commutation rules hold,  $[\hat{a}_\pm, \hat{a}_\pm^\dagger] = 1$  and  $[\hat{a}_\pm, \hat{a}_\mp^\dagger] = 0 = [\hat{a}_\pm, \hat{a}_\mp]$ ,

$$\begin{aligned}\dot{\hat{a}}_+ &= i[\hat{H}, \hat{a}_+] - \kappa\hat{a}_+ \\ &= -i\Delta_c[\hat{a}_+^\dagger\hat{a}_+, \hat{a}_+] + i\eta e^{-ikz}\hat{\sigma}^-[\hat{a}_+^\dagger, \hat{a}_+] + i\eta e^{ikz}\hat{\sigma}^+[\hat{a}_+, \hat{a}_+] + \eta_+[ \hat{a}_+ - \hat{a}_+^\dagger, \hat{a}_+] - \kappa\hat{a}_+ \\ &= (-\kappa + i\Delta_c)\hat{a}_+ - i\eta\hat{\sigma}^- e^{-ikx} + \eta_+ ,\end{aligned}\tag{22.9}$$

and similarly for  $\hat{a}_-$ . For the Pauli deexcitation matrix, using the following commutation rules,  $[\hat{\sigma}^-, \hat{\sigma}^+] = \hat{\sigma}_z$ ,  $\hat{\sigma}^\pm\hat{\sigma}_z = \pm\hat{\sigma}^\pm$ , and  $[\hat{\sigma}^-, \hat{\sigma}^-] = 0$ , we calculate,

$$\begin{aligned}\dot{\hat{\sigma}}^- &= i[\hat{H}, \hat{\sigma}^-] - \gamma\hat{\sigma}^- \\ &= -i\Delta_a[\hat{\sigma}^+\hat{\sigma}^-, \hat{\sigma}^-] + i\eta e^{ikz}\hat{a}_+[\hat{\sigma}^+, \hat{\sigma}^-] + i\eta e^{-ikz}\hat{a}_-[\hat{\sigma}^+, \hat{\sigma}^-] - \gamma\hat{\sigma}^- \\ &= (-\gamma + i\Delta_a)\hat{\sigma}^- + i\eta e^{ikz}\hat{a}_+\hat{\sigma}_z + i\eta e^{-ikz}\hat{a}_-\hat{\sigma}_z .\end{aligned}\tag{22.10}$$

For the Pauli inversion matrix, using the following commutation rules,  $[\hat{\sigma}^+\hat{\sigma}^+, \hat{\sigma}_z] = 0$  and  $[\hat{\sigma}^\pm, \hat{\sigma}_z] = \pm 2\hat{\sigma}^\pm$ , we calculate,

$$\begin{aligned}\dot{\hat{\sigma}}_z &= i[\hat{H}, \hat{\sigma}_z] - 2\gamma - 2\gamma\hat{\sigma}_z \\ &= i\eta e^{-ikz}\hat{a}_+^\dagger[\hat{\sigma}^-, \hat{\sigma}_z] + i\eta e^{ikz}\hat{a}_-^\dagger[\hat{\sigma}^-, \hat{\sigma}_z] + i\eta e^{ikz}\hat{a}_+[\hat{\sigma}^+, \hat{\sigma}_z] + i\eta e^{-ikz}\hat{a}_-[\hat{\sigma}^+, \hat{\sigma}_z] - 2\gamma\hat{\sigma}_z \\ &= -2\gamma - 2\gamma\hat{\sigma}_z + 2i\eta e^{-ikz}\hat{a}_+^\dagger\hat{\sigma}^- + 2i\eta e^{ikz}\hat{a}_-^\dagger\hat{\sigma}^- - 2i\eta e^{ikz}\hat{a}_+\hat{\sigma}^+ - 2i\eta e^{-ikz}\hat{a}_-\hat{\sigma}^+ .\end{aligned}\tag{22.11}$$

Finally, we need to derive the equations governing the motion of atoms. For the position we obtain,

$$\dot{\hat{z}} = i[\hat{H}, \hat{z}] = i\left[\frac{\hat{p}^2}{2m}, \hat{z}\right] = \frac{1}{m}\hat{p} .\tag{22.12}$$

In order to calculate the momentum, we need to do a small auxiliary calculation. With the commutator  $[\hat{z}, \hat{p}] = \imath$  we derive,

$$\begin{aligned} [\hat{z}^n, \hat{p}] &= \imath \frac{\delta \hat{z}^n}{\delta \hat{z}} = m \hat{z}^{n-1} \\ [e^{\imath k \hat{z}}, \hat{p}] &= \sum_{n=0}^{\infty} \frac{(\imath k)^n}{n!} [\hat{z}^n, \hat{p}] = -k \sum_{n=0}^{\infty} \frac{(\imath k)^{n-1}}{(n-1)!} \hat{z}^{n-1} = -k e^{\imath k \hat{z}}, \end{aligned} \quad (22.13)$$

and with this result,

$$\begin{aligned} \dot{\hat{p}} &= \imath [\hat{H}, \hat{p}] \\ &= \imath g \hat{a}_+^\dagger \hat{\sigma}^- [e^{-\imath k \hat{z}}, \hat{p}] + c.c. + \imath g \hat{a}_-^\dagger \hat{\sigma}^- [e^{\imath k \hat{z}}, \hat{p}] + c.c. \\ &= -\imath g k \hat{a}_+^\dagger \hat{\sigma}^- e^{-\imath k \hat{z}} + c.c. + \imath g k \hat{a}_-^\dagger \hat{\sigma}^- e^{\imath k \hat{z}} + c.c. . \end{aligned} \quad (22.14)$$

The *quantum Langevin equations* [147] describing the dynamics of the internal and external degrees of freedom of the atom and the field are coupled,

$$\begin{aligned} \dot{\hat{a}}_\pm &= (-\kappa + \imath \Delta_c) \hat{a}_\pm - \imath g \hat{\sigma}^- e^{\mp \imath k \hat{z}} + \eta_\pm \\ \dot{\hat{\sigma}}^- &= (-\gamma + \imath \Delta_a) \hat{\sigma}^- + \imath g (e^{\imath k \hat{z}} \hat{a}_+ + e^{-\imath k \hat{z}} \hat{a}_-) \hat{\sigma}_z \\ \dot{\hat{\sigma}}_z &= -2\gamma \hat{\sigma}_z + 2\imath g (e^{-\imath k \hat{z}} \hat{a}_+^\dagger + e^{\imath k \hat{z}} \hat{a}_-^\dagger) \hat{\sigma}^- - 2\imath g (e^{\imath k \hat{z}} \hat{a}_+ + e^{-\imath k \hat{z}} \hat{a}_-) \hat{\sigma}^+ \\ \dot{\hat{z}} &= \hat{p}/m \\ \dot{\hat{p}} &= \imath g \hbar k \hat{\sigma}^- (\hat{a}_+^\dagger e^{-\imath k \hat{z}} - \hat{a}_-^\dagger e^{\imath k \hat{z}}) + c.c. \end{aligned} \quad (22.15)$$

We may also verify,

$$\begin{aligned} \dot{\hat{n}}_+ &= \imath [\hat{H}, \hat{n}_+] \\ &= \imath [-\Delta_c \hat{a}_+^\dagger \hat{a}_+ + g \hat{a}_+^\dagger \hat{\sigma}^- e^{-\imath k \hat{z}} + g \hat{a}_+ \hat{\sigma}^+ e^{\imath k \hat{z}} - \imath \eta_+ (\hat{a}_+ - \hat{a}_+^\dagger), \hat{a}_+^\dagger \hat{a}_+] \\ &= (\eta_+ - \imath g e^{-\imath k \hat{z}} \hat{\sigma}^-) \hat{a}_+^\dagger + (\eta_+ + \imath g \hat{\sigma}^+ e^{\imath k \hat{z}}) \hat{a}_+ , \end{aligned} \quad (22.16)$$

and hence conservation of momentum,

$$[\hat{H}, \hbar k (\hat{n}_+ - \hat{n}_-) - \hat{p}] = \hbar k \eta_+ (\hat{a}_+^\dagger + \hat{a}_+) - \hbar k \eta_- (\hat{a}_-^\dagger + \hat{a}_-) , \quad (22.17)$$

in the absence of pumping,  $\eta_+ = 0 = \eta_-$ .

### 22.1.3 Adiabatic elimination of the excited state

Under certain conditions, however, the internal and external dynamics occur at very different time scales, which allows a decoupling of the differential equations<sup>4</sup>. When the light fields are very detuned from atomic resonances,  $\Delta_a \gg \Gamma$ , the internal dynamics of the atoms is very fast, that is, the internal state adapts very rapidly to the boundary conditions defined by the external state and the state of the light field.

<sup>4</sup>In good cavity the limit the degrees of freedom of atomic excitation  $\hat{\sigma}^\pm$  drop out of the dynamics, in the bad cavity limit, the fields  $\hat{a}^\pm$  drop out of the dynamics.

Therefore, the internal state has no separate dynamics of its own, and we can adiabatically eliminate the internal degrees of freedom. Thus, we can neglect correlations between degrees of freedom,  $\langle \hat{a}_\pm \hat{\sigma}^\pm \rangle = \langle \hat{a}_\pm \rangle \langle \hat{\sigma}^\pm \rangle$  etc. [542, 254]. **The adiabatic elimination of the excited state comes down to treating the atom as a classical antenna.**

We obtain the stationary solutions for  $t \rightarrow \infty$  in the same way as for the optical Bloch equations [see Eq. (14.99)], assuming in Eq. (22.15),

$$\dot{\hat{\sigma}}^- = 0 = \dot{\hat{\sigma}}_z \quad (22.18)$$

where  $\langle \hat{\sigma}^- \rangle = \rho_{21}$ . Introducing the position-dependent Rabi frequency of the atom in the standing wave <sup>5</sup>,

$$\hat{\Omega}(z) = 2g(e^{ikz} \hat{a}_+ + e^{-ikz} \hat{a}_-), \quad (22.19)$$

we write,

$$0 = (-\gamma + i\Delta_a) \hat{\sigma}^- + \frac{1}{2} i \hat{\Omega} \hat{\sigma}_z \quad (22.20)$$

$$0 = -2\gamma - 2\gamma \hat{\sigma}_z + i \hat{\Omega}^\dagger \hat{\sigma}^- - i \hat{\Omega} \hat{\sigma}^+.$$

These equations are solved by,

$$\hat{\sigma}_z(\infty) = \frac{-2(\gamma^2 + \Delta_a^2)}{2(\gamma^2 + \Delta_a^2) + \hat{\Omega}^\dagger \hat{\Omega}} \quad (22.21)$$

$$\text{and } \hat{\sigma}^-(\infty) = \frac{-i(\gamma + i\Delta_a) \hat{\Omega}}{2(\gamma^2 + \Delta_a^2) + \hat{\Omega}^\dagger \hat{\Omega}} \simeq \frac{-i(\gamma + i\Delta_a)}{2\Delta_a^2} \hat{\Omega}.$$

Inserting the approximated expression for  $\hat{\sigma}^-(\infty)$  into the equation of motion (22.15) for the light modes,

$$\begin{aligned} \dot{\hat{a}}_\pm &= (-\kappa + i\Delta_c) \hat{a}_\pm - ig \hat{\sigma}^-(\infty) e^{\mp ikz} + \eta_\pm \\ &= \left( -\kappa + i\Delta_c - \frac{g^2 \gamma}{\Delta_a^2} - \frac{ig^2}{\Delta_a} \right) \hat{a}_\pm - \left( \frac{g^2 \gamma}{\Delta_a^2} + \frac{ig^2}{\Delta_a} \right) e^{\mp 2ikz} \hat{a}_\mp + \eta_\pm, \end{aligned} \quad (22.22)$$

and for the atomic momentum,

$$\begin{aligned} \dot{\hat{p}} &= ig\hbar k \hat{\sigma}^-(\infty) (\hat{a}_+^\dagger e^{-ikz} - \hat{a}_-^\dagger e^{ikz}) - ig\hbar k \hat{\sigma}^+(\infty) (\hat{a}_+ e^{ikz} - \hat{a}_- e^{-ikz}) \\ &= \frac{2\hbar k \gamma g^2}{\Delta_a^2} (\hat{a}_+^\dagger \hat{a}_+ - \hat{a}_-^\dagger \hat{a}_-) - \frac{2i\hbar k g^2}{\Delta_a} (e^{2ikz} \hat{a}_+ \hat{a}_-^\dagger - e^{-2ikz} \hat{a}_+^\dagger \hat{a}_-). \end{aligned} \quad (22.23)$$

Defining the light-shift  $U_0$  caused by only one photon and the scattering rate  $\gamma_0$  by,

$$U_0 \equiv \frac{g^2}{\Delta_a} \quad \text{and} \quad \gamma_0 \equiv \frac{\Gamma g^2}{\Delta_a^2}, \quad (22.24)$$

with  $\Gamma = 2\gamma$ , we finally get a set of equations, where the internal degree of freedom of the atom has been eliminated,

$$\boxed{\begin{aligned} \dot{\hat{a}}_\pm &= (-\kappa - \gamma_0 + i\Delta_c - iU_0) \hat{a}_\pm - (\gamma_0 + iU_0) e^{\mp 2ikz} \hat{a}_\mp + \eta_\pm \\ \dot{\hat{p}} &= 2\hbar k \gamma_0 (\hat{a}_+^\dagger \hat{a}_+ - \hat{a}_-^\dagger \hat{a}_-) + 2i\hbar k U_0 (e^{-2ikz} \hat{a}_+^\dagger \hat{a}_- - e^{2ikz} \hat{a}_+ \hat{a}_-^\dagger) \end{aligned}}. \quad (22.25)$$

<sup>5</sup>Note that the factor of 2 ensure consistency with previous definitions of the Rabi frequency, such as in (15.23). Note also, that  $[\hat{\Omega}, \hat{\Omega}^\dagger] = 8g^2 \neq 0$ , but this is negligible when the fields are large enough to be considered as classical. On the other hand the quadratic terms  $\hat{\Omega}^\dagger \hat{\Omega}$  are negligible when they are small compared to  $\gamma^2$  or  $\Delta_a^2$ .



### 22.1.3.1 Radiation pressure and the adiabatically approximated Hamiltonian

The impact of radiation pressure should be considered when the pumping laser is close to a resonance. Then  $\gamma_0 \ll U_0$  is no longer satisfied [254], and we get one more term from the equation for the atomic force:  $\propto \hbar\gamma_0(|\alpha_+|^2 - |\alpha_-|^2)$ .

For the adiabatically approximated Hamiltonian we get immediately from (22.4) [473],

$$\hat{H} = \frac{\hat{p}^2}{2m} + \sum_{\pm} (U_0 - \Delta_c) \hat{a}_{\pm}^{\dagger} \hat{a}_{\pm} + U_0 (e^{-2\nu k \hat{z}} \hat{a}_{+}^{\dagger} \hat{a}_{-} + e^{2\nu k \hat{z}} \hat{a}_{+} \hat{a}_{-}^{\dagger}) - \imath \sum_{\pm} \eta_{\pm} (\hat{a}_{\pm} - \hat{a}_{\pm}^{\dagger}), \quad (22.26)$$

as shown in Exc. 22.1.7.3. Note that dissipative terms are (naturally) absent from this Hamiltonian, so that it shall not be used for the description of radiation pressure. On the other hand, all coherent terms of the equations of motion can be derived from this Hamiltonian (22.26), and we can verify momentum conservation (22.17) and deduce transformation properties.

These equations, which we will call CARL equations for reasons that we will become clear in Sec. 22.2, describe the coupled dynamics of atoms being accelerated by the *kick*  $e^{\imath k \hat{z}}$  imparted by the photonic recoil received upon scattering a photon from one mode into the counterpropagating one. In the same time, the backscattering *annihilates* a photon  $\hat{a}_{\pm}$  in one mode and *creates* a photon  $\hat{a}_{\mp}^{\dagger}$  in the counterpropagating mode. From now on we will exclusively use the CARL equations.

Finally, let us summarize, how the operators act on states and observables of the coupled system, noting that the same transformation rules as for free and trapped atoms (3.124) also hold for the optical lattice,

$$\begin{array}{ll} e^{\imath k \hat{z}} |z\rangle = |z\rangle & , \quad e^{-\imath k \hat{z}} \hat{z} e^{\imath k \hat{z}} = \hat{z} \\ e^{\imath k \hat{z}} |p\rangle = |p + \hbar k\rangle & , \quad e^{-\imath k \hat{z}} \hat{p} e^{\imath k \hat{z}} = \hat{p} + \hbar k \\ \hat{a}_{\pm} |n\rangle = \sqrt{n} |n-1\rangle & , \quad e^{-\imath k \hat{z}} \hat{H}(\hat{z}, \hat{p}) e^{\imath k \hat{z}} = \hat{H}(\hat{z}, \hat{p} - \hbar k) \\ \hat{a}_{\pm}^{\dagger} |n\rangle = \sqrt{n+1} |n+1\rangle & , \quad e^{\imath a \hat{p} / \hbar} \hat{H}(\hat{z}, \hat{p}) e^{-\imath a \hat{p} / \hbar} = \hat{H}(\hat{z} - a, \hat{p}) \end{array} . \quad (22.27)$$

For  $ka = \pi$  the phase shift vanishes:  $[e^{\imath \pi \hat{p} / \hbar k}, \hat{H}(\hat{z}, \hat{p})] = 0$ .

The dynamics is given by the time evolutions,

$$e^{-(\imath/\hbar)\hat{H}t} \hat{z}(0) e^{(\imath/\hbar)\hat{H}t} \quad , \quad e^{-(\imath/\hbar)\hat{H}t} \hat{p}(0) e^{(\imath/\hbar)\hat{H}t} \quad , \quad e^{-(\imath/\hbar)\hat{H}t} \hat{n}(0) e^{(\imath/\hbar)\hat{H}t} . \quad (22.28)$$

In Exc. 22.1.7.4 we calculate the photon number superposition state resulting from a kick  $e^{\imath k_{\text{cck}} \hat{z}}$ .

## 22.1.4 Adiabatic elimination of the cavity modes

We have seen in Sec. 22.1.3 how to eliminate the internal atomic degrees of freedom, once the condition  $|\Delta_a| \gg \Gamma$  is satisfied. We may try an analogous treatment accounting for the limit  $|\Delta_c| \gg \kappa$ . In this case, the cavity fields evolve on a fast time

scale, adiabatically following the evolution of the other degrees of freedom. Hence, we set,

$$\dot{\hat{a}}_{\pm} = 0, \quad (22.29)$$

and obtain from the first Heisenberg equation (22.15),

$$\hat{a}_{\pm}(\infty) = \frac{i g \hat{\sigma}^{-} e^{\mp i k \hat{z}} - \eta_{\pm}}{-\kappa + i \Delta_c}. \quad (22.30)$$

Defining,

$$U_c \equiv \frac{g^2 \Delta_c}{\kappa^2 + \Delta_c^2} \quad \text{and} \quad \kappa_c \equiv \frac{g^2 \kappa_c}{\kappa^2 + \Delta_c^2}, \quad (22.31)$$

we can write the position-dependent Rabi frequency (22.19) as,

$$\begin{aligned} \Omega(z) = 2g(e^{i k \hat{z}} \hat{a}_+ + e^{-i k \hat{z}} \hat{a}_-) &= 2(\kappa_c + i U_c) \left( \frac{\eta_+ e^{i k \hat{z}} + \eta_- e^{-i k \hat{z}}}{g} - 2i \hat{\sigma}^{-} \right) \\ &\xrightarrow{\eta_{\pm}=0} -4i(\kappa_c + i U_c) \hat{\sigma}^{-}, \end{aligned} \quad (22.32)$$

in the limit of no pumping  $\eta_{\pm} = 0$ . Inserting this into the other Heisenberg equations (22.15), we immediately get,

$$\dot{\hat{\sigma}}^{-} = (-\gamma + i \Delta_a) \hat{\sigma}^{-} + \frac{i}{2} \Omega(z) \hat{\sigma}_z \xrightarrow{\eta_{\pm}=0} (-\gamma + i \Delta_a) \hat{\sigma}^{-} + 2(\gamma_c + i U_c) \hat{\sigma}^{-} \hat{\sigma}_z, \quad (22.33)$$

and

$$\dot{\hat{\sigma}}_z = -2\gamma \hat{\sigma}_z + i \Omega^{\dagger}(z) \hat{\sigma}^{-} - i \hat{\sigma}^{+} \Omega(z) \xrightarrow{\eta_{\pm}=0} -2\gamma \hat{\sigma}_z - 4\kappa_c \hat{\mathbb{I}}, \quad (22.34)$$

as well as,  $\dot{\hat{z}} = \hat{p}/m$  and

$$\dot{\hat{p}} = i g \hbar k \hat{\sigma}^{-} (e^{-i k \hat{z}} \hat{a}_+^{\dagger} - e^{i k \hat{z}} \hat{a}_-^{\dagger}) - i g \hbar k \hat{\sigma}^{+} (e^{i k \hat{z}} \hat{a}_+ - e^{-i k \hat{z}} \hat{a}_-) \xrightarrow{\eta_{\pm}=0} 0. \quad (22.35)$$

That is, in summary,

$$\left. \begin{aligned} \dot{\hat{\sigma}}^{-} &= (-\gamma - 2\gamma_c + i \Delta_a - 2i U_c) \hat{\sigma}^{-} \\ \dot{\hat{\sigma}}_z &= -2\gamma \hat{\sigma}_z - 4\kappa_c \hat{\mathbb{I}} \\ \dot{\hat{p}} &= 0 \end{aligned} \right\}. \quad (22.36)$$

Alternatively, the coherent part of these equations can be derived by insert  $\hat{a}_{\pm}(\infty)$  directly in the Hamiltonian (22.4). This will be done in Exc. 22.1.7.5. The equations (22.36) tell us that, in the absence of cavity decay and spontaneous emission, the atomic population will not undergo nutation, but the dipole moment will rotate with a velocity which depends on the inversion. The dynamics becomes interesting in the presence of several atoms, as studied in ??.

### 22.1.5 General rules for deriving equations of motion

We have, in the previous sections, derived Heisenberg equations (22.15), respectively (22.25) which, together with the Schrödinger equation for the system's state  $|\psi(t)\rangle$  or the master equation for the density operator  $\hat{\rho}(t)$  form an *over-complete* set. This

section aims at providing a general recipe for choosing the right set of equations depending on two basic criteria for the nature of the degrees of freedom involved in the dynamics: (i) Do judge it necessary to treat the degree of freedom as quantum or may a classical description be sufficient; and (ii) Is the degree of freedom subject to dissipation (e.g. spontaneous emission of the electronic excitation, cavity decay of the field mode, or collisions messing up the center-of-mass motion), or not. The procedure, which will be applied throughout the remaining part of this chapter, leads to very different descriptions of the system depending on the specific parameter regime.

1. The procedure is generally applicable to coupled systems: We first need to *identify all relevant degrees of freedom and set up the Hamiltonian*, possibly eliminating irrelevant degrees of freedom, e.g. via adiabatic elimination or by tracing over them, if they contribute to dissipation. In the context of atoms coupled to a ring cavity, we assume our system to be in some state <sup>6</sup>,

$$|\psi(t)\rangle = |\mathbf{r}\rangle \otimes |\alpha_+\rangle \otimes |\alpha_-\rangle \otimes |i\rangle, \quad (22.37)$$

coupling the atomic motion, the light fields and the electronic excitation, although the electronic excitation  $|i\rangle$  is often eliminated adiabatically. The dissipative degrees of freedom related to vacuum modes leading to spontaneous emission and cavity decay, as well as collisions between moving atoms are traced away, but may be considered in the master equation for the density operator and in the Heisenberg equations, where the corresponding decay rates are added phenomenologically.

This first item has already been solved in the previous sections and led us to the Hamiltonian (22.4) and the corresponding Heisenberg equations (22.15), or the adiabatically approximated Hamiltonian (22.26) and the corresponding Heisenberg equations (22.25).

2. Now, we must decide which degrees of freedom  $B$  can be treated as *classical*. Typically, those are highly excited degrees of freedom (e.g. fast velocities of many photons in a mode). The corresponding operators can be substituted by their expectation value. Purely classical energy terms in the Hamiltonian can be ignored and removed. For the degrees of freedom  $\hat{A}$  we want to treat as *quantum*, we chose an appropriate common basis, which can be discrete  $\{|m\rangle\}$  where  $m$  is a complete set of quantum numbers. It can also be continuous  $\{|\mathbf{r}\rangle\}$  or a combination of both  $\{|\mathbf{r}, m\rangle\}$ . Now, we need to expand all operators on the chosen basis.
3. For the quantized degrees of freedom must now decide, whether they all evolve coherently or whether they are subject to dissipation. In the first case, perform steps A4 to A7, in the second case, perform steps B4 to B7.
- A4. In the case of coherent dynamics, we *expand the state* of the system  $|\psi(t)\rangle$  on the whole basis. For example, expanded on a partially continuous basis, the

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<sup>6</sup>Throughout this chapter we will denote momentum states by the Greek letters  $|\mu\rangle$  or  $|\nu\rangle$ . Photonic states will be labeled by the Latin letters  $|n\rangle$  or  $|m\rangle$ . Electronic excitation states will be labeled by the Latin letters  $|i\rangle$  or  $|j\rangle$ . Finally, expansion coefficients  $c_{\nu,i,n_+,n_-}$  of the state or of the density matrix elements will sometimes be emphasized in red.

coupled atom-ring cavity state may read,

$$|\psi(t)\rangle = \sum_{n_+, n_-, i} \int d^3r c_{n_+, n_-, i}(\mathbf{r}, t) |\mathbf{r}\rangle \otimes |n_+\rangle \otimes |n_-\rangle \otimes |i\rangle, \quad (22.38)$$

where  $\langle \mathbf{r}, \alpha_+, \alpha_-, i | \psi(t) \rangle = c_{n_+, n_-, i}(\mathbf{r}, t)$  are the expansion coefficients depending on photon numbers  $n_{\pm}$  in the counterpropagating light modes, the electronic excitation state  $i$ , and the atomic position  $\mathbf{r}$  treated in terms of a continuous wavefunction in space <sup>7</sup>. When we want to treat the atomic motion as being quantized in discrete momentum states labeled by some integer number  $\mu$ , we adopt the notation,

$$|\psi(t)\rangle = \sum_{\nu, n_+, n_-, i} c_{\nu, n_+, n_-, i}(t) |\nu\rangle \otimes |n_+\rangle \otimes |n_-\rangle \otimes |i\rangle, \quad (22.39)$$

where  $\langle \nu, \alpha_+, \alpha_-, i | \psi(t) \rangle = c_{\nu, n_+, n_-, i}(t)$  are the new expansion coefficients.

- A5. Next, we write down the *Schrödinger equation* for the state  $|\psi(t)\rangle$ , insert the expansion on the basis, and we derive a linear set of equation of motion for the expansion coefficients  $\dot{c}_{\{m\}}(\mathbf{r})$ . This set governs the dynamics of the quantum degrees of freedom.
- A6. The dynamics of the classical degrees of freedom  $B$  is obtained by taking the expectation values of the *Heisenberg equations*. Here, we need to take care that the quantum degrees of freedom appearing in the Heisenberg equations are expressed by their expansions.
- A7. The coupled set of equations for the expectation values of projectors of the system into a particular state, that is,  $\dot{c}_{\{m\}}$  (respectively,  $\dot{c}_{\{m\}}(\mathbf{r})$ ), and of observables  $B$  really represents all we need to describe the system dynamics and to simulate it numerically. Hack everything into your PC, pronto!
- B4. In the case of dissipative dynamics, derive the master equation obeying commutation rules for all quantized degrees of freedom including the Lindblad terms and expand every quantized degrees of freedom on the common basis, we do the same expansions, but,
- $$\hat{\rho}(t) = |\psi(t)\rangle \langle \psi(t)|. \quad (22.40)$$
- B5. Derive the linear set of equation of motion for the matrix elements  $\dot{\rho}_{\{m\}, \{n\}}$ .
- B6. Take the expectation values  $\text{Tr} \hat{\rho} \hat{B}$  of the Heisenberg equations for all degrees of freedom to be handled classical as expanding the quantized degrees of freedom on their basis.
- B7. The coupled set of equations for  $\dot{\rho}_{\{m\}, \{n\}}$  and  $\dot{B}$  is sufficient to describe the dynamics of the system, hack everything into your PC, pronto!

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<sup>7</sup>Note that, in the absence of other quantum numbers, we rather use to write  $c(\mathbf{r}) = \psi(\mathbf{r})$ .

Let us apply the procedure to the simplest case that the electronic excitation has been adiabatically eliminated and *all* remaining degrees of freedom can be treated classical. Then we do not require a Hamiltonian, nor the Schrödinger equation. We just take the expectation value of the Heisenberg equations (22.25) for all degrees of freedom which is easy to do, because there is no quantum state to be expanded: we just can replace the operators by *c*-numbers,

$$\begin{cases} \dot{\alpha}_{\pm} &= (-\kappa + i\Delta_c - iU_0)\alpha_{\pm} - iU_0 e^{\mp 2ikz} \alpha_{\mp} + \eta_{\pm} \\ \dot{p} &= 2i\hbar k U_0 (e^{-2ikz} \alpha_{+}^{\dagger} \alpha_{-} - e^{2ikz} \alpha_{+} \alpha_{-}^{\dagger}) \end{cases}. \quad (22.41)$$

These *totally classical* equations, called CARL equations, will be studied in the subsequent sections, while a thorough discussion of partially quantized equations of motion is postponed to Sec. 22.4.

### 22.1.5.1 CARL as a beam splitter

Neglecting spontaneous emission,  $\gamma_0 = 0$ , cavity pumping,  $\eta = 0$ , cavity decay,  $\kappa = 0$ , and cavity detuning,  $\Delta_c = 0$ , the CARL equations in the adiabatic approximation can be derived from the following Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \sum_{\pm} U_0 \hat{a}_{\pm}^{\dagger} \hat{a}_{\pm} + U_0 (e^{-2ikz} \hat{a}_{+}^{\dagger} \hat{a}_{-} + e^{2ikz} \hat{a}_{+} \hat{a}_{-}^{\dagger}), \quad (22.42)$$

and read,

$$\begin{cases} \dot{\hat{a}}_{\pm} &= -iU_0 \hat{a}_{\pm} - iU_0 e^{\mp 2ikz} \hat{a}_{\mp} \\ \dot{\hat{p}} &= 2i\hbar k U_0 (e^{-2ikz} \hat{a}_{+}^{\dagger} \hat{a}_{-} - e^{2ikz} \hat{a}_{+} \hat{a}_{-}^{\dagger}), \end{cases} \quad (22.43)$$

or with the substitution  $\hat{b}_{\pm} \equiv \hat{a}_{\pm} e^{iU_0 t}$ ,

$$\begin{cases} \dot{\hat{b}}_{\pm} &= -iU_0 e^{\mp 2ikz} \hat{b}_{\mp} \\ \ddot{\hat{b}}_{\pm} &= -U_0^2 \hat{b}_{\pm} - 2kz U_0 e^{\mp 2ikz} \hat{b}_{\mp}, \end{cases} \quad (22.44)$$

we see that, if the motion weren't a dynamic variable,  $\dot{\hat{z}} = 0$ , the field amplitudes would just perform harmonic oscillations.

On the other hand, with the substitution  $\hat{c} \equiv \hat{a}_{+} e^{ikz} + \hat{a}_{-} e^{-ikz}$ <sup>8</sup>, the complete Hamiltonian rephrased as,

$$\hat{H} = \frac{\hat{p}^2}{2m} + U_0 \hat{c}^{\dagger} \hat{c}. \quad (22.45)$$

Here, we see that, if the motion described by  $(\hat{z}, \hat{p})$  weren't a dynamic variable, our system would simply be a harmonic oscillator vibrating with the frequency  $U_0$ .

<sup>8</sup>Provided we are allowed to commute the operators  $\hat{z}$  and  $\hat{a}_{\pm}$ .

**22.1.5.2 Classical limit of the equations of motion**

For atoms much hotter than the recoil limit and macroscopic light intensities we may replace the quantum operators by complex numbers  $z \equiv \hat{z}$ ,  $\alpha_{\pm} \equiv \hat{a}_{\pm}$  and  $\rho_{21} = \hat{\sigma}^-$ . The classical equations of motion (22.41) for the coupled system of a single atom confined at the position  $r = z$  of the dipolar potential of a ring cavity can be cast into the form,

$$\begin{aligned} \begin{pmatrix} \dot{\alpha}_+ \\ \dot{\alpha}_- \end{pmatrix} &= \begin{pmatrix} -\kappa - \gamma_0 + i(\Delta_c - U_0) & -(\gamma_0 + iU_0)e^{-2ikz} \\ -(\gamma_0 + iU_0)e^{2ikz} & -\kappa - \gamma_0 + i(\Delta_c - U_0) \end{pmatrix} \begin{pmatrix} \alpha_+ \\ \alpha_- \end{pmatrix} + \begin{pmatrix} \eta_+ \\ \eta_- \end{pmatrix} \\ \dot{p} &= 2\hbar k\gamma_0(\alpha_+\alpha_+^* - \alpha_-\alpha_-^*) + 2i\hbar kU_0(\alpha_+^*\alpha_-e^{-2ikz} - \alpha_+\alpha_-^*e^{2ikz}) \end{aligned} \tag{22.46}$$

Recalling that  $\alpha_{\pm}^*\alpha_{\pm}$  is the number of photons in the respective mode, we can interpret this equation as a rate equation: The number of photons in a mode  $\alpha_+$  changes by photon losses at a rate  $\kappa$  from resonator, or by gain due to backscattering from the counterpropagating mode, or by pumping with an external incident light field at rate  $\eta_+$ .

The equations (22.46) completely describe our coupled atom-cavity system. They are totally classical and work for both, atoms and macroscopic particles.

**22.1.6 Cumulant expansion for CARL**

The dynamics of quantum correlations such as  $\hat{a}_+^\dagger\hat{a}_-$  or  $\hat{a}_+\sigma^+$  can be derived from Heisenberg equations, as well. As an example, let us consider the adiabatically eliminated Hamiltonian (22.26) and ignore the quantized nature of the atomic motion, the relevant first-order field-field correlations are then  $\hat{a}_+^2$ ,  $\hat{a}_+^\dagger\hat{a}_+$ ,  $\hat{a}_+^{\dagger 2}$ ,  $\hat{a}_-^2$ ,  $\hat{a}_-^\dagger\hat{a}_-$ ,  $\hat{a}_-^{\dagger 2}$ ,  $\hat{a}_+\hat{a}_-$ ,  $\hat{a}_+\hat{a}_-^\dagger$ ,  $\hat{a}_+^\dagger\hat{a}_-$ ,  $\hat{a}_+^\dagger\hat{a}_-^\dagger$ . From the Heisenberg equation we get, for instance,

$$\begin{aligned} \frac{d}{dt}\hat{a}_+^2 &= i[\hat{H}, \hat{a}_+^2] \\ &= -2i(U_0 - \Delta_c)\hat{a}_+^2 + 2U_0 \left( e^{2ik\hat{z}}\hat{a}_+\hat{a}_-^\dagger - e^{-2ik\hat{z}}\hat{a}_+\hat{a}_- \right) - 2\eta_+\hat{a}_+ . \end{aligned} \tag{22.47}$$

This is the lowest order *cumulant expansion*. The expectation values form a system of 10 linear first order differential equations [120] from which we can calculate the steady-state of the system.

The correlation functions and spectra are obtained directly from the CARL equation for the cavity fields (22.25) using the Wiener-Khinchin theorem (15.83) and the quantum regression theorem (15.137). With the substitutions,  $t \rightarrow 0$ ,  $\hat{B} \rightarrow 1$ ,  $\hat{A} \rightarrow d\hat{A}_k/d\tau$ , and  $\xi_i(\tau)\hat{A}_i(0) \rightarrow \zeta_i\hat{A}_i(\tau)$ , the quantum regression theorem can be written in the form,

$$\frac{d}{d\tau}\langle \hat{A}_k(\tau) \rangle = \sum_i \zeta_i \langle \hat{A}_i(\tau) \rangle \implies \frac{d}{d\tau}\langle \hat{A}_k(\tau)\hat{C}(0) \rangle = \sum_i \zeta_i \langle \hat{A}_i(\tau)\hat{C}(0) \rangle . \tag{22.48}$$

Applied, for example, to the correlation function (22.47), we obtain from the CARL equation (22.25), with  $\gamma_0 = 0$  and  $\Delta_c = 0$ ,

$$\frac{d}{d\tau} \langle \hat{a}_+(\tau) \hat{a}_+(0) \rangle = (-\kappa - iU_0) \langle \hat{a}_+(\tau) \hat{a}_+(0) \rangle - iU_0 e^{-2ikz} \langle \hat{a}_-(0) \hat{a}_+(0) \rangle + \eta_+ \langle \hat{a}_+(0) \rangle . \quad (22.49)$$

Repeating this calculation for the other first-order correlations functions we obtain a system of 10 linear first order differential equations, which can be solved via Laplace transform.

## 22.1.7 Exercises

### 22.1.7.1 Ex: Origin of quantum correlations

Derive the Hamiltonian (22.2) from the JCM Hamiltonian (15.23) transforming it into the co-rotating frame.

### 22.1.7.2 Ex: Linear pumping of a cavity mode

Study how the Hamiltonian  $\hat{H}_{pmp} = v\eta^* \hat{a} - v\eta \hat{a}^\dagger$ , describing linear pumping of a cavity mode, fills the cavity with photons in the absence of dissipation (see also (20.2)).

### 22.1.7.3 Ex: The adiabatically approximated Hamiltonian

- Derive the adiabatically approximated Hamiltonian (22.26) from the total Hamiltonian (22.4).
- Derive the CARL equations (22.25) directly from the adiabatically approximated Hamiltonian.
- Show that, in the absence of pumping, the energy stored in the light fields is conserved separately from the mechanical energy of the atom.
- Verify momentum conservation.

### 22.1.7.4 Ex: Periodicity of a lattice

Assume a symmetrically pumped ring cavity in equilibrium with an atom initially at rest. What photonic states are generated in the counterpropagating light modes, when the atom is kicked by an external force imparting a sudden recoil of  $\hbar k_{ck}$ .

### 22.1.7.5 Ex: Adiabatic elimination of the cavity modes

Derive the coherent part of the equations of motion (22.36) directly from the Hamiltonian (22.4) in the absence of pumping,  $\eta_\pm = 0$ , and in the limit of large cavity detunings,  $|\Delta_c| \gg \kappa$ .

### 22.1.7.6 Ex: Hamiltonian after adiabatic elimination of internal states for a linear cavity including counter-rotating terms

Repeat the adiabatic elimination of Sec. 22.1.4 for a linear cavity including counter-rotating terms.

## 22.2 CARL: The collective atomic recoil laser

The *collective atomic recoil laser* (*CARL*) was first predicted in 1994 [91] as an atomic analog of FEL. The idea consists of a monochromatic homogeneous beam of moving two-level atoms (all atoms have the same velocity), a strong counterpropagating pump laser beam and a weak copropagating probe beam tuned to the blue side of the resonance. The lasers form a standing light wave that moves in the same direction as the atoms. Atoms that are faster than the velocity of the standing wave are rejected by the maxima of the dipolar potential created by the standing wave and feel a repulsive force. Atoms that are slower than the standing wave velocity are pushed by the dipole potential maxima and feel an accelerating force. These forces can be interpreted as backscattering of photons from the pump wave into the probe wave. This redistribution of energy amplifies the contrast of the stationary wave, which in turn amplifies the backscattering efficiency, etc. Therefore, the CARL converts kinetic energy into coherent radiation (or more precisely, into an increase of the energy difference between probe and pump) mediated by atomic bunching. It is a self-amplifying mechanism. The CARL signature is a transient exponential amplification for the incident probe, which defines the frequency of the 'CARL laser'.

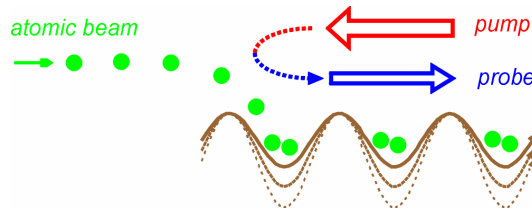


Figure 22.3: Collective atomic recoil laser.

The first experimental realization of CARL used an annular cavity [416].

### 22.2.1 Solutions for many mobile atoms

The preceding sections dealt with a single atom in a ring cavity. The most interesting part of the dynamics, however, only emerge in the presence of several atoms, because their motion can become correlated via their simultaneous interaction with the same two counter-propagating modes of the cavity, as illustrated in the following movie ([watch movie](#)). A talk on CARL can be assisted at ([watch talk](#)).

#### 22.2.1.1 Simulation of the dynamics for many perfectly bunched atoms

In experiment we generally deal with many atoms, which means that we have to extend the equations of motion (22.26) to  $N$  atoms via  $z \rightarrow z_j$  and  $p \rightarrow p_j$ , where  $j = 1, N$ . This will be done in the next chapter. Here, we will assume for simplicity, that the atoms are perfectly bunched,  $z_j = z$  and  $p_j = p$ . This means that we only need to consider a single equation of motion for the atoms. However, their coupling to the cavity modes is  $N$  times stronger, which means that we have to substitute  $U_0 \rightarrow U_N \equiv NU_0$  in the equation of motion for the cavity fields.



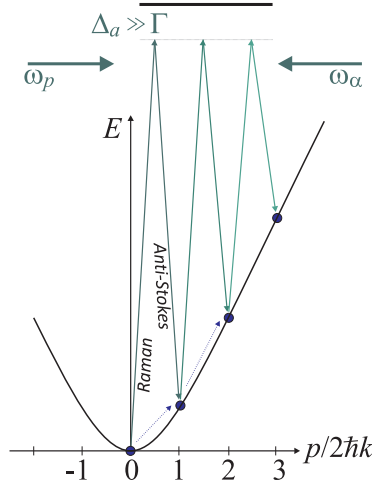


Figure 22.4: In the momentum picture the CARL acceleration process occurs as Raman-anti-Stokes processes along the free-particle dispersion relation.

In general, the equations can not be solved analytically, especially when the pump varies over time. Then we have to iterate numerically the equations,

$$\begin{aligned} \alpha_{\pm}(t + dt) &= \alpha_{\pm}(t) + dt \left[ -(\kappa + iNU_0 - i\Delta_e)\alpha_{\pm} - iNU_0 e^{\mp 2ikz} \alpha_{\mp} + \eta(t) \right] \quad (22.50) \\ z(t + dt) &= z + dt \frac{1}{m} p \\ p(t + dt) &= p - dt \ 2i\hbar k U_0 (\alpha_+ \alpha_-^* e^{2ikz} - \alpha_- \alpha_+^* e^{-2ikz}) . \end{aligned}$$

The kinetic and potential energies are <sup>9</sup>,

$$E_{kin} = \frac{p^2}{2m} \quad , \quad E_{pot} = U_0 I = U_0 |\alpha_+ e^{ikz} + \alpha_- e^{-ikz}|^2 . \quad (22.51)$$

### 22.2.1.2 Analytic approximations for one-sided pumping

Analytical solutions only exist in particular cases. However, they allow a better understanding of the dynamics. So let's consider some limiting cases. In Exc. 20.2.6.11 we determine the steady state of an atom interacting with the modes of a unidirectionally pumped annular cavity. In Exc. 20.2.6.12 we calculate the stationary position of the atom in a unidirectionally pumped ring cavity. In Exc. 20.2.6.13 we derive motion equations for the 'intensities'  $\alpha_{\pm} \alpha_{\pm}^*$  and 'coherences'  $\alpha_{\pm} \alpha_{\mp}^*$ .

When only one atom is in the cavity or when the atoms are perfectly bunched together, it is possible to derive analytical solutions. Particularly interesting is the following situation: We pump the cavity from one side. The pump is supposed to be dominant and locked to a resonance, such that we can neglect the feedback of the system on the pump, that is, we can assume,  $\alpha_+ = \eta/\kappa$ . Using the abbreviations

<sup>9</sup>Note, that there is also a radial motion of the atom coupled to the axial movement. The coupling happens, because the axial motion influences the number of intracavity photons of the radiation field which, in turn, determines the depth of the dipole potential.

$\chi \equiv \kappa + iU_0 - i\Delta_c$  and the photon recoil shift [254],

$$\omega_{rec} \equiv \frac{\hbar k^2}{2m}, \quad (22.52)$$

the equations (22.26) then become,

$$\left[ \begin{array}{l} \dot{\alpha}_- = -\chi\alpha_- - iU_N\alpha_+e^{2ikz} \\ k\dot{v} = 4\omega_{rec}iU_0\alpha_+(\alpha_-e^{-2ikz} - \alpha_-^*e^{2ikz}) \end{array} \right]. \quad (22.53)$$

We consider the stationary case (22.26). Doing the ansatz,

$$\alpha_- \equiv \beta e^{2ikx} \quad \text{where} \quad \dot{\beta} = 0 \quad (22.54)$$

we assume that the atom and the standing wave have the same velocity, that is, they move in phase. We obtain as solution,

$$\beta = \frac{-iU_N\alpha_+}{\kappa + 2ikv}, \quad k\dot{v} = 8\omega_{rec}U_0^2\alpha_+^2 \frac{2\kappa}{\kappa^2 + 4k^2v^2}. \quad (22.55)$$

If  $\kappa \ll 2kv$ , then the differential equation is approximately solved by,

$$(kv)^3 = 3\varepsilon\kappa U_0^2\alpha_+^2 t. \quad (22.56)$$

This means that the CARL frequency, that is, the frequency difference between the emitted probe wave and the incident light, increases temporarily. The frequency corresponds to the double Doppler shift. As the frequency of the probe light gradually shifts away from the cavity resonance, the probe light finally stops being amplified, and the amplitude of the probe field decreases: CARL is only a transient phenomenon. In fact, the behavior described by the equation (22.55) was observed in experiments [415].

### 22.2.1.3 Optical instability in ring cavities

We have until now concentrated on the regime of weak coupling,  $NU_0 < 1$ . If the pump laser is tuned closer to resonance, or if the number of atoms is increased, so that  $NU_0 > 1$ , we observe instabilities in the coupled atom-field dynamics, which critically depend on the pump intensities [515]. Imagine a sample of atoms trapped in an optical lattice formed by a symmetrically pumped ring cavity,  $\eta_+ = \eta_-$ . The system is stationary, the atoms are confined at the antinodes of the standing wave, the light fields are equal in strength,  $\alpha_+ = \alpha_-$ . At time  $t = 0$  we suddenly reduce the pump rate  $\eta_-$  of the non-stabilized mode by only a few percent. The response of the system observed in experiment [515] is to completely break down the field  $\alpha_-$ . The disappearance of the standing wave ejects most atoms and reduces  $NU_0$ , until the coupling gets so weak that the dynamics is essentially governed by the injected fields. The system recovers a stationary state, with much less atoms.

The physical explanation for the instability is reminiscent to the CARL behavior described in previous sections. Because atom-field coupling is strong, a small imbalance of the injected beam intensities is sufficient to displace the atoms to a location,

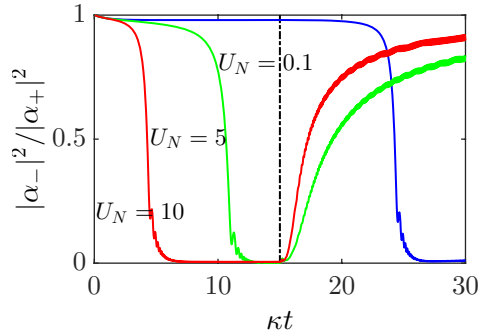


Figure 22.5: (code) Dynamics simulated with equations (22.46). At time  $\kappa t = 0$  the pump rate  $\eta_-$  is reduced by 1%. After a certain time that depends on  $NU_0$ , the standing wave breaks down ejecting atoms from the mode volume. Here, we simulate this via an artificial linear trap loss process setting in at time  $\kappa t = 15$ . As a result of the diminishing  $NU_0$  the standing wave recovers.

where the light which they scatter into the reverse direction interferes destructively with the injected light. A simple argument explains, why the standing wave is attracted towards a position where it gets unstable. We treat the imbalance  $\eta_+ > \eta_-$  as if it was due to a scatterer fixed in space inside the mode volume sitting on an edge of the standing wave (corresponding to a  $\pi/4$  phase shift), such that it only scatters light from  $\alpha_+$  into  $\alpha_-$ , but not the other way round. Whether the phase of the standing wave adjusts itself to that of pump field or such that the scatterer sits at the bottom of the potential well depends on the ratio of the coupling to the external field (given by  $\kappa$ ) and to the scatterer (given by  $U_0$ ). If  $U_0$  is stronger, the field is pulled towards the scatterer dragging along the atoms which are free to move. The stationary situation is therefore a displacement of the standing wave and the atoms by  $\lambda/4$ , which is just the position where the cavity field  $\alpha_-$  and the injected field  $\alpha_-^{(in)}$  are out of phase. The injected light is not transmitted through the cavity any more.

Note that the instability occurs in a plane wave situation, there is no need to consider the transversal motion. Furthermore, it is a single-atom effect, since we assume perfect bunching. We may therefore consider a single atom strongly coupled to the cavity and use the set of equations (22.46). In the *undepleted pump approximation* we assume  $\dot{\alpha}_+ = 0$ , and if the atom adiabatically follows the dynamics of the potential valley,  $\ddot{x} = 0$ , so that,

$$\begin{aligned}
 0 &= -\chi\alpha_+ - iU_0\sqrt{\frac{\alpha_+\alpha_-^*}{\alpha_+\alpha_-}}\alpha_- + \eta_+ , \\
 \dot{\alpha}_- &= -\chi\alpha_- - iU_0\sqrt{\frac{\alpha_+\alpha_-^*}{\alpha_+\alpha_-}}\alpha_+ + \eta_- .
 \end{aligned}
 \tag{22.57}$$

The first equation yields,

$$\alpha_+ = \frac{\eta_+}{\chi + iU_0 \frac{|\alpha_-|}{|\alpha_+|}}, \quad (22.58)$$

$$|\alpha_+| \approx \frac{\eta_+}{\chi} \left( 1 - \frac{U_0^2}{2\eta_+^2} |\alpha_-|^2 \right).$$

Plugging this result into the second equation and assuming the laser on resonance,  $\Delta_c = NU_0$ , so that we may replace  $\chi$  by  $\kappa$ , we get,

$$\dot{\alpha}_- \approx -\kappa\alpha_- - \frac{iU_0\eta_+}{\kappa} \frac{\alpha_-}{|\alpha_-|} + \frac{iU_0^3}{2\kappa\eta_+} |\alpha_-| \alpha_- + \eta_- . \quad (22.59)$$

This equation describes *optical bistability*.

**Example 103 (Locking of the pump laser):** In practice the resonant frequency of a cavity fluctuates due to ambient noise. Hence, it is easier, experimentally, to lock the pump laser on a cavity mode, e.g. using the Pound-Drever-Hall method. This means,

$$\alpha_+ = \frac{\eta_+}{\kappa} . \quad (22.60)$$

In the presence of atoms, however, the resonant frequency can be shifted due to the refractive index of the atomic cloud [226]. Moreover, the shift depends on the atomic bunching and consequently varies during the dynamics of the CARL. The way the locking circuit works, is to continuously adjust the detuning between the laser and the cavity  $\Delta_c$  (defined for the empty cavity) such as to maximize the amplitude of the field  $|\alpha_+|$  and, hence, the transmission of the cavity filled with atoms. The dynamics of the detuning must be incorporated by an additional equation modeling the action of locking. Now that we know the effect, which an ideal lock should have, we can apply the boundary condition (22.60) and eliminate the pump mode  $\alpha_+$  from the dynamics of the system. That is, the following equations are usually sufficient to describe the CARL:

$$\begin{cases} \dot{\alpha}_- &= (-\kappa + i\Delta_c - iU_0)\alpha_- - iU_0 e^{-2ikz} \alpha_+ + \eta_- \\ m\ddot{z} &= 2i\hbar k U_0 \alpha_+ (\alpha_- e^{-2ikz} - \alpha_-^* e^{2ikz}) \end{cases} . \quad (22.61)$$

The frequency offset of the cavity resonances caused by the atom,  $U_0$ , can exceed the width of the cavity  $\kappa$ . From equation (22.26) we know, neglecting  $\gamma = 0$ ,

$$|\alpha_+(\infty)|^2 = \frac{\chi\chi^*}{(\chi^2 + U_0^2)(\chi^{*2} + U_0^2)} \eta_+^2 .$$

The maxima of  $|\alpha_+(\infty)|^2$  as a function of  $\Delta_c$  give the shifted resonances of the modes.

#### 22.2.1.4 Locking on transverse modes

We already mentioned that as the CARL accelerates, the frequency of the light which is backscattered to the probe shifts to the red until it escapes from the resonant mode. What happens if we provide another resonant mode that can receive photons? We will show in the following calculation, that CARL simply picks up the closest

mode to dump the photons. The starting point is generalized CARL equations to accommodate a second reverse mode labeled  $\beta_-$ ,

$$\begin{aligned}\dot{\alpha}_+ &= -(\kappa - i\Delta_c)\alpha_+ - iU_0(u_+^*u_+\alpha_+ + u_+^*u_-\alpha_- + u_+^*u_\beta\beta_-) + \eta_+ \\ \dot{\alpha}_- &= -(\kappa - i\Delta_c)\alpha_- - iU_0(u_-^*u_-\alpha_- + u_-^*u_+\alpha_+ + u_-^*u_\beta\beta_-) \\ \dot{\beta}_- &= -(\kappa - i\Delta_\beta)\beta_- - iU_0(u_\beta^*u_\beta\beta_- + u_\beta^*u_+\alpha_+ + u_\beta^*u_-\alpha_-) \\ m\ddot{x} &= -U_0\nabla|\alpha_+u_+ + \alpha_-u_- + \beta_-u_\beta|^2,\end{aligned}\quad (22.62)$$

com  $u_\pm = e^{\pm ikz}$  and  $u_\beta = e^{-ik_\beta x}$ . We obtain,

$$\begin{aligned}\dot{\alpha}_+ &= -(\kappa - i\Delta_c + iNU_0)\alpha_+ - iU_0e^{-2ikz}\alpha_- - iU_1e^{-i(k+k_\beta)x}\beta_- + \eta_+ \\ \dot{\alpha}_- &= -(\kappa - i\Delta_c + iNU_0)\alpha_- - iU_0e^{2ikz}\alpha_+ - iU_1e^{i(k-k_\beta)x}\beta_- \\ \dot{\beta}_- &= -(\kappa - i\Delta_\beta + iNU_1)\beta_- - iU_1e^{i(k+k_\beta)x}\alpha_+ - iU_1e^{-i(k-k_\beta)x}\beta_- \\ m\ddot{x} &= -U_0(2ike^{2ikz}\alpha_-^*\alpha_+ - 2ike^{-2ikz}\alpha_+^*\alpha_-) \\ &\quad - U_1(i(k+k_\beta)e^{i(k+k_\beta)x}\beta_-^*\alpha_+ - i(k+k_\beta)e^{-i(k+k_\beta)x}\alpha_+^*\beta_-) \\ &\quad - U_1(i(k-k_\beta)e^{i(k-k_\beta)x}\alpha_-^*\beta_- - i(k-k_\beta)e^{-i(k-k_\beta)x}\beta_-^*\alpha_-).\end{aligned}\quad (22.63)$$

Note that  $k - k_\beta \approx 0$  and  $k + k_\beta \approx 2k$ . The result of the simulation is displayed in Fig. 22.6.

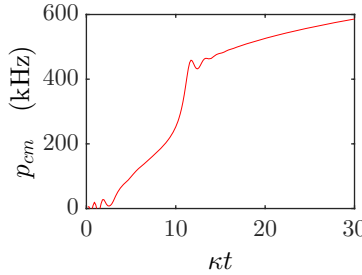


Figure 22.6: (code) The CARL locks to other modes of the cavity.

## 22.2.2 Phononic coupling of atoms mediated by a ring cavity

Phonons can be understood as vibrational excitations of quantum particles (atoms) in quantized traps. When atoms are interconnected in vibrational lattices, phonons can be transferred and shared between atoms<sup>10</sup>. Due to the particularity of the ring cavity of conserving the photonic momentum at each backscattering event, the photonic momentum can be understood as a phononic excitation, propagating in one dimension along the optical axis of the cavity.

We now consider a symmetrically pumped ring cavity [255]. The atoms are very cold and deep in the Lamb-Dicke regime. Using blue-detuned light the atoms will

<sup>10</sup>This is similar to the situation in micromasers, where several atoms can share a single photon.

be trapped at the nodes of the standing wave,  $kz_n = \pi/2 + \varepsilon_n$ , where  $\varepsilon_n$  are small displacements. Hence, we may expand,

$$e^{\mp 2ikz_n} \simeq -(1 \mp 2i\varepsilon_n). \quad (22.64)$$

With the abbreviation  $\chi \equiv \kappa - i(\Delta_c - NU_0)$  and defining the center-of-mass of the small displacements,  $\varepsilon_{cm} = \frac{1}{N} \sum_n \varepsilon_n$ , the equation for the two field modes are,

$$\dot{\alpha}_{\pm} \simeq -\chi\alpha_{\pm} + iNU_0(\mp 2i\varepsilon_0)\alpha_{\mp} + \eta. \quad (22.65)$$

Neglecting the impact of the atom on the amplitudes of the fields, we may derive the steady-state solution,

$$\alpha_{\pm} = \eta \frac{\chi + iNU_0(1 \mp 2i\varepsilon_{cm})}{\chi^2 + N^2U_0^2}. \quad (22.66)$$

As shown in (22.28) the normalized field intensity can be written as,

$$\frac{1}{2\varepsilon_0 c E_1^2} \iota(z, t) = |\alpha_+|^2 + |\alpha_-|^2 + 2|\alpha_+||\alpha_-| \cos(2kz + 2\theta), \quad (22.67)$$

provided the field amplitudes are expressed by,

$$\alpha_{\pm} = |\alpha_{\pm}|e^{\pm i\theta} \quad \text{such that} \quad \alpha_+\alpha_-^* = |\alpha_+||\alpha_-|e^{2i\theta} \quad \text{and} \quad \tan 2\theta = \frac{\text{Im } \alpha_+\alpha_-^*}{\text{Re } \alpha_+\alpha_-^*}. \quad (22.68)$$

Now,

$$\begin{aligned} \tan 2\theta &= \frac{\text{Im } [\chi + iNU_0(1 - 2i\varepsilon_{cm})][\chi^* - iNU_0(1 - 2i\varepsilon_{cm})]}{\text{Re } [\chi + iNU_0(1 - 2i\varepsilon_{cm})][\chi^* - iNU_0(1 - 2i\varepsilon_{cm})]} \\ &= 4NU_0\varepsilon \frac{-\Delta_c + 2NU_0}{-\kappa^2 - \Delta_c^2 + 4\Delta_c NU_0 - 4N^2U_0^2 + 4N^2U_0^2\varepsilon^2} \simeq \frac{4NU_0(\Delta_c - 2NU_0)}{\kappa^2 + (\Delta_c - 2NU_0)^2} \varepsilon. \end{aligned} \quad (22.69)$$

An atom in this optical potential feels the dipolar force,

$$\begin{aligned} m\ddot{z}_n &= [-\hbar U_0 \partial_z I]_{z=z_n} = 4\hbar k U_0 |\alpha_+||\alpha_-| \sin(2kz_n + 2\theta) \\ &= 4\hbar k U_0 \eta^2 \frac{|(\chi + iNU_0)^2 - 4N^2U_0^2\varepsilon_{cm}^2|}{|\chi^2 + N^2U_0^2|^2} \sin\left(2kz_n + \frac{2NU_0(\Delta_c - 2NU_0)}{\kappa^2 + (\Delta_c - 2NU_0)^2} 2\varepsilon_n\right) \\ &\simeq \frac{4\hbar k U_0 \eta^2}{\kappa^2 + \Delta_c^2} \sin\left(2kz_n + \frac{2NU_0(\Delta_c - 2NU_0)}{\kappa^2 + (\Delta_c - 2NU_0)^2} 2\varepsilon_n\right) \equiv \frac{m}{2k} \omega^2 \sin(2kz_n - 2\mu\varepsilon_n), \end{aligned} \quad (22.70)$$

where,

$$m\omega^2 \equiv \frac{8\hbar k^2 U_0 \eta^2}{\kappa^2 + 4U_0^2} \quad \text{and} \quad \mu_N \equiv \frac{2NU_0|2NU_0 - \Delta_c|}{\kappa^2 + (2NU_0 - \Delta_c)^2}. \quad (22.71)$$

Expanding this equation around the nodes we readily obtain,

$$\boxed{\ddot{\varepsilon}_n + \omega^2 \mu_N \varepsilon_n \simeq \mu_N \varepsilon_{cm} = \frac{\mu_N}{N} \sum_m \varepsilon_m}, \quad (22.72)$$

which describes the force on a single atom. Note that the harmonic force,  $\omega^2 \varepsilon_n$ , on the atom is continuously fed by the center-of-mass force,  $\omega^2 \mu_N \varepsilon_{cm}$ . The above equation can be rewritten as,

$$\begin{pmatrix} \ddot{\varepsilon}_1 \\ \dot{\varepsilon}_1 \\ \ddot{\varepsilon}_2 \\ \dot{\varepsilon}_2 \\ \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} 0 & -\omega^2(1 - \frac{\mu_N}{N}) & 0 & -\omega^2 \frac{\mu_N}{N} & \cdot \\ 1 & 0 & 0 & 0 & \cdot \\ 0 & -\omega^2 \frac{\mu_N}{N} & 0 & -\omega^2(1 - \frac{\mu_N}{N}) & \cdot \\ 0 & 0 & 1 & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} \dot{\varepsilon}_1 \\ \varepsilon_1 \\ \dot{\varepsilon}_2 \\ \varepsilon_2 \\ \cdot \\ \cdot \end{pmatrix}. \quad (22.73)$$

The eigenvalues of the matrix are  $e = i\omega, i\omega\sqrt{1 - \mu_N}$ . Therefore, we expect, in addition to the secular frequency  $\omega$ , a second oscillation frequency,

$$\omega_{cm} = \omega\sqrt{1 - \mu_N}. \quad (22.74)$$

We find splitting in the strong coupling regime,  $g > \Gamma$ , but we consider the weak coupling regime,  $g < \Gamma$ , to implement the phononic coupling.

### 22.2.2.1 Probing the phonon spectrum

To probe the phonon spectrum, we can measure (or simulate) the oscillation of a single atom  $x_m(t)$  in the presence of several atoms. The Fourier spectrum of the oscillation should reveal the frequency components of the center-of-mass motion  $Z(t)$  and the relative motion. This is actually observed and discussed earlier.

An alternative method for observing normal modes would be to excite an atomic motion and look for a resonant enhancement of the vibration amplitude near the secular frequency,  $\omega_\phi \approx \omega_{cm}, \omega_0$ . For an empty cavity, we expect a low-pass behavior as discussed in Sec. 20.1.2: The modulation frequencies  $\omega_\phi \gg \kappa$  are not transformed into phase oscillations  $\theta$ . However, if the atomic motion can act back on the field, then we expect a resonant enhancement. The atomic vibration can be excited by an external force, for example, by RIR resonances, superimposed on the field gradient of the cavity,

$$\dot{p} = 2i\hbar k U_0 (\alpha_+^* \alpha_- e^{-2ikz} - \alpha_+ \alpha_-^* e^{2ikz}) + F_{rir} \sin \omega_\phi t, \quad (22.75)$$

or by modulating the pump field,

$$\eta(t) = \eta e^{\pm i\phi_0 \sin \omega_\phi t}. \quad (22.76)$$

Fig. 22.7(a,b) shows a typical resonance curve obtained by plotting the maximum transfer of energy to the atoms as a function of the modulation frequency of the phase of the pump field.

Fig. 22.7(c,d) shows the same typical resonance curve, but taken here the atoms were subjected to a periodic external force. The phase does show a dispersive frequency-dependence  $\theta(\omega)$  if  $\eta \simeq \kappa$ . If the pumping is too strong,  $\eta \gg \kappa$ , the phase does not exhibit any resonant enhancement. Even though the phase-oscillations are suppressed as  $\omega_\phi$  is increased, the atomic center-of-mass motion is excited, when the secular resonance,  $\omega_\phi = \omega_{cm}$ , is met. The other modes  $\omega_0$  are not excited. Also the power-imbalance of the beams  $|\alpha_+|^2 - |\alpha_-|^2$  always has a strong resonant enhancement.

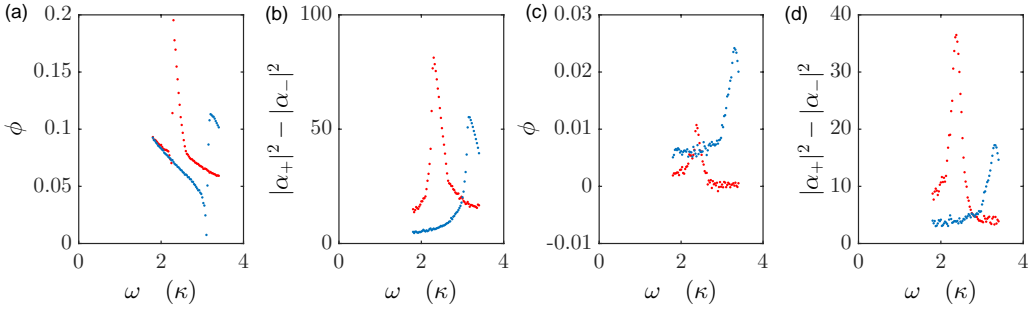


Figure 22.7: (code) The experimental parameters are  $N = 10$ ,  $U_0 = -0.05$ ,  $\gamma_0 \ll \kappa$ ,  $\Delta_c = 2U_0$ ,  $\eta = 10\kappa = \kappa\alpha_{\pm}(0)$ ,  $\omega_{rec} = 0.13$ ,  $\phi_0 = 0.1$ ,  $p_\omega = 10^{-4}$ . The calculated secular frequencies are  $\omega = 3.22\kappa$ ,  $\omega\sqrt{1-\mu} = 3.21\kappa$ ,  $\omega\sqrt{1-\mu_N} = 2.28\kappa$ ,  $\omega\sqrt{1-\mu}\sqrt{1-\mu_N} = 2.27\kappa$ .

The simulations have been done for the two situations that 1. the laser was not locked to the cavity resonance, but fixed to  $\Delta_c = 0$ , and 2. the laser was locked to the cavity resonance, which means  $\Delta_c = (1 + N^{-1}|\sum_m e^{-ikz_m}|)NU_0 \approx 2NU_0$ . This second case is shown in the blue curves in Figs. 22.7(a) to (d). The simulation exactly reproduces the expected deviation of the resonance frequency  $\omega_{cm}$  from the secular frequency  $\omega_0$  (22.74). Obviously, at  $\Delta_c \simeq 2NU_0$  the shift of the CoM mode can not be observed via its resonant enhancement. We can excite the CoM, but at the unshifted frequency  $\omega_0$ . At  $\Delta_c \simeq 0$  where the shift occurs, we can not lock the laser <sup>11</sup>.

**Example 104 (Two-coupled atoms):** Here we rewrite the field equations for two atoms in center-of-mass coordinates,

$$Z = \frac{z_1 + z_2}{2} \quad \text{and} \quad z = z_2 - z_1 ,$$

finding,

$$\dot{\alpha}_{\pm} = (-\kappa + i\Delta_c - 2iU_0)\alpha_{\pm} - 2iU_0\alpha_{\mp}e^{\mp 2ikZ} \cos kz + \eta .$$

**Example 105 (Feasibility analysis):** In order to make some realistic estimates, we choose a reasonably deep potential well  $U \simeq k_B 200 \mu\text{K}$ . This implies a secular frequency on the order of  $\omega_0 = \sqrt{2U/m}k^2 \simeq 12\kappa = 2\pi \times 250 \text{ kHz}$ . With  $N = 10^6$  trapped atoms, we want to reach  $NU_0 \simeq \kappa$ , that is,  $U_0 = 10^{-6}\kappa$ . With a given  $g = 20\kappa$ , this requires detunings  $\Delta_a = g^2/U_0 \simeq 4 \times 10^9\kappa = 2\pi \times 80 \text{ THz}$ . Using  $\varepsilon = 0.26$ , the intracavity photon number should be  $\eta/\kappa = \omega_0/\sqrt{8\varepsilon U_0} \simeq 10^3$ , which gives an intensity of  $I = \frac{\eta^2 \hbar \omega}{\kappa^2 V_{mode}} \simeq 7600 \text{ W/cm}^2$  and a power of  $P = \frac{\pi}{2} w_v w_h \nu \simeq 2.3 \text{ W}$ . This easily achievable with the cavity enhancement factor.

### 22.2.2.2 Phononic quantum gates

The normal mode coupling can be used to create *quantum entanglement*. A suggested procedure to correlate two atoms  $|m\rangle$  and  $|n\rangle$  is shown in Fig. 22.8 [323].

<sup>11</sup>It would also be interesting to calculate the resonance maxima as a function of  $\omega$  to see if the finite cavity bandwidth has an influence on atomic response!



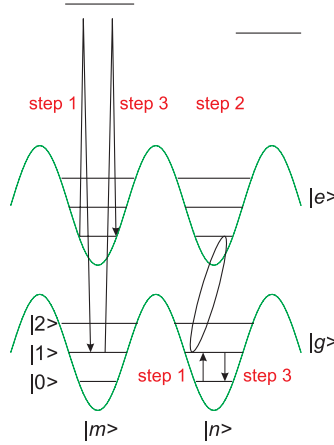


Figure 22.8: Scheme for entanglement in a ring-cavity.

The truth table reads,

$$\begin{array}{cccc}
 |g_m\rangle|g_n\rangle|0\rangle & |g_m\rangle|g_n\rangle|0\rangle & |g_m\rangle|g_n\rangle|0\rangle & |g_m\rangle|g_n\rangle|0\rangle \\
 |g_m\rangle|e_n\rangle|0\rangle & |g_m\rangle|e_n\rangle|0\rangle & |g_m\rangle|g_n\rangle|0\rangle & |g_m\rangle|e_n\rangle|0\rangle \\
 |e_m\rangle|g_n\rangle|0\rangle & \curvearrowright -i|g_m\rangle|g_n\rangle|1\rangle & \curvearrowright +i|g_m\rangle|e_n\rangle|1\rangle & \curvearrowright |e_m\rangle|g_n\rangle|0\rangle \\
 |e_m\rangle|e_n\rangle|0\rangle & -i|g_m\rangle|e_n\rangle|1\rangle & -i|g_m\rangle|e_n\rangle|1\rangle & -|e_m\rangle|e_n\rangle|0\rangle
 \end{array} . \tag{22.77}$$

In a new basis defined by  $|x_m\rangle|\pm_n\rangle \equiv \frac{1}{\sqrt{2}}|x_m\rangle(|g_n\rangle \pm |e_n\rangle)$  the above operation corresponds to a Controlled NOT gate. And if  $|x_m\rangle$  is initially in a superposition state, the states  $|x_m\rangle$  and  $|\pm_n\rangle$  end up entangled.

### 22.2.3 Collective effects

To understand the dynamics of CARL we must understand how atomic ensembles commonly interact with light modes. Let us first consider two atoms: The generalization of the fundamental equations (22.46) to two atoms is,

$$\begin{aligned}
 \dot{\alpha}_+ &= -\kappa\alpha_+ - iU_0e^{-2ikz_1}\alpha_- - iU_0e^{-2ikz_2}\alpha_- + \eta_+ \\
 \dot{\alpha}_- &= -\kappa\alpha_- - iU_0e^{2ikz_1}\alpha_+ - iU_0e^{2ikz_2}\alpha_+ .
 \end{aligned} \tag{22.78}$$

The equations decouple to  $e^{-2ikz_1} = e^{-2ikz_2 - i\pi}$ , such that the impact of the atoms on the light modes vanishes. This situation can be generalized to  $N$  atoms, for which the fundamental equations (22.46) are generalized to,

$$\boxed{
 \begin{aligned}
 \dot{\alpha}_\pm &= (-\kappa - iNU_0)\alpha_\pm - iU_0 \sum_{m=1}^N e^{\mp 2ikz_m} \alpha_\mp + \eta_\pm \\
 \dot{p}_m &= -2i\hbar k U_0 (\alpha_+ \alpha_-^* e^{2ikz_m} - \alpha_- \alpha_+^* e^{-2ikz_m})
 \end{aligned}
 } . \tag{22.79}$$

If the quantity,

$$b \equiv \frac{1}{N} \sum_j e^{-2ikz_j} \neq 0 , \tag{22.80}$$

called *bunching parameter* vanishes, it means that the atomic density distribution is homogeneous. So, the phases of randomly scattered photons destructively interfere, and the impact of the scatterers on the light modes cancels out.

On the other side, when atoms accumulate in the antinodes of the standing wave, it increases the contrast of it can spread more efficiently collectively by Bragg scattering. The particularity of the CARL is that during the temporal evolution the bunching process can amplify itself leading to an exponential growth of the counterpropagant mode, accompanied by an increasingly pronounced self-bunching.

**Example 106 (Universal scaling):** Our formula describing CARL,

$$\begin{aligned}\dot{\alpha}_- &= -\frac{iU_0\eta_+}{\chi} \sum_j e^{2ikz_j} - \chi\alpha_- \\ k\dot{v}_j &= -4\omega_{rec}iU_0\eta_+ \left( \frac{\alpha_-}{\chi^*} e^{-2ikz_j} - \frac{\alpha_-^*}{\chi} e^{2ikz_j} \right) - \gamma_{fric}k v_j,\end{aligned}\quad (22.81)$$

where  $\chi = \kappa + iNU_0 - i\Delta_c$ , can be rewritten in terms of a universal 'scaling' if we define,

$$\begin{aligned}\tau &= 4\omega_{rec}\rho t \quad \text{and} \quad \bar{\gamma} = \frac{\gamma_{fric}}{4\omega_{rec}\rho} \\ \theta_j &= 2kz_j \quad \text{and} \quad P_j = \frac{2kv_j}{4\omega_{rec}\rho} \\ A &= \frac{i|\chi|}{\chi^*\sqrt{\rho N}}\alpha_- \quad \text{and} \quad \bar{\chi} = \frac{\chi}{4\omega_{rec}\rho}.\end{aligned}\quad (22.82)$$

We obtain,

$$\begin{aligned}\dot{A} &= \frac{1}{N} \sum_j e^{i\theta_j} - \bar{\chi}A \\ \dot{\theta} &= P_j \\ \dot{P}_j &= -2(A^*e^{-i\theta_j} + Ae^{i\theta_j}) - \bar{\gamma}P_j.\end{aligned}\quad (22.83)$$

provided that the universal scaling parameter  $\rho$  is set to,

$$\rho \equiv \left( \frac{NU_0^2\eta_+^2}{8\omega_{rec}^2|\chi|^2} \right)^{1/3}.\quad (22.84)$$

The meaning of the  $\rho$  parameter can be gathered by rewriting it in terms of the number of photons of the pump  $|\alpha_+|^2 = \eta_+^2/\kappa^2$  and the depth of the dipolar potential  $U_d = U_0|\alpha_+|^2$ ,

$$\rho^3 = \frac{N}{a_+^2} \frac{U_d^2}{8\omega_{rec}^2}.\quad (22.85)$$

The  $\rho$  parameter therefore indicates the number of atoms per photon and the ratio between the depth of the dipolar trap and the photonic recoil energy. In Exc. 22.2.4.1 we calculate the gain spectrum of the CARL, when the atoms are subjected to an additional harmonic potential.

**Example 107 (Curiosities: Atomic transport around mirrors):** Displacement of the atomic cloud in a unidirectionally pumped ring-cavity. The left and right image in Fig. 22.9 are taken for different pumping directions  $\alpha$ . The upper cloud shows atoms trapped in the main focus of the ring-cavity. The lower

traces stem from atoms transported from the focus passed the mirrors  $T_1$  and  $T_2$  towards the incoupling mirror located at the place where the lower traces intersect. The lower trace are imaged twice, because the imaging beam is reflected from the incoupling mirror surface, before it is sent to a photodiode.

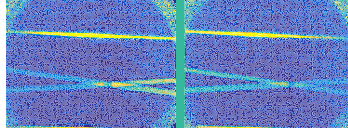


Figure 22.9: Displacement of the atomic cloud in a unidirectionally pumped ring-cavity. The left and right figures are taken for different pumping directions  $\alpha$ . The upper cloud shows atoms trapped in the main focus of the ring-cavity. The lower traces stem from atoms transported from the focus passed the mirrors  $T_1$  and  $T_2$  towards the incoupling mirror located at the place where the lower traces intersect. The lower trace are imaged twice, because the imaging beam is reflected from the incoupling mirror surface, before it is sent to a photodiode.

## 22.2.4 Exercises

### 22.2.4.1 Ex: CARL in a harmonic potential

Extend the CARL dynamics by an additional harmonic potential for the atoms and study the steady state gain as a function of cavity detuning  $\Delta_c$ .

### 22.2.4.2 Ex: Filling and drainage of a ring cavity with one fixed atom

Calculate by simulation of the classical CARL equation, how a laser-pumped ring cavity fills and loses photons in the presence of a single immobile atom.

### 22.2.4.3 Ex: Coupled motion of Rb and Cs atoms in a ring-cavity

Find out by simulation of the classical CARL equation, whether the motion of a Rb atom and a Cs atom can be coupled to the same mode of a ring cavity.

### 22.2.4.4 Ex: Inertially moving atom in a ring-cavity

Illustrate by simulation of the classical CARL equation, how an inertially moving single atom pushes the wave formed by two counterpropagating modes of a ring cavity.

### 22.2.4.5 Ex: Normal switch-off CARL

Do a simulation of the classical CARL equation suddenly switching off one of the two lasers pumping counterpropagating modes of a ring cavity.

### 22.2.4.6 Ex: Impact of an external friction force

Illustrate by simulation of the classical CARL equation, how friction (e.g. induced by an optical molasses) influences the motion of an atom interacting with two counterpropagating modes of a ring cavity.

**22.2.4.7 Ex: Impact of various perturbations**

Illustrate by simulation of the classical CARL equations how (a) radiation pressure, (b) mirror backscattering, (c) an external harmonic trapping potential, and (d) a phase-drifting pump laser influence the dynamics of an atom interacting with two counterpropagating modes of a ring cavity.

**22.2.4.8 Ex: Cavity cooling in a ring cavity**

Study cavity cooling in a ring cavity as a function of (a) friction and (b) detuning.

**22.2.4.9 Ex: Motion of atoms in a ring-cavity**

Discuss whether CARL can be observed without a ring-cavity.

**22.2.4.10 Ex: Further studies on CARL**

- a. Illustrate by simulation of the classical CARL equations the Doppler shift of the accelerated atom by calculating the FFT of the interference signal  $|\alpha_+ - \alpha_-|^2$ .
- b. Illustrate by simulation of the classical CARL equations
- c. Illustrate by simulation of the classical CARL equations the Doppler shift of the accelerated atom by calculating the shape of the RIR signal.
- d. Cavity emission spectrum as a function of detuning.

**22.2.4.11 Ex: Motion of atoms in a ring-cavity including internal states**

Motion of atoms in a ring-cavity, including internal states.

**22.3 Phenomena related to CARL**

The *collective atomic recoil laser* (CARL) unifies the principles of the FEL and LWI. Assume two-level atoms in their ground state moving against the pump beam  $\mathbf{k}_2$ . An (at first) weak probe beam  $k_1$  which is blue detuned with respect to  $\mathbf{k}_2$  builds a together with  $\mathbf{k}_2$  a standing wave fraction moving in direction  $\mathbf{v}$ . This fraction gives rise to a moving dipole potential  $V(\mathbf{r})$  and a light force on the atoms. If the moving standing wave is slower than the atoms (and the light frequency detuning from the atomic resonance is suitable), the atoms fall into the potential valleys by rescattering photons from the pump into the probe wave. This way they amplify the probe (they push the ponderomotive wave like the FEL), deepen the light potential valleys, are therefore further focused, etc.. We get a self-amplifying avalanche and feedback. In this process, the kinetic energy of the atoms is transformed into laser light. Or to resume: Collective recoil with self-bundling produced by cooperative Compton-scattering generates coherent laser light [91].

The following notes first discuss the basic equations of motion in the limit of very far detuning, where the internal dynamics can be adiabatically eliminated. Then we turn our attention to some characteristic features of CARL.

### 22.3.1 Recoil-induced resonances

The *recoil-induced resonances* (RIR) can be explained in two complementary pictures [157]. In the Raman picture, an atomic transition stimulates Raman transitions between momentum states of the free atom without influencing the atomic excitation (the atom remains in a dark state)  $\rho_{atom} \otimes |\mathbf{p}\rangle\langle\mathbf{p} + 2\hbar\mathbf{k}|$ . Absorption  $\Delta > 0$  or amplification  $\Delta < 0$  of the probe field  $\mathbf{k}_s$  by the pump field  $\mathbf{k}_p$  is a result of the population imbalance. However, it is not an excitation imbalance (compare LWI)  $\rho_{atom} \otimes |\mathbf{p} + 2\hbar\mathbf{k}\rangle\langle\mathbf{p} + 2\hbar\mathbf{k}| - \rho_{atom} \otimes |\mathbf{p}\rangle\langle\mathbf{p}|$ . In the Rayleigh picture the RIRs are an effect of coherent backward *Bragg scattering* of the probe wave at the phase-lag between the induced light-shift grating and the atomic density grating resulting from the periodic optical potential.

#### 22.3.1.1 RIR-spectroscopy

Two laser beams 1 and 2 having each two different frequencies  $\omega - \Delta\omega/2$  and  $\omega + \Delta\omega/2$  are irradiated from two different directions enclosing a small angle  $\theta$  into the atomic trap,

$$\begin{aligned} E(\mathbf{r}, t) &= E_1 + E_2 & (22.86) \\ &= E^{(0)} \left[ \cos(\mathbf{k}_1 \cdot \mathbf{r} - (\omega - \frac{1}{2}\Delta\omega)t) + \cos(\mathbf{k}_2 \cdot \mathbf{r} - (\omega + \frac{1}{2}\Delta\omega)t) \right] \\ &\approx 2E^{(0)} \cos(\mathbf{K} \cdot \mathbf{r} - \omega t) \cos(\frac{1}{2}\mathbf{q} \cdot \mathbf{r} - \frac{1}{2}\Delta\omega t), \end{aligned}$$

where  $\mathbf{q} \equiv \mathbf{k}_2 - \mathbf{k}_1$  and  $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_2 + \mathbf{k}_1)$ . The cycle-averaged intensities are  $I_i(t) = 2\varepsilon_0 c |E_i|^2 = 4\varepsilon_0 c E^{(0)^2} \cos^2(\frac{1}{2}\mathbf{q}\mathbf{r} - \frac{1}{2}\Delta\omega t)$ . Atoms coherently interacting with the light fields (which are tuned far from any atomic resonance) can redistribute the photons between the optical modes in a *nearly-degenerate* four-wave mixing process (4WM) thus modifying the amplitudes  $E_i^{(0)}$  so that a signal occurs.

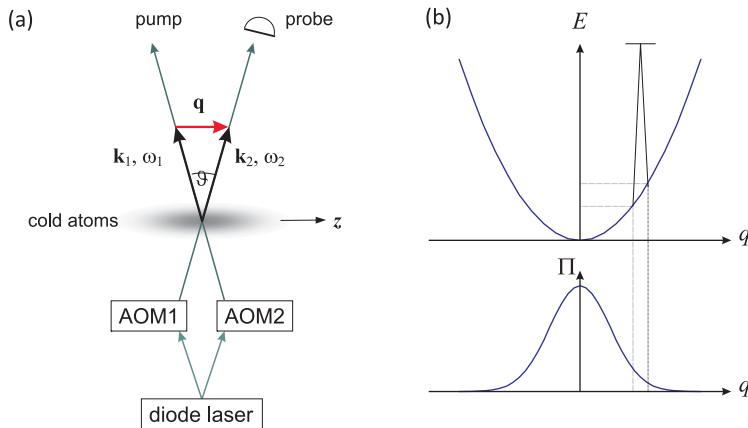


Figure 22.10: Principle scheme for RIR spectroscopy.

From symmetry considerations, it is easy to see that a homogeneous density distribution (along  $\mathbf{q}$ ) of the motionless atoms does not give rise to a signal, neither. So

let us assume that the atoms be bunched inside an optical grating according to some periodic distribution  $n(z) = n_0 \sin^2 k_\lambda z$ , but disregard their kinetics. The signals then generalize to,

$$\begin{aligned} E_1(z, t) &= E_1 + \beta n(z) \chi^{(3)}(E_1 + E_2) E_1 E_2 E_1 + \beta n(z) \chi^{(3)}(E_1 + E_2) E_1 E_2 E_1 \quad (22.87) \\ &= E_1 + \beta n(z) \chi^{(3)} \left( 2E^{(0)} \cos \left( \frac{1}{2} qz - \frac{1}{2} \Delta\omega t \right) \right) E_1 E_2 E_1 \end{aligned}$$

and analogous for  $E_2(z, t)$ . Or following Lambert-Beer [411],

$$\begin{aligned} I_1(x, z, t) &= |E_1|^2 \exp \left( 2i \frac{\pi}{\lambda} \int \chi^{(3)} \left( 2E^{(0)} \cos \left( \frac{1}{2} qz - \frac{1}{2} \Delta\omega t \right) \right) dy \right) \quad (22.88) \\ &= |E_1|^2 \exp \left( 2i \frac{\pi}{\lambda} \int n(x, y, z) \dots dy \right) \\ &= |E_1|^2 \exp \left( 2i \frac{\pi}{\lambda} n_0 \sin^2 k_\lambda z \int \dots dy \right) \\ I_1(t) &= \int I_1(x, z, t) dx dz . \end{aligned}$$

Regarding the momentum transfer, the 4WM process can be interpreted as Bragg scattering of the atoms at one of the two counterpropagating standing waves. We develop the theory of Bragg scattering in Sec. 28.2.

### 22.3.1.2 Temperature measurements via RIR

Temperature measurement are usually carried out by the time-of-flight method followed by absorption imaging. Alternatively, one can perform spectroscopy of RIR resonances. In the latter case, we detect intensity variations in a probe laser beam, *i.e.* the polarisation of the sample under the influence of *all* irradiated laser beams. In Sec. 13.3.6, we have seen that  $\alpha \propto \text{Im} \chi \propto \text{Im} P \propto \text{Im} \rho_{12}$ . It is thus sufficient to calculate the atomic coherences, if necessary including the motional states of the atoms. Calculated by [295]

$$W(t) = \frac{\pi}{2} \frac{\Omega_1 \Omega_2}{\Delta} \sqrt{\frac{mv}{k_B T}} \left[ \frac{\partial}{\partial v} e^{-mv^2/2k_B T} \right]_{v=\Delta\omega(t)/q} . \quad (22.89)$$

### 22.3.1.3 RIR-spectroscopy on trapped atoms

In the case of free particles, the Raman beams interact for every detuning with a different velocity class of atoms. The atoms are almost not disturbed. In the case of trapped atoms, a coherence can be excited, and since the atoms periodically change their velocity, be read out or reexcited at a later time. The same atom can thus interact with the Raman beams at different times/detunings. If the trap is a standing wave, the situation is complicated by the fact that there are two overlapping gratings: The standing wave and the Raman grating. However, if the trap is much deeper than the Raman grating the atoms can be considered as localized.

The signature of atomic oscillation is a modulation in the RIR signal with the periodicity of the secular frequency [410, 567].

Let us consider a standing-wave dipole-trap with  $\omega_z = 2\pi \times 700$  kHz,  $\omega_r = 2\pi \times 1$  kHz and  $U_{dip} = h \times 30$  MHz =  $4000 \times 2\varepsilon = 45\omega_z = 2100\omega_r$ . The 100  $\mu$ K cold atoms are therefore deep inside at the bottom of trap. This implies that the atomic energy levels are sharp and equally distant, and that the transitions are degenerate upon coupling by Raman-beams. If we apply a scan of  $\pm 2\pi \times 300$  kHz, we will not excite the longitudinal motion. But the radial motion can be excited. As seen earlier the absorption signal is  $\alpha \propto \text{Im} \rho_{12}$ . What happens to the coherence, if the radiation is swept across a resonance depends on the scanning speed. If the scan is slow, we expect  $\alpha \propto \text{Im} \rho_{12}(\infty)$ . We should be able to resolve the resonances [295, 297, 296] as peaks at  $\pm\omega_r, \pm 2\omega_r, \dots$ . In contrast, if the scan is fast, as long as  $\Delta_c$  is far from resonance, the population of the excited level  $\rho_{22}$  is just too small and nothing happens. When  $\Delta_c$  passes through 0, the coherence  $\rho_{12}$  is excited, and can now be driven by the laser even when  $\Delta_c$  is tuned far away. The coherence precesses faster and faster.

Let us compare to the situation of a laser swept across an electric dipole resonance. In analogy to the cavity response in reflection to a laser scanned across an eigenfrequency, we might expect a ringing coming from interference of the radiating electric dipole (which has been induced while the laser was close to resonance) with the original laser frequency. The radiated electric field is proportional to the excited state population. If we allow for a change of the input field, for example  $\Delta_c(t)$ , the Bloch-equations must be numerically integrated,

$$\rho(t + dt) = \rho(t) + dt M\rho(t) . \quad (22.90)$$

It is already clear that we should expect a ringing with exactly the time-dependent frequency  $\Delta_c(t)$ . Fig. 22.11 shows

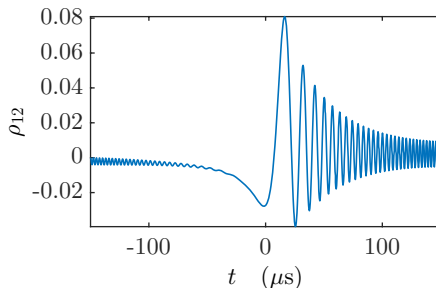


Figure 22.11: (code) Time-evolution of the atomic coherence as the driving laser frequency is swept across resonance. The parameters are  $\Gamma = 2\pi \times 8$  kHz,  $\Omega = 0.2\Gamma$ ,  $\Delta = -50\Gamma..50\Gamma$  and  $t = -150..150 \mu$ s.

This simple mathematical model only assumes a resonance with a given width and a frequency-scanned oscillator. The physical nature of the resonance and the level splitting are not specified and the formalism should be applicable to a variety of situations. A ringing is, in fact, observed for RIR scans, if the scanning speed is too fast, in particular for atoms trapped in optical lattices. Ringing can also be generated in classical harmonic oscillators and laser-driven two-level systems as we will see in Exc. 28.5.4.1.

### 22.3.1.4 RIR versus CARL

The dynamics is characterized by backaction of the atomic motion onto the cavity field. In this respect there is a connection to RIR resonances in the limit investigated by [411]. While normal RIR is the action of the atomic motion on light fields, they demonstrate that in the same time the Raman-lattice influences the atomic motion. The coherence is limited by the time the photon spends in the sample (similar to the limitation of superradiant Rayleigh scattering, without photonic recycling by a ring-cavity). Real backaction in the sense of coherent interdependence of the photonic and the kinetic degrees of freedom requires recycling of the photons.

## 22.3.2 FEL: the free electron laser

Normal lasers work by an inversion in the internal degrees of freedom, that is, bound electrons are excited to energetically higher orbitals, from where they can decay by emitting monochromatic light of well-defined frequency. Because, the *free electron laser* (*FEL*) works with beams of *free* electrons, they are tunable over wide frequency ranges. They have much higher efficiencies above 65%.

The principle is the following: Relativistic electrons are guided through an *undulator*, which is a device producing a magnetic field with periodically alternating polarization. Here, the electrons are subjected to a Lorentz force,  $\mathbf{F} = -e\mathbf{v} \times \mathbf{B}$ , forcing the electrons to oscillate with the periodicity of the undulator field. This corresponds to a dipole moment interacting with the incident light field. The transverse velocity of the electrons within the magnetic field of an incident light produces a Lorentz force in the axial direction called *ponderomotive force*. This force accelerates the electrons when they are a bit slower than the ponderomotive wave. Otherwise the electrons are decelerated. In the second case, the energy of the electrons is transmitted to the light field, which leads to a *bunching* of the atoms. Because it is a parametric process, there is a continuous energy flow between the field and the motion of the  $e^-$  (analogous to parametric Raman cooling). Thus, the FEL converts the kinetic energy of the electron beam into laser radiation. The inversion in a FEL can be interpreted as a relative displacement of the probability distributions for absorption and emission of photons in momentum space,

$$\begin{aligned} W_{abs}(\Delta) &= \text{sinc}^2 \frac{1}{2}(\Delta + \varepsilon/2) \\ W_{abs}(\Delta) &= \text{sinc}^2 \frac{1}{2}(\Delta - \varepsilon/2) , \end{aligned} \quad (22.91)$$

where  $\varepsilon = \hbar k^2/2m_e$ . The gain is a convolution of the difference of the above distribution with the momentum distribution of the electrons [621].

There various kinds of FELs. In stimulated Compton FELs, described by the shown Feynman graphs, the electrons are scattered by virtual (momentum transfer without energy transfer) photons of the wiggler. In Bremsstrahlungs FEL, the electrons are scattered at a static field. Virtual photons of the static field are scattered at the electrons, who then emit Bremsstrahlung and change their propagation direction. In Raman FELs very dense electron beams produce charge density oscillations, which provides an additional effect. Free Electron Lasers already have a wide range of application ranging from biology and medicine to lithography and material science.



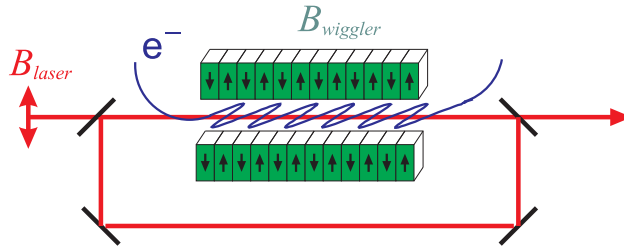


Figure 22.12: Free electron laser.

### 22.3.3 CARL in an ion storage ring

Bonifacio *et al.* [92] suggested to study collective atomic recoil lasing (CARL) with relativistic atoms. They found that using very fast atoms it should, in principle, be possible to get large CARL frequency shifts and much higher power enhancement factors than observed in free-electron lasers (FEL). Relativistic atomic velocities can be achieved in heavy ion accelerators such as the GSI heavy ion accelerator in Darmstadt and TSR ion storage ring in Heidelberg. Therefore the question arises, if CARL could be an alternative way to produce very energetic and intense UV radiation in concurrence to the FEL. In fact, CARL-based systems may prove more powerful and versatile as their electronic counterparts: Cooling techniques based on electron beams or on hybrid optical-radiofrequency friction forces are able to cool the ionic beams down to mK temperatures.

The CARL which has been predicted ten years ago by Bonifacio *et al.* [91], has recently been observed with cold atoms stored in a high-finesse ring cavity [416, 701]. This proof of principle, now may motivate a deeper study of the figure of merit of a relativistic CARL. This short note, however, shows that a relativistic CARL is still, in my opinion, far from being realizable.

### 22.3.4 Matter wave superradiance

There is a close relationship between CARL and the phenomenon of *matter wave superradiance* (or *superradiant Rayleigh scattering*) [90, 599], which will be discussed in the following sections.

In 1999 the group of W. Ketterle at the MIT made a surprising observation, when it illuminated an elongated Bose-Einstein condensate with a short linearly polarized laser pulse traversing the condensate perpendicularly to the long axis [352]<sub>DOI</sub>. Instead of producing radiation with a dipole pattern, as we might expect for a polarized atomic cloud undergoing Rayleigh scattering, they observed emission of directional light bursts along the symmetry axis of the condensate. They also observed that some of the atoms were accelerated at angles of  $45^\circ$ . And these atoms could emit other generations of atoms at angles of  $45^\circ$ .

The phenomenon was explained as follows. Let us imagine a first photon scattered by an atom into the direction of the long axis of the condensate. This atom will be accelerated by the photonic recoil in a direction of  $135^\circ$  with respect to the direction of the photon, and it will interfere with the rest of the condensate thus generating

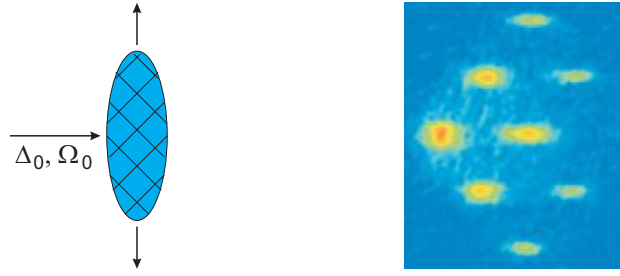


Figure 22.13: (code) Flight-of-time measurement of the atomic momentum distribution after matter wave superradiance.

a standing matter wave of oriented in such a way, that the following photons are scattered into the same direction as the first one via Bragg scattering. This reinforces the contrast of the matter wave, etc.. We obtain an exponential gain of photons in the mode defined by the first scattered photon, as well as of the mode receiving the scattered matter wave. As the path of the gain is longer along the long axis of the condensate, this mode is favored. That is, the condensate can be considered as a cavity embracing the solid angle  $\Omega_{sol}$ .

The Rayleigh scattering rate for a single atom is,

$$R_1 = \sin^2 \theta \sigma(\Delta_a) \frac{I}{\hbar\omega} \frac{3\Omega_{sol}}{8\pi} , \tag{22.92}$$

where  $\theta$  is the angle between the polarization of the incident laser (intensity  $I$ ) and the direction into which the light is scattered. The cross-section is  $\sigma(\Delta_a) = \sigma_0 \frac{\Gamma^2}{4\Delta^2 + 2\Omega^2 + \Gamma^2}$ , where  $\sigma_0 = 3\frac{\lambda^2}{2\pi}$ . Now, for the set of atoms, the superradiant scattering rate is not only amplified by the number of condensed atoms,  $N$ , but also by the number of atoms,  $N_r$ , already being in the mode receiving scattered atoms,

$$R_{sr} = R_1 N \frac{N_r + 1}{2} . \tag{22.93}$$

This is the *superradiance matter wave*.

### 22.3.5 Exercises

#### 22.3.5.1 Ex: Good and bad cavity regime

What are the characteristics distinguishing the good from the bad cavity limit.

#### 22.3.5.2 Ex: Ringing in resonant systems

In this exercise we study ringing in (a) an excited classical harmonic oscillator and (b) in a laser-driven two-level system.

## 22.4 Quantization of the atomic motion in cavities

At the beginning of this chapter we set up the complete Hamiltonian of the coupled atom-cavity system. Then tracing over dissipative degrees of freedom, we derived the master equation or derived the Heisenberg equations for the operators appearing in the remaining Hamiltonian quantum mechanically. But then for CARL we restricted to a classical treatment of the motion, as well as of the cavity modes.

Resuming the discussion started in Sec. 22.1.5 we will, in the remaining sections of this chapter, analyze effects due to the *quantization* of degrees of freedom represented by operators. The present section will (i) on a quantum description of the motion (with and without adiabatic elimination of the internal atomic dynamics and (ii) on issues arising from the presence of many atoms.

### 22.4.1 Quantum description of the motion

Concretely, let us analyze again the situation of a single atom interacting with a ring cavity. We assume validity of the adiabatic elimination of the internal atomic excitation and want to treat the light fields as classical. In contrast, the atomic motion is considered as quantum:

$$|\psi\rangle = |z\rangle_{\text{motion}} \otimes |\alpha_+\rangle \otimes |\alpha_-\rangle \xrightarrow{\text{classical}} \otimes |i\rangle_{\text{electron}} \xrightarrow{\text{adiab.elim.}} |z\rangle . \quad (22.94)$$

Since the motion, being the only quantum degree of freedom, is not subject to dissipation, we may use the Schrödinger equation in addition to Heisenberg equations for the light fields. Then, following the procedure outlined in Sec. 22.1.5, with  $z$  being the only quantum number, we find that the system is completely described by the dynamics of the expansion coefficients,

$$\begin{aligned} i\hbar \frac{d}{dt} \langle z | \psi(t) \rangle &= \langle z | \hat{H} | \psi(t) \rangle \\ \dot{\alpha}_{\pm} &= \langle z | \frac{i}{\hbar} [\hat{H}, \hat{a}_{\pm}] - \kappa \hat{a}_{\pm} | z \rangle . \end{aligned} \quad (22.95)$$

Plugging in the Hamiltonian (22.26), we obtain the Schrödinger equation for the particle's motional wavefunction <sup>12</sup>,

$$i\hbar \frac{d}{dt} \langle z | \psi(t) \rangle = \frac{p^2}{2m} \langle z | \psi(t) \rangle + U_0 \langle z | \hat{a}_+^\dagger \hat{a}_- e^{-2ikz} + \hat{a}_+ \hat{a}_-^\dagger e^{2ikz} | \psi(t) \rangle , \quad (22.96)$$

and the Heisenberg equations for the light fields,

$$\begin{aligned} \dot{\alpha}_{\pm} &= \langle z | (-\kappa + i\Delta_c - iU_0) \hat{a}_{\pm} + iU_0 e^{\mp 2ikz} \hat{a}_{\mp} + \eta_{\pm} | z \rangle \\ &= (-\kappa + i\Delta_c - iU_0) \alpha_{\pm} + iU_0 \alpha_{\mp} \langle z | \int dz |\psi(t)\rangle \langle \psi(t) | e^{\mp 2ikz} | z \rangle + \eta_{\pm} \\ &= (-\kappa + i\Delta_c - iU_0) \alpha_{\pm} + iU_0 \alpha_{\mp} \int dz |\psi(z, t)|^2 e^{\mp 2ikz} + \eta_{\pm} . \end{aligned} \quad (22.97)$$

<sup>12</sup>Terms of the Hamiltonian (22.26) which do not depend on  $z$  or  $p$  have been ignored, as they can be removed from the Schrödinger equation by a simple unitary transformation. Note that this can be done even though these terms depend on the field amplitudes  $\alpha_{\pm}$ .

In summary,

$$\begin{cases} \dot{\psi}(z) = \frac{i\hbar}{2m} \frac{d^2}{dz^2} \psi(z) - iU_0 \left( \alpha_+^\dagger \alpha_- e^{-2ikz} + \alpha_+ \alpha_-^\dagger e^{2ikz} \right) \psi(z) \\ \dot{\alpha}_\pm = (-\kappa + i\Delta_c - iU_0) \alpha_\pm + iU_0 \alpha_\mp \int dz |\psi(z)|^2 e^{\mp 2ikz} + \eta_\pm \end{cases} . \quad (22.98)$$

These are the new CARL equations that should be used in cases when the particle is *slower than the recoil velocity*, in which its motion must be described as a propagating matter wave. Note, that under this form, the equations can easily be generalized to apply to macroscopic wavefunctions such as a Bose-Einstein condensate.

The expectation value of the particle's position is then calculated via,

$$\begin{aligned} z(t) &= \langle \psi(0) | \hat{z}(t) | \psi(0) \rangle = \langle \psi(0) | e^{-i\hat{H}t} | \hat{z} | e^{i\hat{H}t} \psi(0) \rangle \\ &= \langle \psi(t) | \hat{z} | \psi(t) \rangle = \int \langle \psi(t) | z \rangle \langle z | \hat{z} | z' \rangle \langle z' | \psi(t) \rangle dz dz' = \int z |\psi(t, z)|^2 dz . \end{aligned} \quad (22.99)$$

We can verify that the expectation value of the particle's position satisfies the classical equation of motion,

$$\begin{aligned} m\ddot{z} &= \langle \psi(t) | m\ddot{\hat{z}} | \psi(t) \rangle = 2i\hbar k U_0 \left( \hat{a}_+^\dagger \hat{a}_- \langle \psi(t) | e^{-2ik\hat{z}} | \psi(t) \rangle - \hat{a}_+ \hat{a}_-^\dagger \langle \psi(t) | e^{2ik\hat{z}} | \psi(t) \rangle \right) \\ &= 2i\hbar k U_0 \left( \hat{a}_+^\dagger \hat{a}_- e^{-2ik\langle \psi(t) | \hat{z} | \psi(t) \rangle} - \hat{a}_+ \hat{a}_-^\dagger e^{2ik\langle \psi(t) | \hat{z} | \psi(t) \rangle} \right) \\ &= 2i\hbar k U_0 \left( \hat{a}_+^\dagger \hat{a}_- e^{-2ikz} - \hat{a}_+ \hat{a}_-^\dagger e^{2ikz} \right) . \end{aligned} \quad (22.100)$$

### 22.4.1.1 About the origin of quantized motion

The quantization of the light field into photons is, as discussed in Chp. 15.7.3, an intrinsic property of light. In contrast, the quantization of atomic motion is less obvious, because the atoms are not confined in a trapping potential. The reason for it lies in the monochromaticity of the driving laser fields and the one-dimensional geometry of the system, which allow us to write the recoil operator (2.190) or (3.127) as,

$$e^{2ik\hat{z}} = \int |p + 2\hbar k\rangle \langle p| dp . \quad (22.101)$$

Inserting it into the interaction part of the CARL Hamiltonian,

$$\hat{H}_{int} = U_0 (e^{-2ik\hat{z}} \hat{a}_+^\dagger \hat{a}_- + e^{2ik\hat{z}} \hat{a}_+ \hat{a}_-^\dagger) , \quad (22.102)$$

the Schrödinger equation for the expanded wavefunction

$$|\psi\rangle = \int c(p) |p\rangle dp \quad (22.103)$$

yields,

$$\begin{aligned} i\hbar \frac{d}{dt} \langle p | \psi \rangle &= U_0 \hat{a}_+^\dagger \hat{a}_- \langle p | e^{-2ik\hat{z}} | \psi \rangle + U_0 \hat{a}_+ \hat{a}_-^\dagger \langle p | e^{2ik\hat{z}} | \psi \rangle \\ &= i\hbar \frac{d}{dt} c(p) = U_0 [\hat{a}_+^\dagger \hat{a}_- c(p + 2\hbar k) + \hat{a}_+ \hat{a}_-^\dagger c(p - 2\hbar k)] . \end{aligned} \quad (22.104)$$

That is, if the initial momentum distribution is narrow,  $\Delta p \ll 2\hbar k$ , and if CARL-induced recoil due to backscattering of photons between counterpropagating modes is the only force acting on the atoms, the momentum of the atoms can only adopt discrete values in units of  $2\hbar k$ , *as if the atomic velocity were quantized*. That is, the quantization of the field is, in some way, imprinted on the distribution of the atomic moment, so that we may as well use a discrete notation,

$$|\psi\rangle = \sum_{\nu} c_{\nu} |\nu\rangle, \quad (22.105)$$

such that <sup>13</sup>,

$$i\hbar \frac{d}{dt} c_{\nu} = U_0 \hat{a}_+^{\dagger} \hat{a}_- c_{\nu+1} + U_0 \hat{a}_+ \hat{a}_-^{\dagger} c_{\nu-1}. \quad (22.106)$$

**Example 108 (Analogy to the Bose-Hubbard Hamiltonian):** Interestingly the CARL Hamiltonian with quantized motion (22.102) has, in momentum space, a similar shape as the 1D Bose-Hubbard Hamiltonian in position space,

$$\begin{aligned} \hat{H} &= \sum_{\nu} \hbar\omega_{rec}\nu^2 + U_0 \sum_{\nu} \left( |\nu-1\rangle \langle \nu| \hat{a}_+^{\dagger} \hat{a}_- + |\nu-1\rangle \langle \nu| \hat{a}_+ \hat{a}_-^{\dagger} \right) \\ &= \hbar\omega_{rec} \sum_{\nu} \nu^2 + U_0 \hat{a}_+^{\dagger} \hat{a}_- \sum_{\nu} \hat{A}_{\nu-1}^{\dagger} \hat{A}_{\nu} + U_0 \hat{a}_+ \hat{a}_-^{\dagger} \sum_{\nu} \hat{A}_{\nu+1}^{\dagger} \hat{A}_{\nu}. \end{aligned}$$

Now, it is important to understand that the statement that *photonic recoil is quantized does not mean that the dipolar optical force can only be transmitted in units of  $2\hbar k$* , as if the force needed to accumulate a certain amount of energy before it makes a sudden transition to a different momentum state. Rather, the probability to find an initially resting atom subject to a force in the momentum state  $2\hbar k$  gradually increases with time. The atom gradually evolves into a coherent superposition of states  $|0\rangle + |2\hbar k\rangle + |4\hbar k\rangle + \dots$ , and only when we *measure* the momentum distribution will it have to decide in which state it ended up. The expectation value of the center-of-mass momentum linearly, as long as the force is constant. A slide show on the quantized CARL can be viewed at [\(watch talk\)](#).

## 22.4.2 Discretization of the momentum states

We will now assume that, for the physical reasons described above, the motional state of the atom can only exist with momenta corresponding to multiples of twice the photonic recoil.

<sup>13</sup>Note that, instead of expanding the state  $|\psi\rangle$ , we could expand the motional wavefunction into plane waves,

$$\langle z|\tilde{\psi}\rangle = \tilde{\psi}(z) = \frac{1}{\sqrt{2\pi}} \sum_n c_n(t) e^{2imkz} \quad \text{normalized as} \quad \int dz |\tilde{\psi}(z)|^2 = 1 = \sum_n |c_n(t)|^2.$$

Insertion of this expansion into the quantized CARL equations (22.98) yields the same results.

### 22.4.2.1 Schrödinger equation approach

We basically repeat the treatment of Sec. 22.4.1, but now expanding the motion on a discrete basis of momenta labeled by an integer number  $\nu$ ,

$$|\psi\rangle = |\nu\rangle_{\text{motion}} \otimes |\alpha_+\rangle \otimes |\alpha_-\rangle \xrightarrow{\text{classical}} \otimes |i\rangle_{\text{electron}} \xrightarrow{\text{adiab.elim.}} |\nu\rangle. \quad (22.107)$$

Applying the recipe detailed at the beginning of Sec. 22.4, we write down the same Schrödinger equation as in (22.96)<sup>14</sup>, but now projecting on  $\langle\nu|$  rather than on  $\langle z|$  and inserting the expansion (22.105) and,

$$e^{2ik\hat{z}} = \sum_{\nu} |\nu+1\rangle\langle\nu| \quad \text{and} \quad \hat{p} = \sum_{\nu} \nu 2\hbar k |\nu\rangle\langle\nu|. \quad (22.108)$$

We get,

$$\begin{aligned} \langle\nu| i\hbar \frac{d}{dt} \sum_{\nu''} c_{\nu''} |\nu''\rangle = \langle\nu| \sum_{\nu'} \frac{(\nu' 2\hbar k)^2}{2m} |\nu'\rangle\langle\nu'| \\ + U_0 \left( \sum_{\nu'} |\nu'-1\rangle\langle\nu'| \hat{a}_+^\dagger \hat{a}_- + \sum_{\nu'} |\nu'+1\rangle\langle\nu'| \hat{a}_+ \hat{a}_-^\dagger \right). \end{aligned} \quad (22.109)$$

And from the Heisenberg equation (22.15) for light modes,

$$\langle\psi|\dot{\hat{a}}_{\pm}|\psi\rangle = \langle\psi|(-\kappa + i\Delta_c - iU_0)\hat{a}_{\pm} - iU_0 e^{\mp i2k\hat{z}} \hat{a}_{\mp} + \eta_{\pm}|\psi\rangle, \quad (22.110)$$

we get,

$$\sum_{\nu', \nu''} \langle\nu'| c_{\nu'}^* \dot{\hat{a}}_{\pm} c_{\nu''} |\nu''\rangle = \sum_{\nu, \nu', \nu''} \langle\nu'| c_{\nu'}^* [(-\kappa + i\Delta_c - iU_0)\hat{a}_{\pm} - iU_0 |\nu \mp 1\rangle\langle\nu| \hat{a}_{\mp} + \eta_{\pm}] c_{\nu''} |\nu''\rangle. \quad (22.111)$$

Finally,

$$\boxed{\begin{aligned} \dot{c}_{\nu} &= -4i\omega_{\text{rec}} \nu^2 c_{\nu} - iU_0 (\alpha_+^* \alpha_- c_{\nu+1} + \alpha_+ \alpha_-^* c_{\nu-1}) \\ \dot{\alpha}_{\pm} &= (-\kappa + i\Delta_c - iU_0) \alpha_{\pm} - iU_0 \alpha_{\mp} \sum_{\nu} c_{\nu \mp 1}^* c_{\nu} + \eta_{\pm} \end{aligned}}. \quad (22.112)$$

In Exc. 22.4.6.1 and 22.4.6.2 we study the equations (22.112) in the presence of a constant external force.

### 22.4.2.2 Master equation approach

As in the situation under study the motion is the only quantum degree of freedom and not subject to dissipation, a master equation approach is useless, and we will show it here only for completeness.

<sup>14</sup>Here again, as done in Sec. 22.4.1, we ignore terms of the Hamiltonian (22.26) which do not depend on  $z$  or  $p$ .

In 22.4.6.3 we show a derivation obtained by directly inserting the adiabatically simplified Hamiltonian (22.26) into the Liouville equation (22.8). The result is,

$$\begin{aligned}
 \dot{\rho}_{\mu,\nu} &= i(\nu - \mu) [(\nu + \mu)\omega_{rec} - \Delta_c] \rho_{\mu,\nu} \\
 &\quad + iU_0 [\alpha_+^* \alpha_- (\rho_{\mu,\nu-1} - \rho_{\mu+1,\nu}) + \alpha_-^* \alpha_+ (\rho_{\mu,\nu+1} - \rho_{\mu-1,\nu})] \\
 \dot{\alpha}_{\pm} &= (-\kappa + i\Delta_c - iU_0)\alpha_{\pm} - iU_0\alpha_{\mp} \sum_{\nu} \rho_{\nu,\nu\mp 1} + \eta_{\pm}
 \end{aligned} \quad (22.113)$$

### 22.4.3 Quantization of the atomic motion without adiabatic elimination

So far we have discussed the quantization of the atomic motion in the CARL equations, which were obtained by adiabatic elimination of the electronically excited state. In the following, we will quantize the motion directly in the equations of motion (22.15) for the observables and in the Liouville equation for the density operator. We quantize the atomic motion along the optical  $z$ -axis simply by assuming that, in this direction, the momentum only exists in multiples of  $\hbar k$ , and organize up the Hilbert space like this,

$$|\psi\rangle = |\nu\rangle_{\text{motion}} \otimes |i\rangle_{\text{electron}} \otimes \underbrace{|n\rangle_+ \otimes |n\rangle_-}_{\text{classical}} \rightarrow |\nu, i\rangle, \quad (22.114)$$

that is, skipping the quantum number counting the photons, we will treat the light fields classically,  $\hat{a}_{\pm} = \alpha_{\pm}$ ,

$$\begin{aligned}
 \hat{p} &= \sum_{\nu} \nu \hbar k |\nu \hbar k\rangle \langle \nu \hbar k| \otimes \mathbb{I} \\
 e^{-ik\hat{z}} &= \sum_{\nu} |\nu \hbar k - \hbar k\rangle \langle \nu \hbar k| \otimes \mathbb{I} \\
 \hat{\sigma}^+ &= \mathbb{I} \otimes |2\rangle \langle 1| \\
 \hat{\rho} &= |\psi\rangle \langle \psi| = \sum_{\mu,\nu,i,j} c_{\mu,i}^* c_{\nu,j} |\mu\rangle \langle \nu| \otimes |i\rangle \langle j|
 \end{aligned} \quad (22.115)$$

where in the last equation we defined  $c_{\nu,j} = \langle p, j | \psi(t) \rangle = \langle \nu \hbar k, j | \psi(t) \rangle = \langle \nu, j | \psi(t) \rangle$ , such that,

$$\rho_{\mu,\nu;i,j} \equiv \langle \mu, i | \hat{\rho} | \nu, j \rangle = c_{\mu,i}^* c_{\nu,j}. \quad (22.116)$$

Adopting the short notation  $|\nu\rangle \equiv |\nu\hbar k\rangle$  we can write the state of the system,

$$\begin{aligned}
 |\psi(t)\rangle &= \sum_{\nu} c_{\nu,1} |\nu\hbar k, 1\rangle + c_{\nu,2} |\nu\hbar k, 2\rangle & (22.117) \\
 \langle\psi(t)|\hat{p}|\psi(t)\rangle &= \hbar k \sum_{\nu} \nu (|c_{\nu,1}|^2 + |c_{\nu,2}|^2) \\
 \langle\psi(t)|e^{\pm i\nu k \hat{z}}|\psi(t)\rangle &= \sum_{\nu} (c_{\nu\pm 1,1}^* c_{\nu,1} + c_{\nu\pm 1,2}^* c_{\nu,2}) \\
 \langle\psi(t)|\hat{a}|\psi(t)\rangle &= \alpha \sum_{\nu} (|c_{\nu,1}|^2 + |c_{\nu,2}|^2) = \alpha \\
 \langle\psi(t)|\hat{\sigma}^-|\psi(t)\rangle &= \sum_{\nu} c_{\nu,1}^* c_{\nu,2} \\
 \langle\psi(t)|\hat{\sigma}_z|\psi(t)\rangle &= \sum_{\nu} (|c_{\nu,2}|^2 - |c_{\nu,1}|^2) .
 \end{aligned}$$

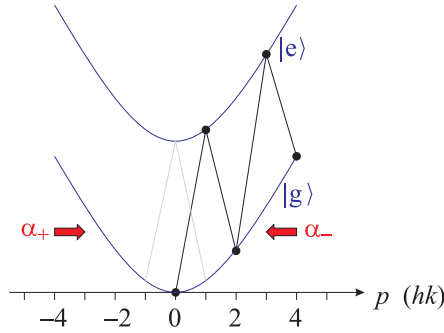


Figure 22.14: Illustration of the quantized motion.

To describe the dynamics of the system we could use the Schrödinger equation, but the Hamiltonian (22.4) does not contain spontaneous emission nor cavity decay. So, let us employ the equations of motion (22.15), which were derived from a master equation. The equation of motion for the field yields,

$$\begin{aligned}
 \dot{\alpha}_{\pm} &= \langle\psi(t)|\dot{\hat{a}}_{\pm}|\psi(t)\rangle = \langle\psi(t)|(-\kappa + i\Delta_c)\hat{a}_{\pm} - ig\hat{\sigma}^- e^{\mp i\nu k \hat{z}} + \eta_{\pm}|\psi(t)\rangle & (22.118) \\
 &= (-\kappa + i\Delta_c)\alpha_{\pm} + \eta_{\pm} - ig \sum_{\nu} c_{\nu\mp 1,1}^* c_{\nu,2} \\
 &= (-\kappa + i\Delta_c)\alpha_{\pm} + \eta_{\pm} - ig \sum_{\nu} \rho_{\nu\mp 1, \nu; 1, 2} .
 \end{aligned}$$

For the atomic motion we get,

$$\dot{x} = \langle\psi(t)|\dot{\hat{x}}|\psi(t)\rangle = \frac{1}{m} \langle\psi(t)|\hat{p}|\psi(t)\rangle = \frac{\nu\hbar k}{m} , \quad (22.119)$$



and

$$\begin{aligned}
\dot{p} &= \langle \psi(t) | \dot{\hat{p}} | \psi(t) \rangle & (22.120) \\
&= \langle \psi(t) | \imath g \hbar k \hat{\sigma}^- \left( \hat{a}_+^\dagger e^{-\imath k \hat{z}} - \hat{a}_-^\dagger e^{\imath k \hat{z}} \right) - \imath g \hbar k \hat{\sigma}^+ \left( \hat{a}_+ e^{\imath k \hat{z}} - \hat{a}_- e^{-\imath k \hat{z}} \right) | \psi(t) \rangle \\
&= \sum_{\nu} \imath g \hbar k \left( \alpha_+^* c_{\nu-1,1}^* c_{\nu,2} - \alpha_-^* c_{\nu+1,1}^* c_{\nu,2} - \alpha_+ c_{\nu+1,1} c_{\nu,2}^* + \alpha_- c_{\nu-1,1} c_{\nu,2}^* \right) \\
&= \sum_{\nu} \imath g \hbar k \left( \alpha_+^* \rho_{\nu-1,\nu;1,2} - \alpha_-^* \rho_{\nu+1,\nu;1,2} - \alpha_+ \rho_{\nu,\nu+1;2,1} - \alpha_- \rho_{\nu,\nu-1;2,1} \right).
\end{aligned}$$

### 22.4.3.1 Maxwell-Bloch equations without adiabatic elimination

Analogously to the treatment in Sec. 14.2.1, we will now derive the master equation without adiabatic elimination of the excited state (in this case called *Maxwell-Bloch equations* from the Liouville equation [first line of Eq. (22.8)] using the Hamiltonian (22.4). The coherent part is,

$$\begin{aligned}
\dot{\rho}_{\mu,\nu;i,j} &\equiv \langle \mu, i | \dot{\hat{\rho}} | \nu, j \rangle = -\imath \langle \mu, i | [\hat{H}, \hat{\rho}] | \nu, j \rangle & (22.121) \\
&= -\imath \sum_{p,u} \langle \mu, i | \hat{H} | p, u \rangle \rho_{p,\nu;u,j} + \imath \sum_{p,u} \rho_{\mu,q;i,v} \langle p, u | \hat{H} | \nu, j \rangle \\
&= -\imath \left[ \frac{(\mu \hbar k)^2}{2m} - \Delta_a \delta_{i2} - \Delta_c (|\alpha_+|^2 + |\alpha_-|^2) - \imath \eta_+ (\alpha_+ - \alpha_+^*) - \imath \eta_- (\alpha_- - \alpha_-^*) \right] \rho_{\mu,\nu;i,j} \\
&\quad - \imath g \left[ \alpha_+^* \delta_{i1} \rho_{\mu+1,\nu;2,j} + \alpha_+ \delta_{i2} \rho_{\mu-1,\nu;1,j} + \alpha_-^* \delta_{i1} \rho_{\mu-1,\nu;2,j} + \alpha_- \delta_{i2} \rho_{\mu+1,\nu;1,j} \right] \\
&\quad + \imath \left[ \frac{(\nu \hbar k)^2}{2m} - \Delta_a \delta_{j2} - \Delta_c (|\alpha_+|^2 + |\alpha_-|^2) - \imath \eta_+ (\alpha_+ - \alpha_+^*) - \imath \eta_- (\alpha_- - \alpha_-^*) \right] \rho_{\mu,\nu;i,j} \\
&\quad + \imath g \left[ \alpha_+^* \delta_{j2} \rho_{\mu,\nu-1;i,1} + \alpha_+ \delta_{j1} \rho_{\mu,\nu+1;i,2} + \alpha_-^* \delta_{j2} \rho_{\mu,\nu+1;i,1} + \alpha_- \delta_{j1} \rho_{\mu,\nu-1;i,2} \right] \\
&= \left[ \imath \frac{(\nu^2 - \mu^2) (\hbar k)^2}{2m} + \imath \Delta_a (\delta_{i2} - \delta_{j2}) \right] \rho_{\mu,\nu;i,j} \\
&\quad + \imath g \left[ \alpha_+^* (\delta_{j2} \rho_{\mu,\nu-1;i,1} - \delta_{i1} \rho_{\mu+1,\nu;2,j}) + \alpha_+ (\delta_{j1} \rho_{\mu,\nu+1;i,2} - \delta_{i2} \rho_{\mu-1,\nu;1,j}) \right. \\
&\quad \quad \left. + (\alpha_-^* \delta_{j2} \rho_{\mu,\nu+1;i,1} - \delta_{i1} \rho_{\mu-1,\nu;2,j}) + \alpha_- (\delta_{j1} \rho_{\mu,\nu-1;i,2} - \delta_{i2} \rho_{\mu+1,\nu;1,j}) \right].
\end{aligned}$$

The incoherent part comprises the spontaneous decay [second line of Eq. (22.8)],

$$\begin{aligned}
\langle \mu, i | \mathcal{L}_{atom-vac} \hat{\rho} | \nu, j \rangle &= -\gamma \langle \mu, i | [\hat{\sigma}^+ \hat{\sigma}^- \hat{\rho} - 2\hat{\sigma}^- \hat{\rho} \hat{\sigma}^+ + \hat{\rho} \hat{\sigma}^+ \hat{\sigma}^-] | \nu, j \rangle & (22.122) \\
&= -\gamma \sum_{p,u} \langle \mu, i | \hat{\sigma}^+ \hat{\sigma}^- | p, u \rangle \rho_{p,\nu;u,j} + 2\gamma \sum_{p,u,q,v} \langle \mu, i | \hat{\sigma}^- | p, u \rangle \rho_{p,q;u,v} \langle q, v | \hat{\sigma}^+ | \nu, j \rangle \\
&\quad - \gamma \sum_{p,u} \rho_{\mu,p;i,u} \langle p, u | \hat{\sigma}^+ \hat{\sigma}^- | \nu, j \rangle \\
&= -\gamma [\delta_{i2} \rho_{\mu,\nu;i,j} - 2\delta_{i1} \delta_{j1} \rho_{\mu,\nu;2,2} + \delta_{j2} \rho_{\mu,\nu;i,j}]
\end{aligned}$$

and the cavity decay [third line of Eq. (22.8)],

$$\langle \mu, i | \mathcal{L}_{cavity-vac, \pm} \hat{\rho} | \nu, j \rangle = -\kappa \langle \mu, i | \hat{a}_{\pm}^\dagger \hat{a}_{\pm} \hat{\rho} - 2\hat{a}_{\pm} \hat{\rho} \hat{a}_{\pm}^\dagger + \hat{\rho} \hat{a}_{\pm}^\dagger \hat{a}_{\pm} | \nu, j \rangle = 0. \quad (22.123)$$

Finally, using the definition of the recoil shift  $\omega_{rec} = \hbar k^2/2m$  we get,

$$\begin{aligned}
 \dot{\rho}_{\mu,\nu;1,1} &= i(\nu^2 - \mu^2)\omega_{rec}\rho_{\mu,\nu;1,1} + 2\gamma\rho_{\mu,\nu;2,2} \\
 &+ i\hbar g [-\alpha_+^*\rho_{\mu+1,\nu;2,1} + \alpha_+\rho_{\mu,\nu+1;1,2} - \alpha_-^*\rho_{\mu-1,\nu;2,1} + \alpha_-\rho_{\mu,\nu-1;2,1}] \\
 \dot{\rho}_{\mu,\nu;1,2} &= [i(\nu^2 - \mu^2)\omega_{rec} - i\hbar\Delta_a] \rho_{\mu,\nu;1,2} - \gamma\rho_{\mu,\nu;1,2} \\
 &+ i\hbar g [\alpha_+^*\rho_{\mu,\nu-1;1,1} - \alpha_+^*\rho_{\mu+1,\nu;2,2} + \alpha_-^*\rho_{\mu,\nu+1;1,1} - \alpha_-^*\rho_{\mu-1,\nu;2,2}] \\
 \dot{\rho}_{\mu,\nu;2,1} &= [i(\nu^2 - \mu^2)\omega_{rec} + i\hbar\Delta_a] \rho_{\mu,\nu;2,1} - \gamma\rho_{\mu,\nu;2,1} \\
 &- i\hbar g [\alpha_+\rho_{\mu-1,\nu;1,1} - \alpha_+\rho_{\mu,\nu+1;2,2} + \alpha_-\rho_{\mu+1,\nu;1,1} - \alpha_-\rho_{\mu,\nu-1;2,2}] \\
 \dot{\rho}_{\mu,\nu;2,2} &= i(\nu^2 - \mu^2)\omega_{rec}\rho_{\mu,\nu;2,2} - 2\gamma\rho_{\mu,\nu;2,2} \\
 &+ i\hbar g [\alpha_+^*\rho_{\mu,\nu-1;2,1} - \alpha_+\rho_{\mu-1,\nu;1,2} + \alpha_-^*\rho_{\mu,\nu+1;2,1} - \alpha_-\rho_{\mu+1,\nu;1,2}] \\
 \dot{\alpha}_{\pm} &= (-\kappa + i\Delta_c - iU_0)\alpha_{\pm} + \eta_{\pm} - ig \sum_{\nu} \rho_{\nu\mp 1,\nu;1,2}
 \end{aligned} \tag{22.124}$$

We note  $\hat{\rho}_{\mu,\nu;2,1} = \hat{\rho}_{\nu,\mu;1,2}^*$ .

The equations (22.124) form a set of equations to describe the quantized CARL without adiabatic elimination. And as shown in the derivation of the CARL equations (22.25), they contain radiation pressure. In Exc. 22.4.6.4 we study the quantized CARL Maxwell-Bloch equations without adiabatic elimination of the excited state for a three-level system.

## 22.4.4 Quantized motion with many particles

The Hamiltonian (22.96) holds for a single atom. If clouds of thermal atoms are considered, we may switch to a classical description of the motion, as done in (22.46). In the case of very cold (below the recoil limit) but still independent atoms, we may assume that they all are coherently distributed over the same momentum states. We may then apply a unique momentum state expansion for all atoms, as shown in the subsequent section.

If on the other hand quantum statistics play a role, then we need to replace the wavefunction in the Schrödinger equation (22.96) by field operators, as done in Sec. 28.5. In the following sections, we will restrict to single atoms that can be in a coherent superposition of momentum states or many atoms in a matter wave that can be treated as a  $c$ -number, e.g. a Bose-condensate without fluctuations.

### 22.4.4.1 Modal expansion of the motion of many independent atoms in the adiabatic approximation for one-sided pumping

Our starting point is the quantum version of the CARL equations (22.25), where we neglect spontaneous emission,  $\gamma_0 = 0$ . Setting  $\alpha_+ = \eta_+/\kappa$  and  $\eta_- = 0$  we get,

$$\begin{aligned}
 \dot{\hat{a}}_- &= (-\kappa + i\Delta_c - iU_0)\hat{a}_- - iU_0 \frac{\eta_+}{\kappa} e^{-2ik\hat{z}_j} \\
 m\ddot{\hat{z}}_j &= 2i\hbar k U_0 (\hat{a}_+^\dagger \hat{a}_- e^{-2ik\hat{z}_j} - \hat{a}_+ \hat{a}_-^\dagger e^{2ik\hat{z}_j})
 \end{aligned} \tag{22.125}$$

where the index  $j$  runs over all atoms. For this case, the total momentum is a constant of motion for  $N$  atoms is,

$$[\hat{H}, 2\hbar k \hat{a}_-^\dagger \hat{a}_- + \sum_{j=1}^N \hat{p}_j] = 0. \quad (22.126)$$

where the Hamiltonian is obtained from (22.26) by eliminating the mode  $\alpha_+$  and summing over all atoms,

$$\hat{H} = \sum_j \left[ \frac{\hat{p}_j^2}{2m} + \frac{\eta_+}{\kappa} U_0 \left( e^{-2\imath k \hat{z}_j} \hat{a}_- + e^{2\imath k \hat{z}_j} \hat{a}_-^\dagger \right) \right] + (U_0 - \Delta_c) \hat{a}_-^\dagger \hat{a}_-. \quad (22.127)$$

To treat the motion as being quantized we define a base  $|\nu\rangle_j$ ,

$$\hat{p}_j |\nu\rangle_j = 2\hbar k \nu |\nu\rangle_j \quad \text{and} \quad |\psi(z_j)\rangle = \sum_\nu c_{j,\nu} |\nu\rangle_j, \quad (22.128)$$

and calculate the expected value of the equations (22.125) regarding the atomic motion,

$$\begin{aligned} \frac{d\hat{a}_-}{dt} &= (-\kappa - \imath\Delta_c) \hat{a}_- - \imath U_0 \frac{\eta_+}{\kappa} \sum_j \langle \psi(z_j) | e^{-2\imath k \hat{z}_j} | \psi(z_j) \rangle \\ &= (-\kappa + \imath\Delta_c - \imath U_0) \hat{a}_- - \imath U_0 \frac{\eta_+}{\kappa} \sum_{j,\mu,\nu} c_{j,\mu}^* c_{j,\nu} \langle \mu | e^{-2\imath k z_j} | \nu \rangle_j \\ &= (-\kappa + \imath\Delta_c - \imath U_0) \hat{a}_- - \imath U_0 \frac{\eta_+}{\kappa} \sum_{j,\nu} c_{j,\nu}^* c_{j,\nu+1}. \end{aligned} \quad (22.129)$$

We do not use the second equation (22.125), but instead we use the Schrödinger equation  $\imath\hbar \frac{d|\psi(z_j)\rangle}{dt} = \hat{H}|\psi(z_j)\rangle$ , which yields,

$$\begin{aligned} \imath\hbar \sum_\nu \frac{dc_{j,\nu}}{dt} |\nu\rangle_j &= \sum_\nu \frac{1}{2m} p_j^2 c_{j,\nu} |\nu\rangle_j + \hbar\Delta_c \hat{a}_-^\dagger \hat{a}_- \sum_\nu c_j(\nu) |\nu\rangle_j \\ &\quad + \hbar U_0 \eta \sum_\nu (\hat{a}_-^\dagger e^{-2\imath k z_j} + \hat{a}_- e^{2\imath k z_j}) c_{j,\nu} |\nu\rangle_j. \end{aligned} \quad (22.130)$$

Projecting on  ${}_j\langle\mu|$ , we obtain [143],

$$\boxed{\begin{aligned} \dot{c}_{j,\mu} &= -4\imath\omega_{rec} \mu^2 c_{j,\mu} - \imath\Delta_c \hat{a}_-^\dagger \hat{a}_- c_{j,\mu} - \imath U_0 \eta [\hat{a}_-^\dagger c_{j,\mu+1} + a_- c_{j,\mu-1}] \\ \dot{\hat{a}}_- &= -(\kappa + \imath\Delta_c) \hat{a}_- + N U_0 \eta \sum_\nu c_{j,\nu}^* c_{j,\nu+1} \end{aligned}}, \quad (22.131)$$

where we took the expectation value of Eq. (22.129). The equations (22.131) can be used for numerical simulations [581].

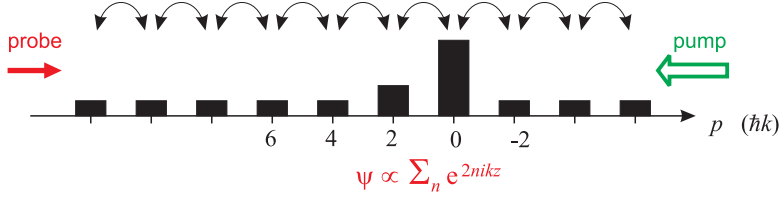


Figure 22.15: Probe light and 'bunching' when the temperature is raised.

#### 22.4.4.2 Equations for the density matrix

The equations (22.131) allow to calculate the derivatives of the density matrix given by,

$$\varrho_{\mu,\nu} \equiv e^{-\imath(\mu-\nu)\Delta_c t} \frac{1}{N} \sum_j c_j^*(\mu) c_j(\nu) , \quad (22.132)$$

yielding,

$$\begin{aligned} \frac{d\varrho_{\mu,\nu}}{dt} &= e^{-\imath(\mu-\nu)\Delta_a t} N^{-1} \sum_j (\dot{c}_{j,\mu}^* c_{j,\nu} + c_{j,\mu}^* \dot{c}_{j,\nu} - \Delta_c c_{j,\mu}^* c_{j,\nu} \imath(\mu-\nu)) \quad (22.133) \\ &= e^{-\imath(\mu-\nu)\Delta_a t} N^{-1} \sum_j [\imath\omega_r(\mu^2 - \nu^2) - \Delta_c \imath(\mu-\nu)] c_{j,\mu}^* c_{j,\nu} + \\ &\quad + \imath U_0 \eta [a c_{j,\mu+1}^* c_{j,\nu} - a c_{j,\mu}^* c_{j,\nu-1} + \hat{a}^\dagger c_{j,\mu-1}^* c_{j,\nu} - \hat{a}^\dagger c_{j,\mu}^* c_{j,\nu+1}] . \end{aligned}$$

Introducing  $\tilde{a} \equiv a e^{\imath\Delta_c t}$  we finally obtain,

$$\begin{aligned} \frac{d\varrho_{\mu,\nu}}{dt} &= \imath(\mu-\nu)[\omega_r(\mu+\nu) - \Delta_c] \varrho_{\mu,\nu} \\ &\quad + \imath U_0 \eta [\tilde{a}(\varrho_{\mu+1,\nu} - \varrho_{\mu,\nu-1}) + \tilde{a}^\dagger(\varrho_{\mu-1,\nu} - \varrho_{\mu,\nu+1})] . \quad (22.134) \\ \frac{d\tilde{a}}{dt} &= -\kappa \tilde{a} - \imath N U_0 \eta \sum_\nu \varrho_{\nu,\nu+1} \end{aligned}$$

These are the CARL equations for the density matrix. In 22.4.6.3 we show an alternative derivation obtained by directly inserting the adiabatically simplified Hamiltonian (22.26) into the Liouville equation (22.8).

We note, that  $\sum_\nu \varrho_{\nu,\nu+1}$  is the 'bunching' and that  $\varrho_{\mu,\nu}^* = \varrho_{\nu,\mu}$ . The average moment is given by  $\langle p \rangle = \sum_\nu \nu \varrho_{\nu,\nu}$ . In the Figs. 22.16 and 22.17 we show simulations in the semi-classical regimes  $\rho \gg 1$  in the 'bad-cavity' limit,  $\kappa > 1$ , and the 'good-cavity' limit  $\kappa \ll 1$ .

Here are some movies illustrating the quantum CARL dynamics, simulated using the momentum state expansion ([watch movie](#)) and ([watch movie](#)). The following dynamics were calculated via direct integration of the Schrödinger equation without momentum state expansion: Bloch oscillations ([watch movie](#)), CARL dynamics ([watch movie](#)), and joint Bloch and CARL dynamics ([watch movie](#)). See also ([watch talk](#)).

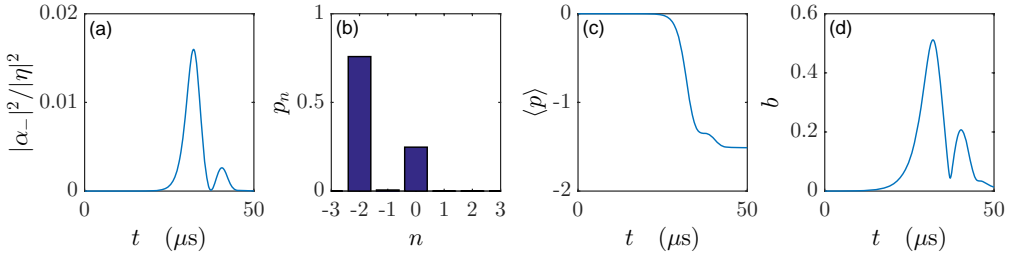


Figure 22.16: (code) Simulation of the CARL equation (22.131) in the superradiant, semi-classical, 'bad-cavity' regime for  $\kappa_c = 4$ ,  $\rho = 4$ ,  $\Delta_c = 0$ .

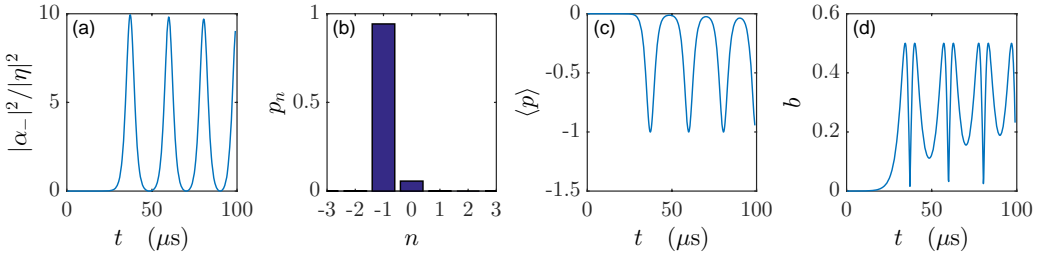


Figure 22.17: (code) Simulation of the CARL equation (22.131) in the superradiant, semi-classical, 'good-cavity' regime for  $\kappa_c = 0.02$ ,  $\rho = 4$ ,  $\Delta_c = 0$ .

### 22.4.5 Approximation for a bimodal momentum distribution

We observe that in the quantum regime the momentum distribution of the matter wave is bimodal, that is, only two momentum states are simultaneously populated. This justifies a simplification of the equations (22.134), assuming that at a given time, atoms must either be in a specific state  $|\mu\rangle_j$  or in a superposition of this state is an adjacent state  $|\mu - 1\rangle_j$ . Hence,

$$\begin{aligned} \frac{d\varrho_{\mu,\mu}}{dt} &= -iU_0\eta(\tilde{a}\varrho_{\mu,\mu-1} - \tilde{a}^\dagger\varrho_{\mu-1,\mu}) = -\frac{d\varrho_{\mu-1,\mu-1}}{dt} \\ \frac{d\varrho_{\mu-1,\mu}}{dt} &= -i[(2\mu - 1)\omega_r - \Delta_c]\varrho_{\mu-1,\mu} + iU_0\eta\tilde{a}(\varrho_{\mu,\mu} - \varrho_{\mu-1,\mu-1}) \\ \frac{d\tilde{a}}{dt} &= -iNU_\mu\eta\varrho_{\mu-1,\mu} - \kappa_c\tilde{a}. \end{aligned} \quad (22.135)$$

Introducing the coherence  $S_\mu = \varrho_{\mu-1,\mu}$  and the inversion  $W_\mu = \varrho_{\mu,\mu} - \varrho_{\mu-1,\mu-1}$  and postulating the normalization  $1 = \varrho_{\mu,\mu} + \varrho_{\mu-1,\mu-1}$ ,

$$\begin{aligned} \frac{dW_\mu}{dt} &= -2iU_0\eta(\tilde{a}S_\mu^* - \tilde{a}^\dagger S_\mu) \\ \frac{dS_\mu}{dt} &= -i[(2\mu - 1)\omega_r - \Delta_c]S_\mu + iU_0\eta\tilde{a}W_\mu \\ \frac{d\tilde{a}}{dt} &= -iNU_0\eta S_\mu - \kappa_c\tilde{a}. \end{aligned} \quad (22.136)$$

### 22.4.5.1 Linearization and stability analysis

We assume that the atoms are initially 'bunched' in a specific state  $|\mu\rangle_j$ . Only adjacent momentum states are coupled,

$$\begin{aligned}\frac{d\varrho_{\mu+1,\mu}}{dt} &= i[\omega_r(2\mu+1) - \Delta_c]\varrho_{\mu+1,\mu} + iU_0\eta\tilde{a}^\dagger(\varrho_{\mu,\mu} - \varrho_{\mu+1,\mu+1}) \\ \frac{d\varrho_{\mu-1,\mu}}{dt} &= -i[\omega_r(2\mu-1) - \Delta_c]\varrho_{\mu-1,\mu} + iU_0\eta\tilde{a}(\varrho_{\mu,\mu} - \varrho_{\mu-1,\mu-1}) \\ \frac{d\tilde{a}}{dt} &= -iNU_0\eta(\varrho_{\mu,\mu+1} + \varrho_{\mu-1,\mu}) - \kappa_c\tilde{a}.\end{aligned}\quad (22.137)$$

Conjugate the upper equation and build the sum and difference,  $B_\mu \equiv \varrho_{\mu,\mu+1} + \varrho_{\mu-1,\mu}$  and  $D_\mu \equiv \varrho_{\mu,\mu+1} - \varrho_{\mu-1,\mu}$ ,

$$\begin{aligned}\frac{dB_\mu}{dt} &= i(\Delta_c - 2\mu\omega_r)B_\mu - i\omega_\mu D_\mu + iU_0\eta\tilde{a}(\varrho_{\mu+1,\mu+1} - \varrho_{\mu-1,\mu-1}) \\ \frac{dD_\mu}{dt} &= i(\Delta_c - 2\mu\omega_r)D_\mu - i\omega_r B_\mu - 2iU_0\eta\tilde{a} + iU_0\eta\tilde{a}(\varrho_{\mu+1,\mu+1} - 2\varrho_{\mu,\mu} + \varrho_{\mu-1,\mu-1}) \\ \frac{d\tilde{a}}{dt} &= -iNU_0\eta B_\mu - \kappa_c\tilde{a}.\end{aligned}\quad (22.138)$$

Use  $\varrho_{\mu,\mu} \simeq 1$  and abbreviate  $\delta_\mu \equiv 2r\omega_\mu - \Delta_c$ ,

$$\begin{aligned}\frac{dB_\mu}{dt} &= -i\delta_\mu B_\mu - i\omega_r D_\mu \\ \frac{dD_\mu}{dt} &= -i\omega_r B_\mu - i\delta_r D_\mu - 2iU_0\eta\tilde{a} \\ \frac{d\tilde{a}}{dt} &= -iNU_0\eta B_\mu - \kappa_c\tilde{a}.\end{aligned}\quad (22.139)$$

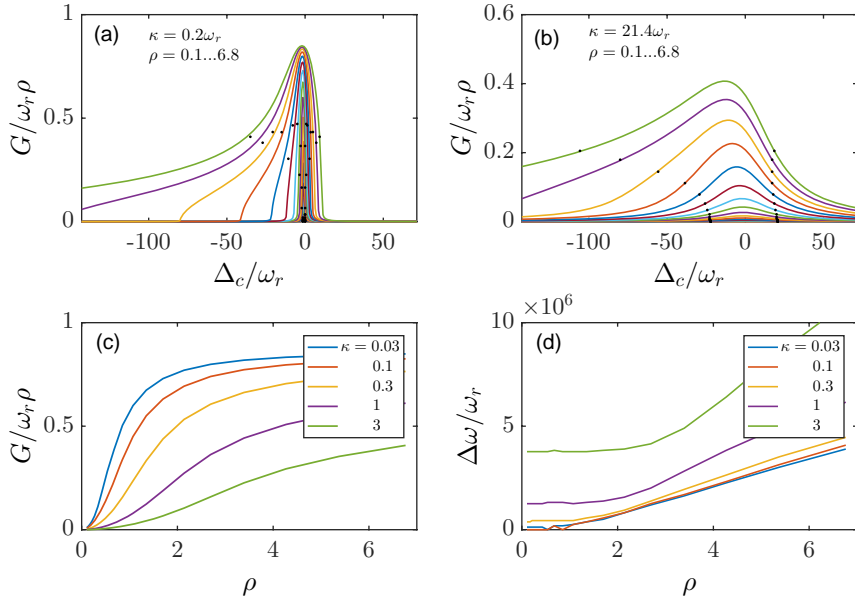
Seeking solution proportional to  $x \equiv \bar{x}e^{(\lambda - \delta_\mu)t}$ ,

$$\begin{aligned}i\lambda\bar{B}_\mu &= -i\omega_\mu\bar{D}_\mu \\ i\lambda\bar{D}_\mu &= -i\omega_r\bar{B}_\mu - 2iU_0\eta\bar{a} \\ i(\lambda - \delta_\mu)\bar{a} &= -iNU_0\eta\bar{B}_\mu - \kappa_c\bar{a}.\end{aligned}\quad (22.140)$$

Abbreviating  $\Lambda_m \equiv \delta_m + i\kappa_c$ , the characteristic equation is,

$$\det \begin{pmatrix} \lambda & \omega_r & 0 \\ \omega_r & \lambda & 2U_0\eta \\ NU_0\eta & 0 & \lambda - \Lambda_\mu \end{pmatrix} = \lambda^3 - \Lambda_\mu\lambda^2 - \omega_r^2\lambda + \omega_r^2\Lambda_\mu + 2NU_0^2\eta^2\omega_r = 0. \quad (22.141)$$

The gain is given by the imaginary part of  $\lambda$ . We have exponential amplification if  $\text{Im } \lambda < 0$ . Hence, we search for solution with the lowest imaginary value.

Figure 22.18: (code) Gain dependence on  $\rho$  and  $\kappa$ .

### 22.4.5.2 Universal scaling

To simplify the formulae simplify, we rescale them. We start from Eq. (22.134) and use the substitution for universal scaling,

$$\begin{aligned}
 \theta_j &\equiv 2kz_j & \text{and} & & \bar{p}_j &\equiv 2kv_j/\rho\omega_r & (22.142) \\
 \tau &\equiv \rho\omega_r t & \text{and} & & \kappa &\equiv \kappa_c/\omega_r \rho \\
 \bar{\lambda} &\equiv \lambda/\omega_r \rho & \text{and} & & \bar{\delta}_\mu &\equiv \delta_\mu/\omega_r \rho = 2\mu/\rho + \Delta_c/\omega_r \rho \\
 \bar{A} &\equiv (2/N\rho)^{1/2}\bar{a} & \text{and} & & \eta U_\mu &\equiv \sqrt{\rho^3\omega_r^2/2N} .
 \end{aligned}$$

This reproduces the Bonifacio notation,

$$\begin{aligned}
 \bar{\lambda}\bar{B}_\mu + \rho^{-1}\bar{D}_\mu &= 0 & (22.143) \\
 \bar{\lambda}\bar{D}_\mu + \rho^{-1}\bar{B}_\mu + \rho\bar{A} &= 0 \\
 (\bar{\lambda} - \bar{\delta}_\mu - \imath\kappa)\bar{A} + \bar{B}_\mu &= 0 .
 \end{aligned}$$

Skipping the bars, the characteristic equation reads,

$$\det \begin{pmatrix} \lambda & \rho^{-1} & 0 \\ \rho^{-1} & \lambda & \rho \\ 1 & 0 & \lambda - \delta_\mu - \imath\kappa \end{pmatrix} = (\lambda - \delta_\mu - \imath\kappa)(\lambda^2 - \rho^{-2}) + 1 = 0 . \quad (22.144)$$

Let us first discuss the semiclassical limit,  $\rho \gg 1$ . In the good-cavity regime,  $\kappa \simeq 0$ , we may neglect the recoil shift,  $2m\omega_r \rightarrow 0$ , so that  $\Lambda = \Delta_c$ . The gain is largest

when  $\Delta_c \rightarrow 0$ . The characteristic equation reduces to  $\lambda^3 = -1$ , yielding the solutions  $\lambda = 1, \frac{1}{2}(1 \pm i\sqrt{3})$ . Hence, the gain  $G = -\text{Im } \lambda$ , is

$$G = \frac{1}{2}\omega_r\rho\sqrt{3} \quad (22.145)$$

$$\Delta\omega_G \simeq \omega_r\rho \gg \kappa_c, \omega_r .$$

The gain bandwidth  $\Delta\omega_G$  being much larger than the recoil frequency, the Bragg condition for scattering between different momentum states is approximately fulfilled for a large number of initial momenta. I.e. although the momentum transfer is quantized,  $\Delta_c = n\omega_r$ , the atoms can be accelerated to high velocities. From Eq. (22.138)(a) we see  $|\bar{D}_\mu/\bar{B}_\mu| = \rho|\bar{\lambda}| \gg 1$ , i.e.  $\varrho_{\mu,\mu+1} \simeq \varrho_{\mu-1,\mu}$ .

In the superradiant regime,  $\kappa > 1$ , of the semiclassical limit the characteristic equation reduces to  $\lambda^2 = -i/\kappa$ , i.e.  $\lambda = \pm(1-i)/\sqrt{2\kappa}$ .<sup>15</sup> Hence, the gain is,

$$G = \frac{1}{2}\omega_r\rho\sqrt{2/\kappa} \quad (22.146)$$

$$\Delta\omega_G \simeq \kappa_c = \omega_r\rho\kappa \gg \omega_r .$$

In fact, the relative gain bandwidth is on the order of  $\Delta\omega_G/\omega_r \simeq \rho \propto (nNU_0^2)^{1/3}$ . Since recoil can be neglected we can have absorption or emission. The gain results from the difference between the average rates of both.

Now we turn to the quantum limit,  $\rho < 1$ . In the good-cavity regime,  $\kappa \simeq 0$ ,  $\lambda = \rho^{-1} + \frac{1}{2}(\delta_m - \rho^{-1}) - \frac{1}{2}\sqrt{(\delta_m - \rho^{-1})^2 - 2\rho}$ . Hence, the gain is,

$$G = \frac{1}{2}\omega_r\rho\text{Im} \sqrt{(\delta_m - \rho^{-1})^2 - 2\rho} \simeq \frac{1}{2}\omega_r\rho\sqrt{2\rho} \quad (22.147)$$

$$\Delta\omega_G = \omega_r\rho^{3/2} < \omega_r .$$

In fact, the relative gain bandwidth is on the order of  $\Delta\omega_G/\omega_r \simeq \rho^{3/2} \propto \sqrt{nNU_0^2}$ . Here recoil plays a role so that we have emission without absorption. Gain results exclusively from emission. From Eq. ((22.138)a) we see  $|\bar{D}_m/\bar{B}_m| = \rho|\bar{\lambda}| \simeq 1$ , i.e.  $\varrho_{m,m+1} \ll \varrho_{m-1,m}$ .

In the superradiant regime,  $\kappa > 1$ , of the quantum limit,  $\lambda = \rho^{-1} + \frac{\rho}{2}[(\delta_m - \rho^{-1}) + i\kappa]^{-1}$ . Hence,

$$G = \frac{1}{2}\omega_r\rho\frac{\rho\kappa}{(\delta_m - \rho^{-1})^2 + \kappa^2} \simeq \frac{1}{2}\frac{\omega_r\rho^2}{\kappa} \quad (22.148)$$

$$\Delta\omega_G = \kappa_c > \omega_r\rho .$$

The various regimes may be summarized in the following phase diagram. We will see later, that each region produces qualitatively different solutions of the full (non-linearized) equations.

<sup>15</sup>The assertion  $\text{Re } \lambda \ll \kappa$  used to simplify the characteristic equation is compatible with the solution.



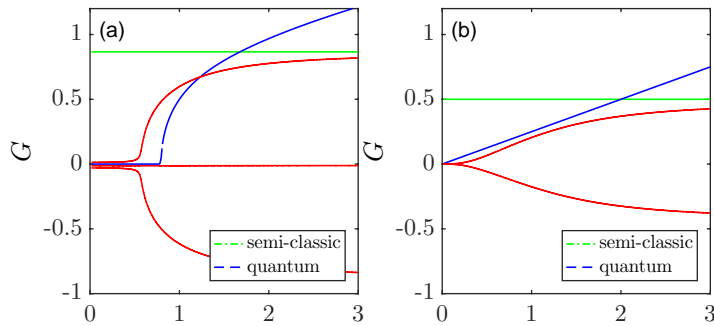


Figure 22.19: (code) Analytical approximations of the characteristic equation for the various regimes in the good-cavity limit  $\kappa = 0.03$  (a) and the superradiant limit  $\kappa = 2$  (b).

## 22.4.6 Exercises

### 22.4.6.1 Ex: Quantized CARL equations in the presence of a constant external force

- Generalize the quantized CARL equations (22.98), respectively, (22.112) for the presence of a constant external force.
- Now, we consider a unidirectionally pumped ring cavity, with the pump laser locked to a cavity mode, in the presence of an external periodic potential. Show that this system is equivalent to CARL in a ring cavity pumped from both sides.

### 22.4.6.2 Ex: Competition between CARL and Bloch oscillations

Reproduce the simulations of [601].

### 22.4.6.3 Ex: Alternative derivation of the Maxwell-Bloch with adiabatic elimination

Derive the directly from the Liouville equation (22.8) using the Hamiltonian (22.26) in adiabatic elimination.

### 22.4.6.4 Ex: Maxwell-Bloch equations without adiabatic elimination

Derive the Maxwell-Bloch equations for a three-level system coupled to a ring cavity without adiabatic elimination, but with quantized motion.

### 22.4.6.5 Ex: Linearized quantum CARL

Analyze the quantum CARL according to [552].

## 22.5 Quantized light interacting with atoms moving in cavities

*Cavity QED* has been studied extensively in the context of the Jaynes-Cummings model in Sec. 15.2 and of cooperative scattering in Sec. 20.2, however, without addressing the issue of atomic motion which, via photonic recoil, inevitably influences the dynamics. We also started a discussion on the role of photonic recoil in Sec. 18.3, which will be continued in the following sections in the context of ring cavities,

$$\begin{aligned}\dot{c}_{n_+, n_-, i} &= \frac{d}{dt} \langle \mathbf{r}, \alpha_+, \alpha_-, i | \psi(t) \rangle = \langle \mathbf{r}, \alpha_+, \alpha_-, i | \frac{-i}{\hbar} \hat{H} | \psi(t) \rangle \\ \dot{\alpha}_{\pm} &= \langle \psi(t) | \hat{a}_{\pm} | \psi(t) \rangle = \langle \psi(t) | \frac{i}{\hbar} [\hat{H}, \hat{a}_{\pm}] - \kappa \hat{a}_{\pm} | \psi(t) \rangle.\end{aligned}\quad (22.149)$$

Concretely, we will be using the Hamiltonian (22.26), obtained after adiabatic elimination of the excited state.

### 22.5.1 QED in ring cavities

Macroscopic high-finesse ring cavities interacting with a cloud of cold atoms allowed to enter the regime of strong collective coupling. However, new interesting aspects arise from the regime of strong coupling on the level of individual atoms.

Today's research projects on cold atoms in cavities are essentially divided into two classes, each class realizing an opposite regime: Cavity quantum electrodynamics (CQED) experiments as they are done by the groups of Rempe [417] and Kimble use microcavities having mode volumes so small that few photons give rise to macroscopic field strength. In such cavities the atom-field coupling is made to exceed all other decay rates. The other regime is that of cavity-cooling mainly investigated by Vuletic at the MIT and, in the case of ring cavities, of the collective atomic recoil laser (CARL) realized in the Tübingen research group. In this second regime the cavities are so large that the light fields can be considered as classical.

An interesting question is, whether the two regimes can be married to realize a system, where collective effects and entanglement between optical and atomic modes can be observed. The central idea is not to increase the coupling strength by reducing the mode volume, but to reduce the decay rates, in particular the natural linewidth of the atomic transition by choosing an atomic species that can be laser-cooled on a narrow intercombination line.

**Example 109 (CQED by reducing the ring cavity mode volume):** Technically a ring cavity design with  $(w, L, F) = (30 \mu\text{m}, 4 \text{ cm}, 200000)$  is feasible. This is enough to get below the critical atom number, but this is not sufficient to get into the CQED regime. Reducing  $\Gamma$  seems unavoidable. The isotope  $^{88}\text{Sr}$  possesses a narrow transition which can be used for optical cooling. The following table compares the various systems, i.e. a CQED example taken from Rempe, the macroscopic ring cavity with rubidium used in our Tübingen CARL experiments and a cavity tuned close to the strontium intercombination line.

experiment	Rempe, Rb	Tübingen, Rb	São Carlos, Sr
$\Gamma$	$(2\pi)6$ MHz	$(2\pi)6$ MHz	$(2\pi)7.6$ kHz
$F$	440000	80000	200000
$\kappa$	$(2\pi)0.7$ MHz	$(2\pi)22$ kHz	$(2\pi)19$ kHz
$w$	$29 \mu\text{m}$	$100 \mu\text{m}$	$30 \mu\text{m}$
$L$	$500 \mu\text{m}$	$8.5$ cm	$4$ cm
$g$	$(2\pi)4$ MHz	$(2\pi)88$ kHz	$(2\pi)13$ kHz
$N_{crit}$	0.5	34	1.6
$n_{sat}$	1.1	2312	0.16

With  $N = 10^4$  the cooperativity parameter  $N/N_{crit}$  is in all cases well above 1.

## 22.5.2 Description of quantized light fields in cavities

In order to calculate the evolution of photon distributions in the counter-propagating modes  $\hat{a}_{\pm}$  of a ring cavity, we develop CARL in a Fock basis. For simplicity, we first consider the *motion of a single atom as classical* and fixed (i.e. not as a degree of freedom), and we apply the adiabatic approximation. I.e. we have only two quantized degrees of freedom, which we organize like,

$$|\psi\rangle = |\nu\rangle_{\text{motion}} \otimes |i\rangle_{\text{electron}} \otimes |n\rangle_+ \otimes |n\rangle_- \rightarrow |n_+, n_-\rangle, \quad (22.150)$$

Expanding the fields into Fock states,

$$|\psi\rangle = \sum_{n_+, n_-} c_{n_+, n_-} |n_+, n_-\rangle, \quad (22.151)$$

the field operators and the density matrix read,

$$\begin{aligned} \hat{a}_+ &= \sum_{n_+} \sqrt{n_+} |n_+ - 1\rangle \langle n_+| \otimes \mathbb{I} = \sum_{n_+, n_-} \sqrt{n_+} |n_+ - 1, n_-\rangle \langle n_+, n_-| \\ \hat{a}_- &= \mathbb{I} \otimes \sum_{n_-} \sqrt{n_-} |n_- - 1\rangle \langle n_-| = \sum_{n_+, n_-} \sqrt{n_-} |n_+, n_- - 1\rangle \langle n_+, n_-| \\ \hat{\rho} &= |\psi\rangle \langle \psi| = \sum_{m_+, m_-, n_+, n_-} c_{m_+, m_-}^* c_{n_+, n_-} |m_+, m_-\rangle \langle n_+, n_-|. \end{aligned} \quad (22.152)$$

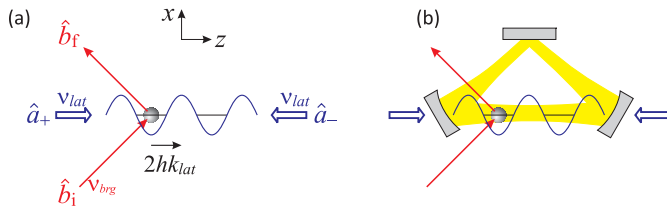


Figure 22.20: (a) Bragg scattering at a 1D optical lattice. (b) Same as in (a), but now the optical lattice is generated by the mode of an optical ring cavity.

Note that the master equation using the Lindblad operator traces over the reservoir. Hence, the master equation only treats the cavity modes, but does not allow predictions on the quantum behavior of outcoupled fields. In order to describe e.g. quantum correlations in output field, one needs an input-output theory [147, 258].

In the case of classical motion quantum light fields,

$$\begin{aligned}
\dot{c}_{n_+,n_-} &= i(\Delta_c - U_0)(n_+ + n_-) c_{n_+,n_-} \\
&- iU_0 \left( e^{-2ikz} \sqrt{n_+(n_- + 1)} c_{n_+-1,n_-+1} - e^{2ikz} \sqrt{(n_+ + 1)n_-} c_{n_++1,n_- -1} \right) \\
&- \eta_+ \left( \sqrt{n_+ + 1} c_{n_++1,n_-} - \sqrt{n_+} c_{n_+-1,n_-} \right) \\
&- \eta_- \left( \sqrt{n_- + 1} c_{n_+,n_-+1} - \sqrt{n_-} c_{n_+,n_- -1} \right) \\
\dot{z} &= 2i\hbar k U_0 \sum_{n_+,n_-} \left( e^{-2ikz} \sqrt{(n_+ + 1)n_-} c_{n_++1,n_- -1}^* c_{n_+,n_-} \right. \\
&\quad \left. - e^{2ikz} \sqrt{n_+(n_- + 1)} c_{n_+-1,n_-+1}^* c_{n_+,n_-} \right)
\end{aligned}
\tag{22.153}$$

### 22.5.3 Photon backscattering for fixed atomic position

To tackle the problem of quantized light field we first assume an atom fixed in space, that is, we completely *disregard the motional degree of freedom* by setting  $\hat{p} = 0$  and restricting to the Hamiltonian,

$$\hat{H} = \sum_{\pm} \omega_{\pm} \hat{a}_{\pm}^{\dagger} \hat{a}_{\pm} - \eta_{\pm} (\hat{a}_{\pm} - \hat{a}_{\pm}^{\dagger}) + U_0 (\hat{a}_+^{\dagger} \hat{a}_- e^{-2ik\hat{z}} + \hat{a}_+^{\dagger} \hat{a}_+ e^{2ik\hat{z}}). \tag{22.154}$$

In Exc. 22.5.7.1 we show how to cast the Hamiltonian into a matrix form using an appropriate basis already used in the discussion of the beam splitter in the photon representation in Sec. 15.6.1.

In Exc. 22.5.7.2(a) we derive the equations of motion for the components  $c_{n_+,n_-}$  of the state vector from the Schrödinger equation cavity decay. In Exc. 22.5.7.3(a) we derive the equations of motion for the components  $\rho_{m_+,n_+;m_-,n_-} = \langle m_+, m_- | \hat{\rho} | n_+, n_- \rangle$  of the density operator. Simulations performed based on these equations of motion are shown in Fig. 22.21).

The simulations reveal a number of interesting facts:

- The field amplitudes  $|\alpha_{\pm}|^2$  execute oscillations due to CARL coupling, but with preserved Poissonian shape of the photon number distributions.
- When simulations are done with initial Fock states, they eventually relax to a Glauber state.
- The mean photon numbers and the atomic coordinates evolve in a continuous way.

These observations are not surprising, once we understood the backscattering as a linear coupling between the modes being mediated by a beam splitter Hamiltonian

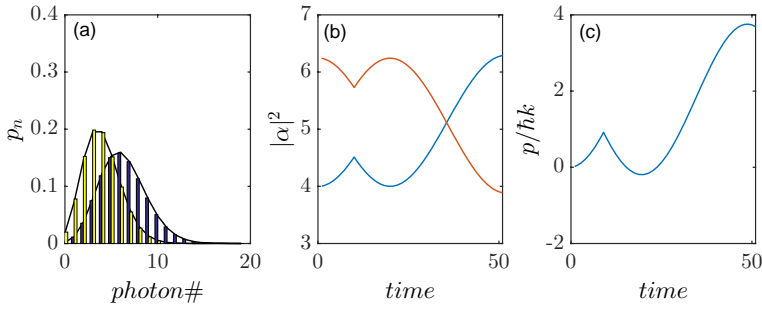


Figure 22.21: (code) Time-evolution of CARL with one classical atom and two quantized field modes. (a) Photon number distributions of two modes after some evolution time  $t$ . (b) Time-evolution of the mean photon number; at time  $t = 10$ , the atom is suddenly displaced. (c) Time-evolution of the (classical) atomic trajectory.

of type (15.198)<sup>16</sup>,

$$\hat{H}_{int} = U_0(\hat{a}_+^\dagger \hat{a}_- e^{-2ikz} + \hat{a}_+ \hat{a}_-^\dagger e^{2ikz}), \quad (22.155)$$

for which we found the relationship (15.199),

$$e^{-i\hat{H}_{int}t} \hat{a}_\pm e^{i\hat{H}_{int}t} = \hat{a}_\pm \cos U_0 t \pm \hat{a}_\mp e^{\mp 2ikz} \sin U_0 t. \quad (22.156)$$

This means, that we expect (for a fixed location  $z$  of the atom) an oscillatory behavior of the field amplitudes  $|\alpha_\pm|^2$  and also of the phase (encoded in  $\alpha_\pm^* \alpha_\pm$ ), but no modification of the coherent photon statistics. On the contrary, as shown in Sec. 15.6.1, a beam splitter tends to transform sub-Poissonian states into Poissonian ones. In fact, *CARL is nothing else than a movable beam splitter*.

Non-linearity may come into play, if photonic recoil is included, i.e. if the *atomic motion itself becomes a degree of freedom*. This is the next step of our problem, that needs to be solved.

#### 22.5.4 Quantized light fields and quantized recoil

The simulations of the preceding section show that the CARL Hamiltonian (22.155), despite the appearance of photon creation and annihilation operator, does not request recoil to be quantized: If an arbitrary momentum kick of the atom can be absorbed by the light fields, then an arbitrary dipole force can be transmitted to the atomic momentum! The momentum conservation law (22.17) does not imply quantization of

<sup>16</sup>Which itself represents a generalized displacement operator,

$$\hat{H}_{int} \simeq U_0(\alpha_+^* e^{-2ikz} \hat{a}_- + \alpha_+ e^{2ikz} \hat{a}_-^\dagger) \equiv i\hbar\beta^* \hat{a}_- - i\hbar\beta \hat{a}_-^\dagger,$$

since defining  $\beta \equiv \frac{iU_0}{\hbar} \alpha_+ e^{2ikz}$ , we find,

$$B(\beta t) = e^{-i\hat{H}_{int}t/\hbar} = e^{\beta^* t \hat{a}_- - \beta t \hat{a}_-^\dagger}.$$

photonic recoil. The question is now, how to conceal this fact with the observation of discrete momentum sidemodes [640]. We have seen earlier, that the quantization of the motion is transferred from the quantized photon fields via the operator (22.101) to the atom: An initially resting atom can only adopt motional states with momenta equal to a multiple of  $2\hbar k$ .

We will now take the quantization of the atomic momentum for granted and study quantized light modes coupled by *recoiling atoms*, we extend our Hilbert space like,

$$|\psi\rangle = |\nu\rangle_{\text{motion}} \otimes |i\rangle_{\text{electron}} \xrightarrow{\text{adiab.elim.}} \otimes |n\rangle_+ \otimes |n\rangle_- \rightarrow |\nu, n_+, n_-\rangle, \quad (22.157)$$

Expanding the motion and fields <sup>17</sup>,

$$|\psi\rangle = \sum_{\nu, n_+, n_-} c_{\nu, n_+, n_-} |\nu, n_+, n_-\rangle, \quad (22.158)$$

the momentum kick operator reads,

$$e^{-2\mathbf{a}k\hat{z}} \otimes \mathbb{I} \otimes \mathbb{I} = \sum_{\nu} |\nu\hbar k - 2\hbar k, n_+, n_-\rangle \langle \nu\hbar k, n_+, n_-|. \quad (22.159)$$

The equations of motions derived in Exc. 22.5.7.2 from the Schrödinger equation are now generalized to,

$$\begin{aligned} \dot{c}_{\nu, n_+, n_-} &= i(\Delta_c - U_0)(n_+ + n_-)c_{\nu, n_+, n_-} \\ &- iU_0 \left( \sqrt{n_+(n_- + 1)}c_{\nu-1, n_+-1, n_-+1} - \sqrt{(n_+ + 1)n_-}c_{\nu+1, n_++1, n_- - 1} \right) \\ &- \eta_+ (\sqrt{n_+ + 1}c_{\nu, n_++1, n_-} + \sqrt{n_+}c_{\nu, n_+-1, n_-}) \\ &- \eta_- (\sqrt{n_- + 1}c_{\nu, n_+, n_-+1} + \sqrt{n_-}c_{\nu, n_+, n_- - 1}) \end{aligned} \quad (22.160)$$

Note that the general shape of fully quantized Schrödinger equations looks like,

$$\dot{c}_{\nu', n'_+, n'_-} = \begin{pmatrix} \ddots & & \vdots \\ \cdots & \mathcal{B}_{\{\nu', n'_+, n'_-\}; \{\nu, n_+, n_-\}} & \cdots \\ & & \ddots \end{pmatrix} c_{\nu, n_+, n_-} \quad (22.161)$$

and for fully quantized master equations,

$$\begin{aligned} \dot{\rho}_{\{\mu', m'_+, m'_-\}; \{\nu', n'_+, n'_-\}} & \\ = \begin{pmatrix} \ddots & & \vdots \\ \cdots & \mathcal{L}_{\{\mu', m'_+, m'_-\}; \{\nu', n'_+, n'_-\}; \{\mu, m_+, m_-\}; \{\nu, n_+, n_-\}} & \cdots \\ & & \ddots \end{pmatrix} \rho_{\{\mu, m_+, m_-\}; \{\nu, n_+, n_-\}} \cdot \end{aligned} \quad (22.162)$$

<sup>17</sup>Note the fact, which is important for computation, that the dimension of the Hilbert space increases a lot, that is like  $\dim \nu \cdot \dim n_+ \cdot \dim n_-$ , where  $\nu, n_{\pm}$  are the numbers of states considered.

However, the mere inclusion of a third degree of freedom coupled to the other two degrees in the same linear fashion will modify the behavior of the system, which will continue to oscillate as it did before, now just involving the atomic motion in this dynamics. This behavior can only change, when we additionally consider the force equation,

$$\dot{\hat{p}} = 2\hbar k U_0 (\hat{a}_+^\dagger \hat{a}_- e^{-2ikz} - \hat{a}_+ \hat{a}_-^\dagger e^{2ikz}) , \quad (22.163)$$

which will lead to feedback. Inserting the expansion (22.158),

$$\dot{c}_{\nu, n_+, n_-} = 2\hbar k U_0 \left( c_{\nu, n_+, n_-} \sqrt{n_+(n_- + 1)} - c_{\nu, n_+, n_-} \sqrt{n_+(n_- + 1)} \right) . \quad (22.164)$$

Note that, in contrast to CARL equations, the fully quantized equations (22.160) are *linear*. That is, it is the 'classization'<sup>18</sup> of the degrees of freedom which introduces the non-linearities, which are typical for CARL, e.g. the feedback introduced by classical light fields. The process of 'classization' corresponds to *tracing* over degrees of freedom, which we want to treat classically and thus remove from the Hamiltonian.

#### 22.5.4.1 Calculation of observables

Once the time evolution of the coefficients  $c_{\nu, n_+, n_-}(t)$  has been determined by solving the differential equation (22.160) we can calculate the observables in the following way. The probability distribution for photon numbers in the mode  $\alpha_+$  is given by,

$$\begin{aligned} P_{n_+}(t) &= \langle \psi(t) | \mathbb{I} \otimes |n_+\rangle \langle n_+| \otimes \mathbb{I} | \psi(t) \rangle \\ &= \sum_{\nu, n_-} \langle \nu, n_+, n_- | \nu, n_+, n_- \rangle = \sum_{\nu, n_-} |c_{\nu, n_+, n_-}(t)|^2 , \end{aligned} \quad (22.165)$$

the mean photon number by,

$$\langle \hat{n}_+(t) \rangle = |\alpha_+(t)|^2 = \sum_{n_+} n_+ P_{n_+}(t) = \sum_{\nu, n_+, n_-} n_+ |c_{\nu, n_+, n_-}(t)|^2 , \quad (22.166)$$

and similarly for  $\alpha_-$ . The probability distribution for momentum states is given by,

$$P_\nu(t) = \sum_{n_+, n_-} |c_{\nu, n_+, n_-}(t)|^2 , \quad (22.167)$$

the mean momentum by,

$$\langle \hat{p}(t) \rangle = \sum_{\nu, n_+, n_-} \nu \hbar k |c_{\nu, n_+, n_-}(t)|^2 , \quad (22.168)$$

the mechanical kinetic energy by,

$$\begin{aligned} E_{kin}(t) &= \frac{\langle \hat{p}^2 \rangle}{2m} = \sum_{\nu, n_+, n_-} \frac{(\nu \hbar k)^2}{2m} |c_{\nu, n_+, n_-}(t)|^2 \\ &= \sum_{\nu, n_+, n_-} \nu^2 \hbar \omega_{rec} |c_{\nu, n_+, n_-}(t)|^2 , \end{aligned} \quad (22.169)$$

---

<sup>18</sup>As opposed to the term quantization.

and the potential energy by,

$$\begin{aligned}
 E_{pot}(t) &= \hbar U_0 \langle e^{-2ik\hat{z}} \hat{a}_+^\dagger \hat{a}_- + e^{2ik\hat{z}} \hat{a}_+ \hat{a}_-^\dagger \rangle \\
 &= \hbar U_0 \sum_{\nu, n_+, n_-} \left( c_{\nu+1, n_++1, n_- -1}^* c_{\nu, n_+, n_-} \sqrt{(n_+ + 1)n_-} \right. \\
 &\quad \left. + c_{\nu-1, n_+-1, n_- +1}^* c_{\nu, n_+, n_-} \sqrt{n_+(n_- + 1)} \right) .
 \end{aligned} \tag{22.170}$$

With this we can check conservation of the total photon number,

$$\langle \hat{n}_+(t) \rangle + \langle \hat{n}_-(t) \rangle = const , \tag{22.171}$$

of the mechanical energy,

$$E_{kin}(t) + E_{pot}(t) = const , \tag{22.172}$$

and of total linear momentum,

$$\hbar k [\langle \hat{n}_+(t) \rangle - \langle \hat{n}_-(t) \rangle] - \langle \hat{p}(t) \rangle = const . \tag{22.173}$$

#### 22.5.4.2 Master equation for CQED with atomic recoil in the adiabatic approximation

Using the Hamiltonian (22.26) or (22.96), the expansion of the recoil operator (22.101), the expansion of the photon field operators (22.152), and the matrix representation of the density operator (14.16), that is,

$$\hat{\rho} = \sum_{\mu, \nu; m_+, n_+; m_-, n_-} |\mu, m_+, m_-\rangle \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \langle \nu, n_+, n_- | , \tag{22.174}$$

the master equation (22.8) becomes,

$$\boxed{\langle \mu, m_+, m_- | \dot{\hat{\rho}} | \nu, n_+, n_- \rangle = -i \langle \mu, m_+, m_- | [\hat{H}, \hat{\rho}] | \nu, n_+, n_- \rangle + \mathcal{L}_{cavity-vac, \pm \hat{\rho}} } , \tag{22.175}$$



with the coherent contributions,

$$\begin{aligned}
\langle \mu, m_+, m_- | [\frac{\hat{p}^2}{2m}, \hat{\rho}] | \nu, n_+, n_- \rangle &= \omega_{rec}(\mu^2 - \nu^2) \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \\
\langle \mu, m_+, m_- | [(U_0 - \Delta_c) \hat{a}_\pm^\dagger \hat{a}_\pm, \hat{\rho}] | \nu, n_+, n_- \rangle &= (U_0 - \Delta_c) n_\pm \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \\
\langle \mu, m_+, m_- | [-\eta_+ (\hat{a}_+ - \hat{a}_+^\dagger), \hat{\rho}] | \nu, n_+, n_- \rangle \\
&= -\eta_+ \left( \sqrt{m_+} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} - \sqrt{m_+ + 1} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \right. \\
&\quad \left. + \sqrt{n_+} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} - \sqrt{n_+ + 1} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \right) \\
\langle \mu, m_+, m_- | [-\eta_- (\hat{a}_- - \hat{a}_-^\dagger), \hat{\rho}] | \nu, n_+, n_- \rangle \\
&= -\eta_- \left( \sqrt{m_-} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} - \sqrt{m_- + 1} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \right. \\
&\quad \left. + \sqrt{n_-} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} - \sqrt{n_- + 1} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \right) \\
\langle \mu, m_+, m_- | [U_0 e^{-2ik\hat{z}} \hat{a}_+^\dagger \hat{a}_-, \hat{\rho}] | \nu, n_+, n_- \rangle \\
&= U_0 \left( \sqrt{m_+ (m_+ + 1)} \rho_{\mu+1, \nu; m_+, n_+; m_-, n_-} + \sqrt{(m_+ + 1) m_-} \rho_{\mu-1, \nu; m_+, n_+; m_-, n_-} \right) \\
\langle \mu, m_+, m_- | [U_0 e^{2ik\hat{z}} \hat{a}_+ \hat{a}_-^\dagger, \hat{\rho}] | \nu, n_+, n_- \rangle \\
&= U_0 \left( \sqrt{(n_+ + 1) n_-} \rho_{\mu, \nu-1; m_+, n_+; m_-, n_-} + \sqrt{n_+ (n_- + 1)} \rho_{\mu, \nu+1; m_+, n_+; m_-, n_-} \right),
\end{aligned} \tag{22.176}$$

and the incoherent contributions,

$$\begin{aligned}
\langle \mu, m_+, m_- | -\kappa [\hat{a}_+^\dagger \hat{a}_+ \hat{\rho} - 2\hat{a}_+ \hat{\rho} \hat{a}_+^\dagger + \hat{\rho} \hat{a}_+^\dagger \hat{a}_+] | \nu, n_+, n_- \rangle \\
&= -\kappa \left( m_+ \rho_{\mu, \nu; m_+, n_+; m_-, n_-} + n_+ \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \right. \\
&\quad \left. - 2\sqrt{(m_+ + 1)(n_+ + 1)} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \right) \\
\langle \mu, m_+, m_- | -\kappa [\hat{a}_-^\dagger \hat{a}_- \hat{\rho} - 2\hat{a}_- \hat{\rho} \hat{a}_-^\dagger + \hat{\rho} \hat{a}_-^\dagger \hat{a}_-] | \nu, n_+, n_- \rangle \\
&= -\kappa \left( m_- \rho_{\mu, \nu; m_+, n_+; m_-, n_-} + n_- \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \right. \\
&\quad \left. - 2\sqrt{(m_- + 1)(n_- + 1)} \rho_{\mu, \nu; m_+, n_+; m_-, n_-} \right).
\end{aligned} \tag{22.177}$$

### 22.5.5 Kicking and forcing an atom in a ring cavity

The question we want to elucidate here is, how a coupled atom-ring cavity system reacts to a kick transferring an arbitrary amount of momentum to the atom. We studied a similar question when studying the kicking of a harmonic oscillator in Sec. 3.6.2, however, the situation is quite different now because, in contrast to the harmonic oscillator, the motion of an atom subject to CARL dynamics is not localized and, hence, *not quantized*. That is, an arbitrarily kicked atom is not bound to join one of those momentum states it would populate when kicked by photonic recoil. Hence, a momentum state expansion like (22.105) is not appropriate, so that we have to go a step back and consider the Hamiltonian (22.26) again. See also (watch talk).

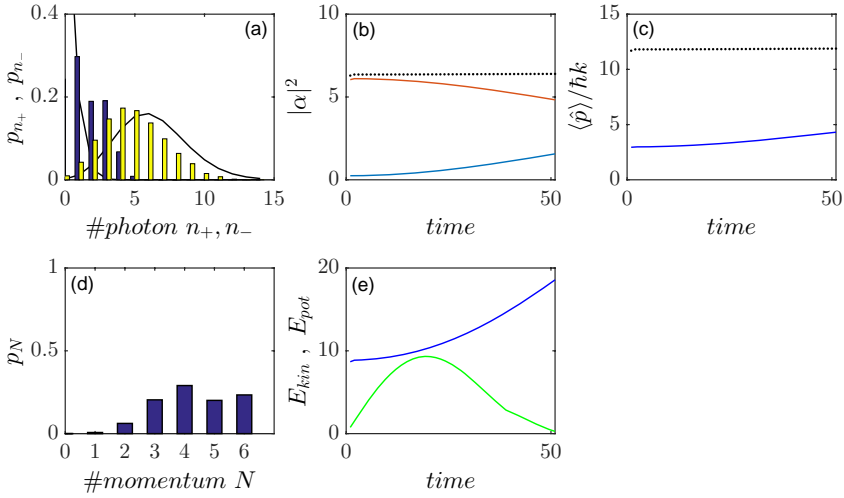


Figure 22.22: (code) Time-evolution of CARL with one classical atom and two quantized field modes. (a) Photon number distributions of two modes after some evolution time  $t$ . (b) Time-evolution of the mean photon number; at time  $t = 10$ , the atom is suddenly displaced. (c) Time-evolution of the (classical) atomic trajectory.

### 22.5.5.1 Kicking

Let us first describe the kick as an incoherent disruptive one time event transforming operators, the Hamiltonian and the system's state like,

$$\hat{A} \longrightarrow e^{-iq\hat{z}} \hat{A} e^{iq\hat{z}} \quad , \quad |\psi\rangle \longrightarrow e^{iq\hat{z}} |\psi\rangle \quad (22.178)$$

and in particular,

$$\hat{H} \longrightarrow e^{-iq\hat{z}} \hat{H} e^{iq\hat{z}} = \hat{H}(\hat{z}, \hat{p} - \hbar q) \quad , \quad \langle p|\psi\rangle \longrightarrow \langle p|e^{iq\hat{z}}|\psi\rangle = \langle p - \hbar q|\psi\rangle . \quad (22.179)$$

The Schrödinger equation tells us the system's evolution after the kick,

$$i\hbar \frac{d}{dt} \langle p|\psi\rangle = \frac{p^2}{2m} \langle p|\psi\rangle + U_0 \left( \langle p|e^{-2ik\hat{z}}|\psi\rangle \hat{a}_+^\dagger \hat{a}_- + \langle p|e^{2ik\hat{z}}|\psi\rangle \hat{a}_+ \hat{a}_-^\dagger \right) . \quad (22.180)$$

We remind that this equations contains CARL feedback via the simultaneous presence of  $\hat{z}$  and  $\hat{p}$ . If we want to disregard the CARL force (assuming, for example, that the motion is totally imposed by an external force, as done in Sec. 20.2.5 in order to focus on the behavior of the light fields), we must not project the Schrödinger equation on  $\langle p|$  but treat the motional degree of freedom as classical.

### 22.5.5.2 Forcing

Let us now describe the kick as a force  $F(t) = mg\theta(t)$  being switched on at a given time, but being constant afterward,

$$\hat{H} = \frac{\hat{p}^2}{2m} + U_0 \left( e^{-2ik\hat{z}} \hat{a}_+^\dagger \hat{a}_- + e^{2ik\hat{z}} \hat{a}_+ \hat{a}_-^\dagger \right) + mg\hat{z} . \quad (22.181)$$

We note that with (2.153) the Hamiltonian transformed into the accelerated frame reads,

$$\begin{aligned} \hat{H} &\longrightarrow e^{-img\hat{z}t/\hbar} \hat{H} e^{img\hat{z}t/\hbar} + i\hbar \left( \frac{d}{dt} e^{img\hat{z}t/\hbar} \right)^\dagger e^{img\hat{z}t/\hbar} = \hat{H}(\hat{z}, \hat{p} - mgt) - mg\hat{z} \\ &= \frac{(\hat{p} - mgt)^2}{2m} + U_0 \left( e^{-2ik\hat{z}} \hat{a}_+^\dagger \hat{a}_- + e^{2ik\hat{z}} \hat{a}_+ \hat{a}_-^\dagger \right). \end{aligned} \quad (22.182)$$

The Schrödinger equation for the transformed wavefunction  $|\psi\rangle = |\tilde{\psi}\rangle e^{img\hat{z}t/\hbar}$ , which tells us the system's evolution during the force,

$$i\hbar \frac{d}{dt} \langle p | \tilde{\psi} \rangle = \frac{(p - mgt)^2}{2m} \langle p | \tilde{\psi} \rangle + U_0 \left( \langle p | e^{-2ik\hat{z}} | \tilde{\psi} \rangle \hat{a}_+^\dagger \hat{a}_- + \langle p | e^{2ik\hat{z}} | \tilde{\psi} \rangle \hat{a}_+ \hat{a}_-^\dagger \right), \quad (22.183)$$

has a similar shape to Eq. (22.180).

### 22.5.5.3 Vibrating

Another option might be to additionally confine the atom in a harmonic potential [741],

$$\begin{aligned} \hat{H} &= \frac{\hat{p}^2}{2m} + U_0 \left( e^{-2ik\hat{z}} \hat{a}_+^\dagger \hat{a}_- + e^{2ik\hat{z}} \hat{a}_+ \hat{a}_-^\dagger \right) + \frac{m}{2} \omega^2 \hat{z}^2 \\ &= \hbar\omega \left( \hat{A}^\dagger \hat{A} + \frac{1}{2} \right) + U_0 \left[ D^\dagger(\alpha) \hat{a}_+^\dagger \hat{a}_- + D(\alpha) \hat{a}_+ \hat{a}_-^\dagger \right], \end{aligned} \quad (22.184)$$

where  $D(\alpha) \equiv e^{\alpha \hat{A}^\dagger - \alpha^* \hat{A}}$  with  $\alpha \equiv \frac{2ik a_{ho}}{\sqrt{2}}$ .

### 22.5.5.4 Quantized equations of motion

In both cases, 'kicking' and 'forcing', we may discretize momentum space, although in the latter case we need to transform back into the lab frame after having solved the Schrödinger equation (22.160).

## 22.5.6 Quantum correlations

Superradiant or CARL scattering exist due to a correlation of subsequent scattering events. In the quantum regime, the emergence of quantum correlations, such as entanglement and squeezing is to be expected as a consequence of CARL dynamics [499, 550, 565, 557, 558, 694, 144, 145, 146]. The advantage of doing CARL with BECs is the possibility to exploit the instability in the good-cavity regime to parametrically amplify optical and matter waves, manipulate matter wave coherence properties and generate entanglement.

For the description of the dynamics of the fields, i.e. the momentum sidemodes and the cavity modes, a first-quantized treatment of the atomic motion [552] would be sufficient. All information can be extracted from a numerical simulation of the quantum CARL equations. However, here we are also interested in quantum correlations. Hence, in a first-quantized treatment of the atomic motion, the coefficients  $\hat{c}_n$  must be treated as field operators. Alternatively, we derive the basic equations rigorously from a second-quantized treatment.

### 22.5.6.1 Generation of squeezing and entanglement via CARL

An experiment by [568] produces squeezing in transmission of a cavity resonantly interacting with single atoms. The effect was induced by vacuum Rabi-splitting. In our case we have a ring cavity, we operate far from equilibrium, we have classical Stark splitting. Hence, we may expect squeezing and entanglement from the CARL dynamics.

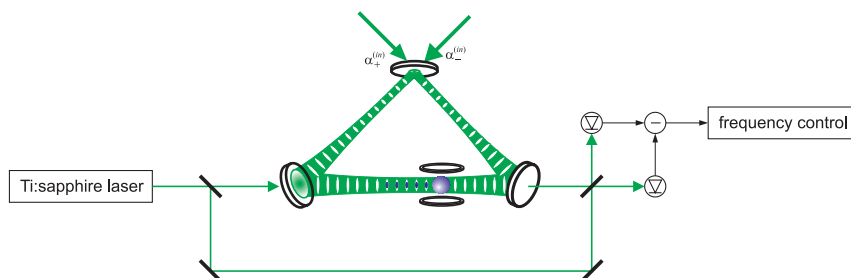


Figure 22.23: Production and detection of squeezing.

Differences between entanglement and correlation (correlations involve time or space coordinates  $g(\tau)$ , particles correlate across space and time, coherence).

Bragg scattering of light at an atomic grating (or simply the splitting of light at a beam splitter) is an irreversible process (see Sec. 15.6). CARL can be interpreted in terms of Bragg scattering of light at an atomic grating, which is generated itself by the Bragg scattering. Hence, the scattering of early photons influences the scattering of late photons, i.e. the scattering processes get correlated, the dynamics gets a history. The correlation between subsequent scattering processes is what preserves the coherence in CARL and superradiant Rayleigh scattering.

It is now interesting to ask how this classical correlations will behave in the quantum regime, i.e. upon 1. quantization of the motion of individual atoms and upon 2. quantization of atomic particle field. Following [499, 498, 501, 500, 550, 551, 557, 558], non-classical correlations such as entanglement of matter wave modes, and entanglement between matter-wave and optical modes is expected.

### 22.5.6.2 Quantum non demolition measurements with CARL

According to [558], a ring cavity could lend itself to quantum non demolition measurements. They consider our ring cavity being pumped from both sides through an incoupling mirror. A so-called pump mode is injected with a  $p$ -polarized light field, and a probe mode with a  $s$ -polarized light field. The light of the probe mode leaking through a mirror gives information about the atoms (e.g. via the refraction index). The counterpropagating pump light gives access to higher-order moments of the atom distribution.

The problem is that the effect is based on photon exchange between the modes, and those are orthogonally polarized. Even more problematic is that, in practice, the modes have different frequencies. Other work on this subject has been done by [36, 221, 473, 474, 128].

## 22.5.7 Exercises

### 22.5.7.1 Ex: Analogy between CARL and two-atom Dicke states

a. Write the Hamiltonian (22.154) in matrix form using the basis,

$$\psi_k = \{|0, 0\rangle, |0, 1\rangle, |1, 0\rangle, |0, 2\rangle, |1, 1\rangle, |2, 0\rangle, \dots\}.$$

b. Now restrict to the finite number of states  $\psi_k = \{|0, 0\rangle, |0, 1\rangle, |1, 0\rangle, |1, 1\rangle\}$  and discuss the analogy between CARL and two-atom Dicke states.

### 22.5.7.2 Ex: Cavity QED with Schrödinger equation

Assume a symmetrically pumped ring cavity in equilibrium with an atom at a fixed position.

a. Derive the equations of motion for the components for the probability amplitudes in a Fock state basis.

b. Express the possible initial states  $|\alpha_+, \alpha_-\rangle$ ,  $|\alpha_+, n_-\rangle$ , and  $|n_+, n_-\rangle$  in the Fock state basis. How to calculate the photon distribution  $p_{n_+}$ , the amplitudes of field modes  $\alpha_{\pm}$ , and the atom's position and momentum at later times of the evolution?

### 22.5.7.3 Ex: Cavity QED with density matrix

Assume a symmetrically pumped ring cavity in equilibrium with an atom at a fixed position.

a. Derive the equations of motion for the components of the density operator.

b. Write down the density operator describing two decoupled Glauber states? How to retrieve the Fock state populations from the density operator?

c. Now, assume that the atom can move. What will be the evolution of the motional state?

### 22.5.7.4 Ex: Photon number and momentum conservation

a. Calculate the evolution under CARL interaction,  $e^{-i\hat{H}_{carl}t}\hat{n}_{\pm}e^{i\hat{H}_{carl}t}$ , of the photon numbers in each mode and show that the total photon number is conserved.

b. Assuming conservation of total momentum calculate the evolution of the atomic momentum.

### 22.5.7.5 Ex: Self-synchronization of Bloch oscillations

Study the Bloch-CARL dynamics for the case of a sinusoidally modulated CARL pump light intensity. Choose as the modulation frequency the expected Bloch oscillation frequency and a variable phase delay.

## 22.6 Further reading

J. Guo et al., *Recoil-induced Resonances in Non-linear Spectroscopy* [DOI]

J.-Y. Courtois et al., *Recoil-induced Resonances in Cesium: An Atomic Analog to the Free Electron Laser* [DOI]

- P. R. Hemmer et al., *Self-Organization, Broken Symmetry, and Lasing in an Atomic Vapor: The Interdependence of Gratings and Gain* [DOI]
- G.-L. Lippi et al., *Spontaneous Generation of a Longitudinal Atomic Density Grating in Sodium Vapor* [DOI]
- D.R. Meacher et al., *Method for Velocimetry of Cold Atoms* [DOI]
- P. Verkerk et al., *Comment on "Spontaneous Generation of a Longitudinal Atomic Density Grating in Sodium Vapor"* [DOI]
- S. Barbay et al., *Pump-probe spectroscopy of the sodium D line and the question of recoil-induced gratings in hot vapors* [DOI]
- P.R. Berman, *Comparison of recoil-induced resonances and the collective atomic recoil laser* [DOI]
- M. Vengalattore et al., *Optical bistability at low light level due to collective atomic recoil* [DOI]
- V. Vuletic et al., *Three-dimensional cavity Doppler cooling and cavity sideband cooling by coherent scattering* [DOI]
- M. Gangl et al., *Cold atoms in a high-Q ring cavity* [DOI]
- S. Ostermann et al., *Atomic self-ordering in a ring cavity with counterpropagating pump fields* [DOI]
- S.C. Schuster et al., *Supersolid properties of a Bose-Einstein condensate in a ring resonator* [DOI]
- J. Léonard et al., *Supersolid formation in a quantum gas breaking continuous translational symmetry* [DOI]
- J.K. Asbóth et al., *Optomechanical coupling in a one-dimensional optical lattice* [DOI]
- G.R.M. Robb, *Dispersive optical bistability in cold atomic vapours* [DOI]
- R. Culver et al., *Collective strong coupling of cold potassium atoms in a ring cavity* [DOI]
- S. Bux et al., *Cavity-controlled matter wave superradiance at the recoil limit* [DOI]
- R.J. Schulze et al., *Optomechanical approach to cooling of small polarizable particles in a strongly pumped ring cavity* [DOI]

### 22.6.1 on CARL

- R. Bonifacio et al., *The self-consistent pendulum picture of the free electron laser revised* [\[DOI\]](#)
- R. Bonifacio et al., *A quantum model for collective recoil lasing* [\[DOI\]](#)
- S. Gupta et al., *Cavity Nonlinear Optics at Low Photon Numbers from Collective Atomic Motion* [\[DOI\]](#)
- M.S. Shahriar et al., *Ultra-high enhancement in absolute and relative rotation sensing using fast and slow light* [\[DOI\]](#)
- F. Zimmer et al., *Sagnac Interferometry Based on Ultraslow Polaritons in Cold Atomic Vapors* [\[DOI\]](#)
- G.E. Stedman et al., *Ring-laser tests of fundamental physics and geophysics* [\[DOI\]](#)
- Shanchao Zhang et al., *A dark-line two-dimensional magneto-optical trap of  $85\text{Rb}$  atoms with high optical depth* [\[DOI\]](#)

# Chapter 23

## Statistical and thermodynamic approaches to CARL

The CARL phenomenon introduced in the previous chapter raises a variety of questions, such as: How does it compare to an ordinary laser? Is there a phase transition? Of what kind would be this transition (in the Ehrenfest or Landau classification scheme)? What are the coherence properties (measured by correlation functions)? How do these properties depend on the random motion (temperature) of the atoms? These issues will be addressed in this chapter and in the later chapter within the models of Langevin, Fokker-Planck, Vlasov, and Kuramoto.

### 23.1 The Langevin model

#### 23.1.1 CARL with damping

We saw in the previous chapter that CARL is a transient phenomenon, the atoms and the phase of the light wave being continuously accelerated. However, it is possible to force stationary behavior by providing additional friction for the atoms. Such friction can be carried out by an *optical molasses* (see Sec. 24.2.1) characterized by a friction coefficient  $\gamma_{fric}$ . The friction force can be added to the CARL equations of motion (22.53),

$$\begin{aligned} \dot{\alpha}_- &= -\kappa\alpha_- - iU_0\alpha_+ \sum_m e^{2ikz_m} \\ \kappa\dot{v}_n &= 4i\omega_{rec}U_0\alpha_+(\alpha_-e^{-2ikz_n} - \alpha_-^*e^{2ikz_n}) - \gamma_{fric}kv_n . \end{aligned} \quad (23.1)$$

Now, the balance of forces happens at a well-defined atomic velocity, which incidentally corresponds to a well-defined CARL frequency. Assuming perfect 'bunching'  $e^{2ikz_m} = e^{2ikz}$ , and balanced forces,  $\dot{v}_m = 0$  e  $\alpha_- = \beta e^{2ikz}$  with  $\beta = 0$ , we obtain for  $\kappa \ll 2kv$ ,

$$\begin{aligned} \alpha_- &= \frac{-iNU_0\alpha_+}{\kappa+2kv} e^{2ikz} \\ (kv)^3 &= \frac{2\omega_{rec}\kappa NU_0^2\alpha_+^2}{\gamma_{fric}} . \end{aligned} \quad (23.2)$$



This result will be derived in Exc. 23.1.3.1.

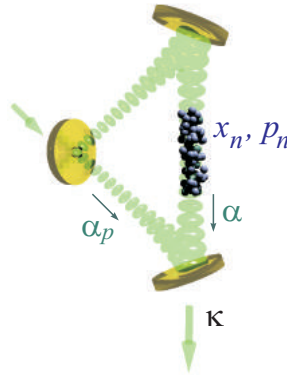


Figure 23.1: Scheme of the ring cavity.

Optical molasses obviously are subject to a cooling limit coming from the random scattering of photons. As a consequence, atoms follow a *random walk* in the momentum space, which leads to the diffusion and heating of atoms and impedes the bunching of atoms. It also turns out that a minimal grouping is required to initialize CARL. Therefore, there is a threshold behavior as a function of the equilibrium temperature of the molasses,

$$\begin{cases} \dot{\alpha}_- = -\kappa\alpha_- - iU_0\alpha_+ \sum_m e^{2ikz_m} \\ k\dot{v}_n = 4i\omega_{rec}U_0\alpha_+(\alpha_-e^{-2ikz_n} - \alpha_-^*e^{2ikz_n}) - \gamma_{frc}kv_n + \xi_n(t) \end{cases}. \quad (23.3)$$

The equation corresponds to a *Langevin equation*, where the stochastic term  $\xi_n(t)$  describes white noise. We can simulate this equation by a Runge-Kutta method, where the atoms are continually exposed to random momentum changes. For  $N$  atoms we need to solve  $2N + 2$  Langevin equations to describe the dynamics of all degrees of freedom. The Langevin equations are associated to so-called *Fokker-Planck equations* [701, 583, 365, 700]. These describe the temporal evolution of the atomic density along the optical  $x$ -axis. With these equations we replace the  $2N$  trajectories of individual particles by a one-dimensional field  $P(x, t)$ . The *Vlasov equation* represents a different approach: Here we assume that the equilibrium between cooling and heating is achieved by a continuous thermalization process described by a single rate  $\gamma_{th}$ <sup>1</sup>.

### 23.1.1.1 Characterization of an optical molasses

Optical molasses is discussed in Sec. 24.2.1. In Exc. 24.2.5.1 we will show how, through a linearization of the radiative pressure force, we arrive at the following approximation,

$$\mathbf{F} = -\gamma_{frc}\mathbf{v} \quad \text{with} \quad \gamma_{frc} \simeq -\sqrt{3}\hbar k^2 s(1+s)^{-3/2}, \quad (23.4)$$

<sup>1</sup>Through a linearization of the CARL equations, the cavity dissipation itself is found to exert a friction force to the atoms [313, 255]. This implies the existence of diffusion and a finite equilibrium temperature even at if the atoms are initially at  $T = 0$ .

where  $s = I/I_s$  is the saturation parameter. This formula estimates the maximum friction force, when the lasers are tuned close to an atomic resonance <sup>2</sup>.

A more fundamental problem is the interdependence of the molasses friction and the CARL. In fact, because the dipole potential influences the detuning of the molasses beams by light-shifting the  $D_2$  line, the  $\gamma_{th}$  coefficient depends on  $\Delta_a$  and  $\eta_+$  (the reverse field  $|\alpha_-|$  may be neglected). The threshold equations must then be solved in a self consistent way. It might however be possible to determine  $\gamma_{th}$  only slightly above threshold, where the modification is small,  $\gamma_{th} \approx \gamma_{th}^{(thresh)}$ .

### 23.1.1.2 Fluctuation-dissipation theorem

Trajectories of ensembles of particles subject to friction and stochastic forces can be described by *Langevin equations*. The friction and the diffusion forces are related by the *fluctuation-dissipation theorem*. This theorem states that, for a thermal sample of atoms whose coordinates  $\theta_n$  follow,

$$\ddot{\theta}_n = -\gamma_{frc}\dot{\theta}_n + \xi_n(t) , \quad (23.5)$$

the Langevin force  $\xi(t)$  fluctuates stochastically with,

$$\langle \xi_n(t) \rangle = 0 \quad \text{and} \quad \langle \xi_n(t)\xi_m(t+\tau) \rangle = 2\gamma_{frc}^2 D_T \delta_{mn} \delta(\tau) . \quad (23.6)$$

Here, the *diffusion coefficient*,

$$D_T = \frac{\sigma^2}{\gamma_{frc}} \quad (23.7)$$

is related to the width of the Maxwell-Boltzmann velocity distribution,

$$\sigma = 2k\sqrt{\frac{k_B T}{m}} . \quad (23.8)$$

## 23.1.2 Langevin simulations

The Langevin equations of CARL can be simulated, including the random term of the Langevin force, using the *Runge-Kutta method* [343]. The procedure consists in propagating a general first order differential equation,

$$\dot{x} = f(x) + g(t) , \quad (23.9)$$

subject to a deterministic force  $f$  and a stochastic noise  $g$  satisfying,

$$\langle g(t) \rangle = 0 \quad \text{and} \quad \langle g(t)g(t') \rangle = 2D\delta(t-t') \quad (23.10)$$

---

<sup>2</sup>We note that atomic species exhibiting a hyperfine structure in the ground state are subject to cooling phenomena called 'polarization gradient cooling', which can cause much higher friction coefficients.

We also note that, when the molasses is applied to atoms confined to a potential, the atomic levels can be displaced (e.g., by light-shift or the Zeeman effect). This causes an inhomogeneous effective detuning of the laser beams generating the molasses.

as follows,

$$\boxed{\begin{array}{l} x(dt) = x_0 + \frac{1}{2}dt[f(x_0) + f(\tilde{x})] + \zeta(2Ddt)^{1/2} \\ \text{with } \tilde{x} \equiv x_0 + f(x_0)dt + \zeta(2Ddt)^{1/2} \end{array}}, \quad (23.11)$$

where  $\zeta$  is a random variable distributed according to a normal (Gaussian) distribution normalized as <sup>3</sup>,

$$\langle \zeta \rangle = 0 \quad \text{and} \quad \langle \zeta^2 \rangle = 1. \quad (23.12)$$

### 23.1.2.1 Langevin simulation in the adiabatic approximation

Now, we apply this method to the CARL subject to an optical molasses. Making the adiabatic approximation  $\ddot{\theta}_n = 0$ , the starting point is,

$$\boxed{\begin{array}{l} \dot{\alpha}_- = -\kappa\alpha_- - iU_0\alpha_+ \sum_m e^{i\theta_m} \equiv B(\alpha_-, \theta_n) \\ \dot{\theta}_n = \frac{8i\omega_{rec}U_0\alpha_+}{\gamma_{frc}}(\alpha_- e^{-i\theta_n} - \alpha_-^* e^{i\theta_n}) + \frac{\xi_n(t)}{\gamma_{frc}} \equiv F(\alpha_-, \theta_n) + \frac{\xi_n(t)}{\gamma_{frc}} \end{array}}. \quad (23.13)$$

In order to apply the Runge-Kutta method (23.11), we identify the variables and functions,

$$x(t) \equiv \begin{pmatrix} \alpha_-(t) \\ \theta_n(t) \end{pmatrix}, \quad f(x) \equiv \begin{pmatrix} B(\alpha_-, \theta_n) \\ F(\alpha_-, \theta_n) \end{pmatrix}, \quad g(t) \equiv \begin{pmatrix} 0 \\ \xi_n(t)/\gamma_{frc} \end{pmatrix}, \quad (23.14)$$

such that,

$$\tilde{x} = \begin{pmatrix} \tilde{\alpha}_- \\ \tilde{\theta}_n \end{pmatrix} = \begin{pmatrix} \alpha_-(0) \\ \theta_n(0) \end{pmatrix} + dt \begin{pmatrix} B(\alpha_-(0), \theta_n(0)) \\ F(\alpha_-(0), \theta_n(0)) \end{pmatrix} + \begin{pmatrix} 0 \\ \zeta_n \sqrt{2D_T dt} \end{pmatrix} \quad (23.15)$$

and

$$\begin{aligned} x(dt) &= \begin{pmatrix} \alpha_-(dt) \\ \theta_n(dt) \end{pmatrix} & (23.16) \\ &= \begin{pmatrix} \alpha_-(0) \\ \theta_n(0) \end{pmatrix} + \frac{dt}{2} \left[ \begin{pmatrix} B(\alpha_-(0), \theta_n(0)) \\ F(\alpha_-(0), \theta_n(0)) \end{pmatrix} + \begin{pmatrix} B(\tilde{\alpha}_-, \tilde{\theta}_n) \\ F(\tilde{\alpha}_-, \tilde{\theta}_n) \end{pmatrix} \right] + \begin{pmatrix} 0 \\ \zeta_n \sqrt{2D_T dt} \end{pmatrix}. \end{aligned}$$

The Langevin equation can be used to simulate the temporal evolution of CARL. Fig. 23.2 shows a simulation of the frequency and amplitude of the CARL based on prescription (23.11).

<sup>3</sup>The MATLAB random number generator satisfies this requirement:  $\langle \zeta_n \rangle \triangleq \text{sum}(\text{randn}(1, N))/N = 0$  and  $\langle \zeta_n^2 \rangle \triangleq \text{sum}(\text{randn}(1, N) . \wedge 2)/N = 1$ .

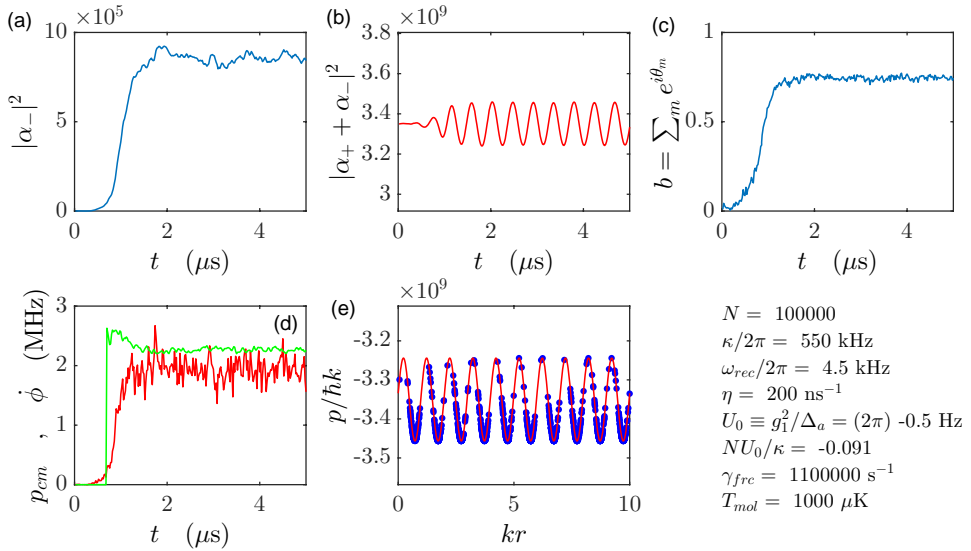


Figure 23.2: (code) Time evolution with phase transition of the viscous CARL in the adiabatic approximation. Shown are (a) the number of photons in the probe mode, (b) the beat signal, (c) the bunching, (d) the phase of the standing wave and the position of the center-of-mass of the cloud, and (e) the dipole potential calculated from (22.21) with the atomic distribution.

### 23.1.2.2 Langevin simulation of the full dynamics

Without adiabatic approximation, the starting point is,

$$\begin{aligned}
 \dot{\alpha}_- &= \kappa\alpha_- - iU_0\alpha_+ \sum_m e^{i\theta_m} && \equiv B(\alpha_-, \theta_n) \\
 \dot{\theta}_n &= V_n \\
 \dot{V}_n &= 8i\omega_{rec}U_0\alpha_+(\alpha_-e^{-i\theta_n} - \alpha_-^*e^{i\theta_n}) - \gamma_{fre}V_n + \xi_n(t) && \equiv F(\alpha_-, \theta_n, V_n) + \xi_n(t)
 \end{aligned}
 \tag{23.17}$$

In order to apply the Runge-Kutta method (23.11), we identify the variables and functions,

$$x(t) \equiv \begin{pmatrix} \alpha_-(t) \\ \theta_n(t) \\ V_n(t) \end{pmatrix}, \quad f(x) \equiv \begin{pmatrix} B(\alpha_-, \theta_n) \\ V_n \\ F(\alpha_-, \theta_n, V_n) \end{pmatrix}, \quad g(t) \equiv \begin{pmatrix} 0 \\ 0 \\ \xi_n(t) \end{pmatrix}, \tag{23.18}$$

such that,

$$\tilde{x} = \begin{pmatrix} \tilde{\alpha}_- \\ \tilde{\theta}_n \\ \tilde{V}_n \end{pmatrix} \equiv \begin{pmatrix} \alpha_-(0) \\ \theta_n(0) \\ V_n(0) \end{pmatrix} + dt \begin{pmatrix} B(\alpha_-(0), \theta_n(0)) \\ V_n(0) \\ F(\alpha_-(0), \theta_n(0), V_n(0)) \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \zeta_n \sqrt{2\gamma_{fre}^2 D_T dt} \end{pmatrix}
 \tag{23.19}$$

and

$$x(dt) = \begin{pmatrix} \alpha_-(dt) \\ \theta_n(dt) \\ V_n(dt) \end{pmatrix} = \begin{pmatrix} \alpha_-(0) \\ \theta_n(0) \\ V_n(0) \end{pmatrix} + \frac{dt}{2} \left[ \begin{pmatrix} B(\alpha_-(0), \theta_n(0)) \\ V_n(0) \\ F(\alpha_-(0), \theta_n(0), V_n(0)) \end{pmatrix} + \begin{pmatrix} B(\tilde{\alpha}_-, \tilde{\theta}_n) \\ \tilde{V}_n \\ F(\tilde{\alpha}_-, \tilde{\theta}_n, \tilde{V}_n) \end{pmatrix} \right] + \begin{pmatrix} 0 \\ 0 \\ \zeta_n \sqrt{2\gamma_{frc}^2 D_T dt} \end{pmatrix}. \quad (23.20)$$

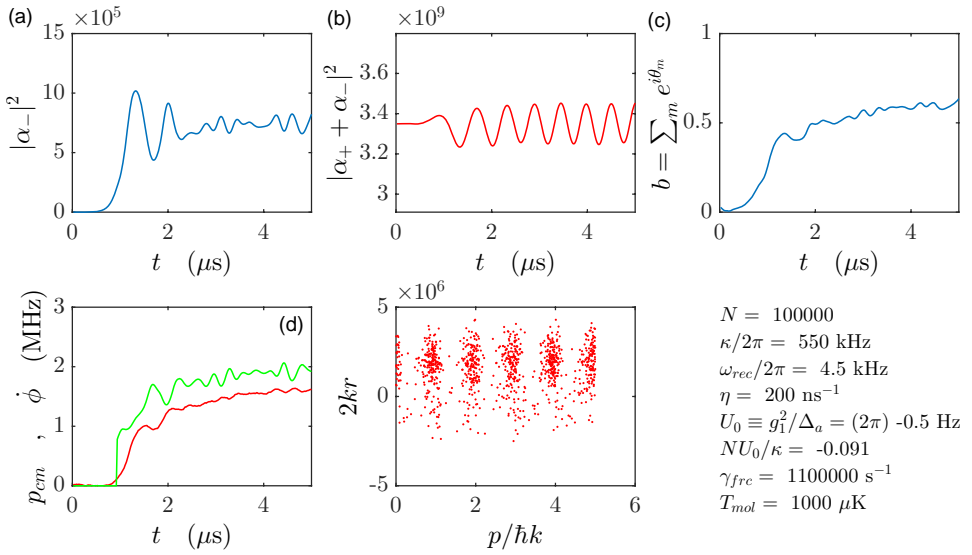


Figure 23.3: (code) Time evolution of the complete dynamics of the viscous CARL with phase transition. Same parameters as in Fig. 23.2. Shown are (a) the number of photons in the probe mode, (b) the beat signal, (c) the bunching, (d) the phase of the standing wave and the position of the center-of-mass of the cloud, and (e) the dipole potential calculated from (22.21) with the atomic distribution.

## 23.1.3 Exercises

### 23.1.3.1 Ex: Viscous CARL

Assuming a perfect 'bunching',  $e^{2ikz_m} = e^{2ikz}$ ,  $e \alpha_- \equiv \beta e^{2ikz}$  with  $\dot{\beta} = 0$  and  $\ddot{z} = 0$  derive the equations (23.2).

### 23.1.3.2 Ex: Langevin simulations

Langevin simulations

## 23.2 The Fokker-Planck and the Vlasov model

The *Fokker-Planck equation* for a density distribution  $Q(\mathbf{r}, t)$ ,

$$\frac{dQ}{dt} + Q\nabla \cdot \mathbf{v} = D\nabla^2 Q, \quad (23.21)$$

represents a generalization of the *continuity equation*, since with  $\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$ , we obtain,

$$\frac{\partial Q}{\partial t} = -\nabla \cdot (\mathbf{v}Q) + D\nabla^2 Q. \quad (23.22)$$

If  $\rho$  is a local density, it the continuity equation reads,

$$\frac{d\rho}{dt} + \rho\nabla \cdot \mathbf{v} = 0. \quad (23.23)$$

Knowing,

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla, \quad (23.24)$$

we obtain,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho\mathbf{v}). \quad (23.25)$$

The Fokker-Planck equation is just a generalization to include a diffusion process,

$$\frac{d\rho}{dt} + \rho\nabla\mathbf{v} = D_x \frac{\partial^2 \rho}{\partial x^2}, \quad (23.26)$$

or

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho\mathbf{v}) + D_x \frac{\partial^2 \rho}{\partial x^2}. \quad (23.27)$$

### 23.2.1 Thermalization in the Fokker-Planck equation

We now apply the Fokker-Planck equation to the density distribution (23.13) of an atomic cloud subjected to the CARL force [701, 583]. As CARL is a one-dimensional process, we can use  $\nabla \rightarrow \partial\theta$  and replace the velocity field  $\mathbf{v} \rightarrow \dot{\theta}$ :

$$\begin{aligned} \dot{\alpha}_- &= -\kappa\alpha_- - iNU_0\alpha_+b \\ \frac{\partial Q}{\partial t} &= \frac{8i\omega_{rec}U_0\alpha_+}{\gamma_{frc}} \frac{\partial}{\partial \theta} [(\alpha_- e^{-i\theta} - \alpha_-^* e^{i\theta})Q] + D_\theta \frac{\partial^2 Q}{\partial \theta^2} \end{aligned} \quad (23.28)$$

The position diffusion coefficient can be estimated by,

$$D_\theta = \frac{\langle k^2 v^2 \rangle}{\gamma_{frc}}. \quad (23.29)$$

The normalization and the 'bunching'  $|b|$  are given by,

$$1 = \int_0^{2\pi} Q(\theta, t) d\theta \quad , \quad b \equiv \int_0^{2\pi} Q(\theta, t) e^{-i\theta} d\theta. \quad (23.30)$$

To simulate the equations (23.28) we expand the distribution function in spatial harmonics [583],

$$Q(\theta, t) \equiv \sum_{\nu} Q_{\nu}(t) e^{i\nu\theta} . \quad (23.31)$$

In this expansion the normalization and the bunching become,

$$Q_0 = 1/2\pi \quad , \quad |b| = 2\pi|Q_1| , \quad (23.32)$$

and the equations (23.28) immediately yield,

$$\boxed{\begin{aligned} \dot{\alpha}_{-} &= -2\pi i N U_0 \alpha_{+} Q_1 - \kappa \alpha_{-} \\ \frac{dQ_{\nu}}{dt} &= \frac{8\omega_{rec} U_0 \alpha_{+}}{\gamma_{frc}} \nu (\alpha_{-} Q_{\nu+1} + \alpha_{-}^{*} Q_{\nu-1}) - \nu^2 D_{\theta} Q_{\nu} \end{aligned}} . \quad (23.33)$$

We will derive the results (23.32) and (23.33) in Exc. 23.2.5.1. Also,

$$kv = \frac{d}{dt} \arctan \frac{\text{Im } \alpha_{-}}{\text{Re } \alpha_{-}} , \quad (23.34)$$

and,

$$\begin{aligned} \langle \dot{\theta} \rangle &\equiv \int_0^{2\pi} \dot{Q}(\theta, t) d\theta = \sum_{\nu} \dot{Q}_{\nu}(t) \int_0^{2\pi} e^{i\nu\theta} d\theta \\ &= \sum_{\nu} \frac{8\omega_{rec} U_0 \alpha_{+}}{\gamma_{frc}} \nu (\alpha_{-} Q_{\nu+1} + \alpha_{-}^{*} Q_{\nu-1}) \delta_{\nu 0} = \frac{16\omega_{rec} U_0 \alpha_{+}}{\gamma_{frc}} \text{Re} (\alpha_{-} Q_1^{*}) . \end{aligned} \quad (23.35)$$

These equations can be easily simulated.

Matlab simulations of the Fokker-Planck equation, shown in Fig. 23.4, reproduce quantitatively the curves previously obtained by simulations of the Langevin equations.

### 23.2.2 Bistability and instability of the viscous CARL

The threshold can be found by simulating the Fokker-Planck equation while varying a control parameter (pumping power, temperature, number of atoms) sufficiently slowly, that the system always remains in a steady state. Fig. 23.5 shows the behavior of the CARL, while the pump power is linearly reduced and then linearly increased at different velocities. We observe a bistability that slightly depends on the speed of the ramp. The behavior of the mass-center velocity  $kv_{cm}$  and the phase of the standing wave,  $\phi$ , are different [582]<sup>4</sup>.

<sup>4</sup>We can expect a second phase transition when the pump power exceeds a critical value, because for  $NU_0 > \kappa$ , the CARL becomes unstable again: It will unlock from the self-determined frequency and start to oscillate strongly. However, this effect is not described by the equations used for the simulation, which suppose an adiabatic elimination of the inertia.

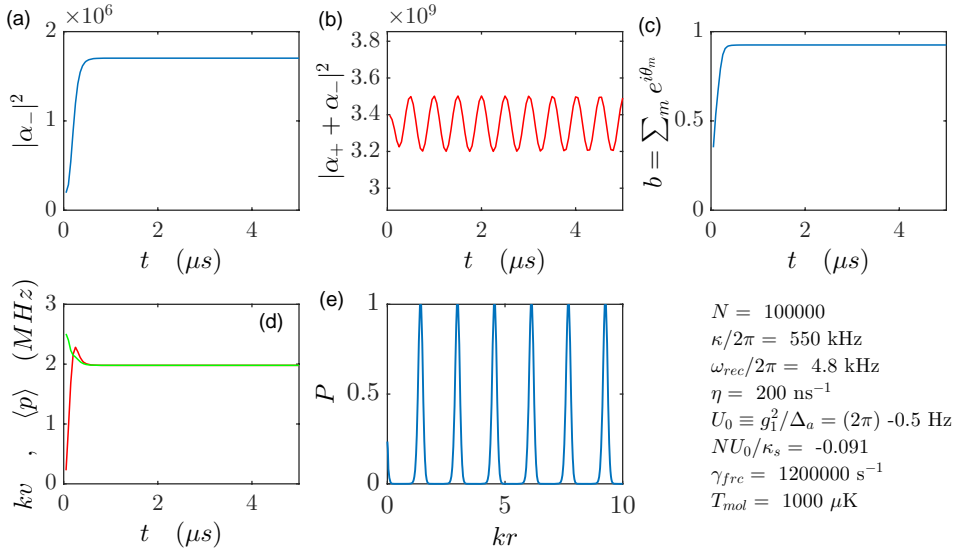


Figure 23.4: (code) Temporal evolution of the complete dynamics with phase transition of the viscous CARL. The same parameters as in Fig. 23.2. Shown are (a) the number of photons in the probe mode, (b) the beat signal, (c) the bunching, (d) the phase of the standing wave and the position of the center-of-mass of the cloud, and (e) the atomic density distribution.

### 23.2.3 Thermalization in the Vlasov equation

The basic equations describing our ring-cavity filled with atoms are [416],

$$\begin{cases}
 \dot{\alpha}_- = \kappa\alpha_- - iU_0\alpha_+ \sum_m e^{i\theta_m} \\
 \dot{\theta}_n = V_n \\
 \dot{V}_n = 8i\omega_{rec}U_0\alpha_+(\alpha_-e^{-i\theta_n} - \alpha_-^*e^{i\theta_n}) - \gamma_{frc}(V_n - V_n^{(0)})
 \end{cases}, \quad (23.36)$$

if we assume the pump mode to be stationary  $\alpha_+ = \eta_+/\kappa^{-1}$  and define the atomic bunching parameter by  $b = \frac{1}{N} \sum_j e^{2ikx_j}$ . A non-zero steady-state temperature is reached, if we allow the steady-state velocities of the atoms  $v_j^{(0)}$  to be *different* for all atoms and distributed according to a Maxwell-Gaussian velocity distribution. The assumption of a common steady-state velocity for all atoms obviously results in perfect bunching and cooling to  $T = 0$ .

Let us introduce a local phase space density of the atomic cloud  $Q(x, p, t)$  as a two-dimensional field in phase space. The time-evolution of this quantity is given by the so-called *Vlasov equation* (or collisionless Boltzmann equation),

$$0 = \partial_t Q + v\partial_x Q + F\partial_p Q + \gamma_{th}(Q - Q_0), \quad (23.37)$$

where  $v$  and  $F$  are the center-of-mass velocity and force taken from equation (23.36) without the friction term. According to this equation the atomic cloud tends to a sta-



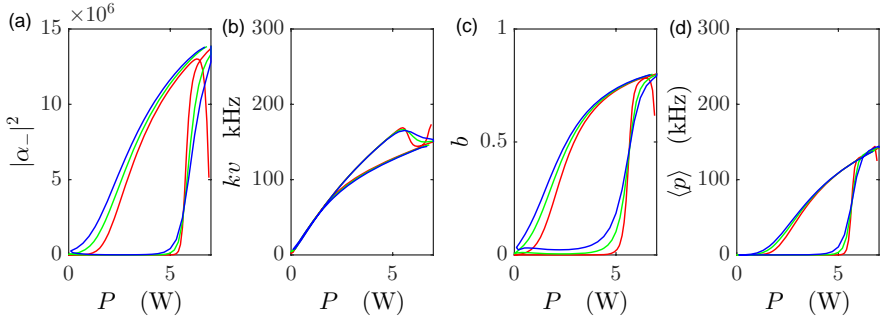


Figure 23.5: (code) Bistability of CARL near the threshold when the power is ramped at different paces.

tionary distribution  $Q_0$  as time goes on. Following Bonifacio *et al.* [93] and Javaloyes [366, 367, 368], we replace the friction term by an additional (Vlasov) equation:

$$\begin{aligned}
 \dot{\alpha}_- &= -iNU_0\alpha_+b - \kappa\alpha_- \\
 \dot{\theta} &= \omega_{rec}V \\
 \dot{V} &= iU_0\alpha_+(\alpha_-e^{-i\theta} - \alpha_-^*e^{i\theta}) \\
 0 &= \partial_t Q + \dot{\theta}\partial_\theta Q + \dot{\varrho}\partial_\varrho Q + \gamma_{frc}(Q - Q_0)
 \end{aligned} \tag{23.38}$$

The bunching parameter can now be rewritten in terms of

$$b = \int_0^{2\pi} d\theta \int_{-\infty}^{\infty} d\varrho Q(\theta, \varrho, t) e^{2i\theta} . \tag{23.39}$$

The equilibrium distribution is chosen to be a homogeneous cloud with a Maxwell-Boltzmann velocity distribution,

$$Q_0 = \frac{1}{2\pi} \sqrt{\frac{\sigma}{\pi}} e^{-\sigma\varrho^2} , \tag{23.40}$$

where  $\sigma \equiv \hbar\omega_{rec}/k_B T$  with  $\omega_{rec} \equiv \hbar k^2/2m$  such that  $\int_0^{2\pi} d\theta \int_{-\infty}^{\infty} Q_0 d\varrho = 1$ . We now perform a linear stability analysis. We expand  $Q$  around the steady state,  $Q(\theta, \varrho, t) = Q_0(\varrho) + Q_1(\theta, \varrho, t)$  and retain to first order,

$$0 = \partial_t Q_1 + \dot{\theta}\partial_\theta Q_1 + \dot{\varrho}\partial_\varrho Q_0 + \gamma_{th}Q_1 . \tag{23.41}$$

Now we look for a time-dependent particular solution by inserting the ansatz,

$$\begin{aligned}
 \alpha_-(t) &= \beta_- e^{i\lambda t} \quad \text{with} \quad \dot{\beta}_- = 0 \\
 Q_1(\theta, \varrho, t) &= H_1(\varrho) e^{-2i\theta} e^{i\lambda t} + c.c. ,
 \end{aligned} \tag{23.42}$$

where  $i\lambda \equiv \lambda_g + i\lambda_\omega$  into the field equation (23.38)a, the first order expansion of the Vlasov equation (23.41) (only retaining co-rotating terms) and into the expression for

bunching (23.39). This ansatz accounts for the fact that, in steady state, we expect a fixed CARL frequency  $\nu$  and a spatially modulated density distribution of the atoms. The set of equations becomes,

$$\begin{aligned} qi\lambda\beta_- &= -\kappa\beta_- - iNU_0\tilde{\eta}_+be^{-i\lambda t} \\ 0 &= i\lambda H_1(\varrho) - 4i\omega_{rec}\varrho H_1(\varrho) + iU_0\tilde{\eta}_+\beta_- \partial_\varrho Q_0 + \gamma_{th}H_1(\varrho) \\ b &= \int_0^{2\pi} d\theta \int_{-\infty}^{\infty} d\varrho H_1(\varrho)e^{i\lambda t}. \end{aligned} \quad (23.43)$$

With the definition,

$$\begin{aligned} \Gamma(\sigma, \gamma_{th}, i\lambda) &\equiv \int_{-\infty}^{\infty} \frac{d\varrho \partial_\varrho Q_0}{i\lambda - 4i\omega_{rec}\varrho + \gamma_{th}} \\ &= - \int_{-\infty}^{\infty} \frac{d\varrho 4i\omega_{rec}Q_0}{(i\lambda - 4i\omega_{rec}\varrho + \gamma_{th})^2}, \end{aligned} \quad (23.44)$$

the solution of the above set of equations is,

$$\begin{aligned} H_1(\varrho) &= \frac{-iU_0\tilde{\eta}_+\beta_- \partial_\varrho Q_0}{i\xi - 4i\omega_{rec}\varrho + \gamma_{th}} \\ b &= -e^{i\xi t} iU_0\tilde{\eta}_+\beta_- 2\pi\Gamma(\sigma, \gamma_{th}, i\lambda) \\ 0 &= [\kappa + i\lambda + NU_0^2\tilde{\eta}_+^2 2\pi\Gamma(\sigma, \gamma_{th}, i\lambda)] \beta_-. \end{aligned} \quad (23.45)$$

### 23.2.4 Calculation of the threshold

The bifurcation where the reverse field crosses the threshold to lasing occurs at  $\lambda_g = 0$ . We divide the field equation in real and imaginary parts,

$$\begin{aligned} \kappa + NU_0^2\tilde{\eta}_+^2 2\pi\text{Re } \Gamma(\sigma, \gamma, i\lambda_\omega) &= 0 \\ \nu + NU_0^2\tilde{\eta}_+^2 2\pi\text{Im } \Gamma(\sigma, \gamma, i\lambda_\omega) &= 0. \end{aligned} \quad (23.46)$$

Now the condition  $\lambda_\omega \text{Re } \Gamma(\sigma, \gamma_{th}, i\lambda_\omega) = \kappa \text{Im } \Gamma(\sigma, \gamma_{th}, i\lambda_\omega)$  leads to,

$$\int_{-\infty}^{\infty} \frac{d\varrho \varrho e^{-\sigma\varrho^2} (\kappa\lambda_\omega - 2\kappa\varepsilon\varrho + \lambda_\omega\gamma_{th})}{(\lambda_\omega - 2\varepsilon\varrho)^2 + \gamma_{th}^2} = 0. \quad (23.47)$$

The values  $\lambda_\omega$  where this integral is zero are inserted into one of the equations (23.46). Finally,

$$\tilde{\eta}_+^2 = \frac{-1}{NU_0^2 2\pi\text{Re } \kappa\Gamma(\sigma, \gamma_{th}, i\lambda_\omega)}, \quad (23.48)$$

is the expression for the pump power threshold as a function of temperature  $\sigma$ , friction  $\gamma_{th}$ , cavity damping  $\kappa$  and coupling constant  $U_0$ . The intracavity CARL power is,

$$P_+ = \hbar\omega\delta \tilde{\eta}_+^2. \quad (23.49)$$

$\lambda_\omega$  is the associated CARL frequency, i.e. the frequency difference between probe and pump.

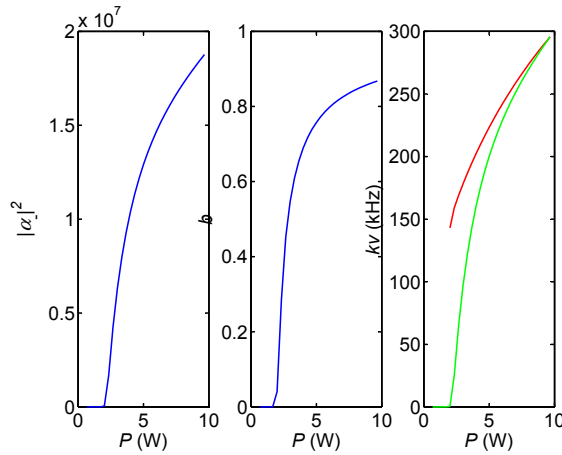


Figure 23.6: (code) Intracavity threshold power as a function of temperature and friction coefficient. The coupling strength is set to  $\tilde{U}_0 = -10^{-7}$ , the atom number is  $N = 10^6$ .

The final equations show that the threshold power drops as  $NU_0^2$  increases. To see the dependencies of the threshold power on  $T$  and  $\gamma_{th}$ , we have to evaluation of the integral (23.47). Fig. 23.6 shows a numerical evaluation of Eqs. (23.47), (23.48) and (23.49) for finite  $T$  and  $\gamma_{th}$ .

Apparently, the threshold pump power drops with vanishing friction and with low temperatures. For typical experimental situations,  $T \approx 100 \mu\text{K}$  and  $\gamma_{th} \approx 10\kappa$ , we expect threshold powers on the order of about  $P_+ = 1 \text{ W}$ , corresponding to  $P_+^{(out)} = 4 \mu\text{W}$  leaking out of the cavity.

## 23.2.5 Exercises

### 23.2.5.1 Ex: Fokker-Planck equations

Derive the equations (23.32) and (23.33) from (23.30) and (23.28) applying the expansion (23.31).

## 23.3 The Kuramoto model

Ripples on a dusty street driven by cars, rapids in a river arising spontaneously or behind an obstacle, wind blowing over a water surface spontaneously creating waves. Imagine a photon wind blowing over an atomic sea. Just like for water waves friction hinders boundless acceleration. The analogies are wind-molasses-friction, water-atoms, wind-acceleration-field, gravitation-dipole-force. The phenomenon is closely related to the *dissipative structure*. See also (watch talk) and (watch talk).

Our system has the advantage over macroscopic systems, that the hypothesis of uniform coupling is exactly satisfied, because the coupling medium, i.e. the light fields are delocalized within the cavity mode. In contrast, rapids develop exclusively behind

the perturbation. There are no delay times effects and no spatial constraints due to a finite size of the individual oscillators.

The viscous CARL system is representative for of the vast class of *Kuramoto systems* [670] introduced in Sec. ???. This can be seen most appropriately by rewriting the CARL equations in terms of phase and amplitude of individual atoms. Another approach is via the Fokker-Planck equation, for which there already exists a Kuramoto equivalence.

Why is it interesting to investigate yet another coupled oscillator system? Our CARL is fully classical, although we deal with microscopic particle, such as atoms and photons. However, our system bears the possibility of being transferred to quantum situations, and thus to study the coupling of large ensembles of quantum oscillators. Furthermore, the coupling mechanism is well understood and controlable by experiment. Because the coupling goes through the standing wave fraction, it depends on the atom number and the coupling strength independently. Furthermore, the tunable friction force (temperature) corresponds to a variable width of the distribution of the oscillator frequencies, which we can manipulate in-situ and on-line.

Another realization of the Kuramoto model would be atoms in a ring cavity standing wave. Cold trapped atoms have the same oscillation frequencies. And thus do not need to synchronize. For hot atoms, however, the oscillation period depends on their kinetic energy.

The equation for the phases of the atoms is similar to the Kuramoto model [368],

$$\dot{\theta}_n = \frac{K}{N} \sum_m \sin(\theta_n - \theta_m) - \xi_n(t) . \quad (23.50)$$

The CARL equations which describes the dynamics of an ensemble of mean-field coupled oscillators, belong to the class of Kuramoto systems [367]. The main differences are: a Dirac-like distribution of eigenfrequencies and a mean-field self-consistently provided by a dynamical equation. Hence, in contrast to the original Kuramoto model, where the collective oscillation frequency is just the mean of the individual frequencies, the CARL frequency is self-determined and depends also on control parameters. This phenomenon is known from other systems like rhythmic applause, which only takes place by a reduction of the individual frequencies of clapping hands, towards a resonance. For this to happen the mean-field must self-adjust while the individual oscillators synchronize, e.g. the noise produce by the audience must adjust to the average desire of the audience to produce a satisfying level of noise.

In [720] is stated: "The essence of the problem is the competition between the intrinsic disorder (i.e. noise and diffusion) and the dynamical coupling strength. In the Kuramoto model, the disorder enters via the distribution of natural frequencies, while the effective coupling strength is set by the parameter combination  $K \cos \alpha_j$ ."

### 23.3.1 Phase formalism of CARL

The starting point is the CARL equations (22.79). We make ansatz,

$$\alpha_+ \equiv \alpha_1 \quad , \quad \alpha_- \equiv \alpha_2 e^{i\phi} \quad , \quad \eta_+ \equiv \eta_1 \quad , \quad \eta_- \equiv \eta_2 e^{i\Delta} \quad , \quad (23.51)$$

where the quantities with numeric suffixes are real, such that,

$$|\alpha_+ + \alpha_-|^2 = \alpha_1^2 + \alpha_2^2 + 2\alpha_1\alpha_2 \cos \phi . \quad (23.52)$$

By this ansatz we assume that a pumping laser is locked to the mode  $\alpha_+$  of the ring cavity, such that the phases of the fields  $\alpha_+$  and  $\eta_+$  are equal and, without loss of generality, zero. On the other hand, the phase  $\phi$  of the probe mode is a dynamic variable. Inserting the ansatz into the equations (22.79) we obtain,

$$\begin{aligned} \dot{\alpha}_1 &= -(\kappa + iNU_0 - i\Delta_c)\alpha_1 - iU_0 \sum_n e^{-i\theta_n + i\phi} \alpha_2 + \eta_1 , \\ \dot{\alpha}_2 + i\dot{\phi}\alpha_2 &= -(\kappa + iNU_0 - i\Delta_c)\alpha_2 - iU_0 \sum_n e^{i\theta_n - i\phi} \alpha_1 + \eta_2 e^{i\Delta - i\phi} , \\ \ddot{\theta}_n &= 16\omega_{rec}U_0\alpha_1\alpha_2 \sin(\theta_n - \phi) . \end{aligned} \quad (23.53)$$

The first two equations, which describe the dynamics of the fields, can be separated into real and imaginary parts,

$$\begin{aligned} \dot{\alpha}_1 &= -\kappa\alpha_1 - U_0 \sum_n \sin(\theta_n - \phi)\alpha_2 + \eta_1 \\ \dot{\alpha}_2 &= -\kappa\alpha_2 + U_0 \sum_n \sin(\theta_n - \phi)\alpha_1 + \eta_2 \cos(\phi - \Delta) , \\ \Delta_c &= NU_0 \left( 1 + N^{-1} \sum_n \cos(\theta_n - \phi) \frac{\alpha_2}{\alpha_1} \right) , \\ \dot{\phi} &= \Delta_c - NU_0 \left( 1 + N^{-1} \sum_n \cos(\theta_n - \phi) \frac{\alpha_1}{\alpha_2} \right) - \frac{\eta_2}{\alpha_2} \sin(\phi - \Delta) . \end{aligned} \quad (23.54)$$

Eliminating  $\Delta_c$ , we can substitute the third and fourth equations for,

$$\dot{\phi} = U_0 \left( \frac{\alpha_2}{\alpha_1} - \frac{\alpha_1}{\alpha_2} \right) \sum_n \cos(\theta_n - \phi) - \frac{\eta_2}{\alpha_2} \sin(\phi - \Delta) . \quad (23.55)$$

Defining the 'bunching' parameter,

$$b \equiv |b|e^{i\psi} \equiv N^{-1} \sum_n e^{i\theta_n} , \quad (23.56)$$

we finally obtain, in the presence of friction and dissipation,

$$\begin{aligned} \dot{\alpha}_1 &= -\kappa\alpha_1 - NU_0\alpha_2|b| \sin(\psi - \phi) + \eta_1 \\ \dot{\alpha}_2 &= -\kappa\alpha_2 + NU_0\alpha_1|b| \sin(\psi - \phi) + \eta_2 \cos(\phi - \Delta) \\ \dot{\phi} &= NU_0 \left( \frac{\alpha_2}{\alpha_1} - \frac{\alpha_1}{\alpha_2} \right) |b| \cos(\psi - \phi) - \frac{\eta_2}{\alpha_2} \sin(\phi - \Delta) \\ \ddot{\theta}_n &= 16\omega_{rec}U_0\alpha_1\alpha_2 \sin(\theta_n - \phi) - \gamma_{frc}\dot{\theta}_n + \xi_n \end{aligned} . \quad (23.57)$$

A particularly interesting case is that of unidirectional pumping,  $\eta_2 = 0$ . Assuming that the pump mode be not affected,  $\dot{\alpha}_1 = 0$ , and that the probe mode be weak,

$\alpha_1 \gg \alpha_2$ , and making the adiabatic approximation,  $\ddot{\theta}_n = 0$ , of the atomic motion, we obtain,

$$\begin{cases} \dot{\alpha}_2 &= -\kappa\alpha_2 + NU_0\alpha_1|b|\sin(\psi - \phi) \\ \dot{\phi} &\simeq -\frac{NU_0\alpha_1}{\alpha_2}|b|\cos(\psi - \phi) \\ \dot{\theta}_n &= \frac{\xi_n}{\gamma_{frc}} + \frac{16\omega_{rec}U_0\alpha_1\alpha_2}{\gamma_{frc}}\sin(\theta_n - \phi) \end{cases}. \quad (23.58)$$

We note that the equation for the phases of the atoms is similar to the Kuramoto equation (23.50).

### 23.3.2 Relationship between CARL and Kuramoto

The viscous CARL described by the formulas (23.58) corresponds to the Kuramoto model [670]. Defining  $\theta_n \equiv 2kx_n$  as the position of the  $n^{th}$  atom, we assume the pump laser to be in resonance and write  $\alpha_+ \equiv \eta_+/\kappa$  [416]. The diffusion in the momentum space is a process that limits the temperature in optical molasses.

We start from the Langevin equations (23.13). In addition, we assume that the standing wave propagates at a constant velocity, which is to say that for a strong viscous damping, the system quickly finds a steady state. This condition is formulated by  $d_t|\alpha_-| = 0$  and  $\dot{\alpha}_- = i\omega_{ca}\alpha_-$  with constant velocity  $\omega_{ca}$ , which may be different from the velocity of the center of mass  $kv$ . We note that this assumption can introduce a considerable error, when used to describe temporal phase transitions, since, as shown by simulations of the complete dynamics (23.17), the mode  $\alpha_-$  exhibits a transient behavior, as well. We obtain from the first Eq. (23.13),

$$\alpha_- = -\frac{iU_0\alpha_+}{i\omega_{ca} + \kappa} \sum_m e^{i\theta_m}. \quad (23.59)$$

Substituting Eq. (23.59) into the second equation (23.13),

$$\begin{aligned} \dot{\theta}_n &= \frac{\xi_n}{\gamma_{fr}} + \frac{8\omega_{rec}NU_0^2\alpha_+^2}{\gamma_{fr}} \frac{1}{N} \sum_m \left( \frac{e^{i\theta_m - i\theta_n}}{i\omega_{ca} + \kappa} + \frac{e^{-i\theta_m + i\theta_n}}{-i\omega_{ca} + \kappa} \right) \\ &= \frac{\xi_n}{\gamma_{fr}} + \frac{16\omega_{rec}NU_0^2\alpha_+^2}{\gamma_{fr}(\omega_{ca}^2 + \kappa^2)} \frac{1}{N} \sum_m [\kappa \cos(\theta_m - \theta_n) + \omega_{ca} \sin(\theta_m - \theta_n)]. \end{aligned} \quad (23.60)$$

Defining the *order parameter*,

$$b \equiv |b|e^{i\psi} \equiv \frac{1}{N} \sum_m e^{i\theta_m}, \quad (23.61)$$

which also implies,

$$|b|\sin(\psi - \theta_n) = \frac{1}{N} \sum_m \sin(\theta_m - \theta_n), \quad (23.62)$$

we can write Eq. (23.62) as,

$$\dot{\theta}_n = \frac{\xi_n}{\gamma_{fr}} + \frac{8\epsilon NU_0^2\alpha_+^2\kappa}{\gamma_{fr}(\omega_{ca}^2 + \kappa^2)} |b| \left[ \cos(\psi - \theta_n) + \frac{\omega_{ca}}{\kappa} \sin(\psi - \theta_n) \right]. \quad (23.63)$$

In the 'good cavity' limit,  $\kappa \ll \omega$ , using  $(2kv)^3 = 8\varepsilon NU_0^2 \alpha_+^2 \kappa / \gamma_{fr}$  and additionally assuming small amplitude oscillations,  $\psi \approx \theta_n$ , that is, good 'bunching',

$$\dot{\theta}_n \approx \frac{\xi_n}{\gamma_{fr}} + \frac{(2kv)^3}{\omega_{ca}^2} |b| + \frac{(2kv)^3}{\kappa \omega_{ca}} |b| \sin(\psi - \theta_n). \quad (23.64)$$

This shows that in the limit of perfect 'bunching'  $\omega_{ca} = 2kv$  must be satisfied. If really  $\kappa \ll \omega$  is valid, we can dispense the cosine. Introducing the Kuramoto coupling constant,

$$K \equiv \frac{16\omega_{rec} NU_0^2 \alpha_+^2 \omega_{ca}}{\gamma_{fr}(\omega_{ca}^2 + \kappa^2)} \approx \frac{1}{\kappa} \left( \frac{16\omega_{rec} NU_0^2 \alpha_+^2 \kappa}{\gamma_{fr}} \right)^{2/3} = (4\omega_{rec} \rho)^2 \left( \frac{4}{\kappa \gamma_{fr}^2} \right)^{1/3}, \quad (23.65)$$

using  $2\varepsilon\rho = (4\varepsilon NU_0^2 \alpha_+^2)^{1/3}$ , Eq. (23.63) is precisely the one used by the *Kuramoto model* of  $N$  coupled harmonic oscillators synchronizing over time,

$$\dot{\theta}_n \approx \frac{\xi_n}{\gamma_{fr}} + \frac{\kappa K}{\omega_{ca}} |b| + K |b| \sin(\psi - \theta_n). \quad (23.66)$$

Oscillators with  $\omega_n \leq K|b|$  are locked. For a reasonable 'bunching' this is satisfied in the 'good cavity' limit.

### 23.3.2.1 Kuramoto model with inertial effects

It is possible to incorporate inertial effects into the Kuramoto model [1]: allowing for  $\ddot{\theta}_n \neq 0$ , but still assuming  $d_t|\alpha_-| = 0$  and  $\dot{\alpha}_- = i\omega\alpha_-$ , the equation (23.60) becomes,

$$\begin{aligned} \ddot{\theta}_n &= -\gamma_{fr}\dot{\theta}_n + \xi_n + \frac{16\omega_{rec} NU_0^2 \alpha_+^2}{\omega^2 + \kappa^2} \frac{1}{N} \sum_m [\kappa \cos(\theta_m - \theta_n) + \omega \sin(\theta_m - \theta_n)] \\ &= -\gamma_{fr}\dot{\theta}_n + \xi_n + \frac{\kappa}{\omega} K |b| \cos(\psi - \theta_n) + K |b| \sin(\psi - \theta_n). \end{aligned} \quad (23.67)$$

### 23.3.3 Fokker-Planck equation

Let us write the *Kuramoto equation* including stochastic noise,

$$\dot{\theta}_n = \omega + K |b| \sin(\psi - \theta_n) + \xi_n(t), \quad (23.68)$$

define the order parameter,

$$b = |b| e^{i\psi}, \quad (23.69)$$

and the Langevin-force  $\langle \xi_n(t) \rangle = 0$  and  $\langle \xi_n(t) \xi_m(\tau) \rangle = 2D \delta_{ij} \delta(t - \tau)$ .

The Fokker-Planck equation associated to Eq. (23.68) reads,

$$\frac{\partial \rho}{\partial t} = - \frac{\partial \rho}{\partial \theta} [\omega + K |b| \sin(\psi - \theta)] + D \frac{\partial^2 \rho}{\partial \theta^2}, \quad (23.70)$$

where  $D = \sigma^2 / \gamma_{fr}$ . Inserting  $\rho(\theta, t) \equiv \sum_\nu \rho_\nu(t) e^{i\nu\theta}$ ,

$$\frac{\partial \rho_\nu}{\partial t} = -(\nu^2 D + i\nu\omega) \rho_\nu + \frac{1}{2} \nu K (b^* \rho_{\nu-1} - b \rho_{\nu+1}), \quad (23.71)$$

especially,

$$\int_0^{2\pi} \rho(\theta, t) d\theta = 1 \quad \implies \quad \rho_0 = \frac{1}{2\pi}, \quad (23.72)$$

and we defined the bunching as  $|b|$ , where,

$$b \equiv \int_0^{2\pi} \rho(\theta, t) e^{-i\theta} d\theta \quad \implies \quad b \equiv 2\pi\rho_1. \quad (23.73)$$

### 23.3.3.1 Laser-type equation for CARL

Defining the displacement of the  $n^{th}$  atomic oscillator as,

$$E_n \equiv e^{i\theta_n}, \quad (23.74)$$

we can rewrite the second equation (23.13) as,

$$\dot{E}_n = \frac{i\xi_n}{\gamma_{fr}} E_n - \frac{8\omega_{rec} U_0 \alpha_+}{\gamma_{fr}} (\alpha_- - \alpha_-^* E_n^2). \quad (23.75)$$

Substituting  $\alpha_-$  by the integral of the first equation (23.13),

$$\dot{E}_n = \frac{i\xi_n}{\gamma_{fr}} E_n + \frac{8\omega_{rec} i N U_0^2 \alpha_+^2}{\gamma_{fr}} \left( \int b e^{-\kappa(t-t')} dt' + E_n^2 \int b^* e^{-\kappa(t-t')} dt' \right). \quad (23.76)$$

In the limit  $e^{-\kappa(t-t')} = \kappa^{-1} \delta(t-t')$  we obtain an equation similar to that of an ordinary laser,

$$\begin{aligned} \dot{E}_n &= \frac{i\xi_n}{\gamma_{fr}} E_n + \frac{8\omega_{rec} i N U_0^2 \alpha_+^2}{\gamma_{fr} \kappa} (b + b^* E_n^2) \\ &= \frac{i\xi_n}{\gamma_{fr}} E_n + \frac{8\omega_{rec} i N U_0^2 \alpha_+^2}{\gamma_{fr} \kappa} \left( \sum_m E_m + \sum_m E_m^* E_n^2 \right). \end{aligned} \quad (23.77)$$

## 23.3.4 Exercises

### 23.3.4.1 Ex: Kuramoto simulations

Implement the Kuramoto model with pendulum clocks.

## 23.4 Thermodynamics of the CARL process

There is an analogy between the laser threshold and a second-order phase transition [626], p. 341 ff: '... The usual treatment of laser behavior is a self-consistent field theory. In the laser analysis each atom develops a radiating dipole in an electromagnetic field due to (i.e. emitted by) all the other atoms. The radiation field produced by an ensemble of radiating atoms is then calculated in a self-consistent fashion. (...This) suggests the identification of the laser electric field as the variable corresponding to the (...) order parameter and the atomic population inversion as that corresponding to the temperature.'



Note that numerical simulations revealed that in certain regimes the CARL corresponds to a first-order phase transition: At high temperatures the probe to pump power diagram shows bistability [366] and [582]<sub>DOI</sub>.

The correspondence between CARL and a common laser is illustrated by the table below. A number of questions arise from the analogy: The CARL being a laser without inversion, what is the equilibrium parameter? Is it the temperature of the atomic cloud? How to calculate the density of states?

	ferromagnet	laser
control parameter	external magnetic field $H$	pump intensity $\mathcal{S}$
equilibrium parameter	temperature $T$	population inversion $\sigma$
order parameter	magnetization $\langle M \rangle = \begin{cases} 0 & T > T_c \\ c\sqrt{\frac{T_c - T}{T}} & T < T_c \end{cases}$	electric field $\langle E \rangle = \begin{cases} 0 & \sigma > \sigma_c \\ c\sqrt{\frac{\sigma_c - \sigma}{\sigma}} & \sigma < \sigma_c \end{cases}$
probability density	$P(M) \propto e^{-F(M)/k_B T}$	$P$ -representation $P(x, y) \propto e^{-G(x, y)/K\sigma}$
thermodyn. free energy	$F = F(T, H)$	$G(x, y)$
heat capacity	$C(T) = \frac{\partial E(T)}{\partial T}$	?

	CARL atoms	CARL light
control parameter	pump intensity $\eta$	pump intensity $\eta$
equilibrium parameter	temperature $T$	?
order parameter	bunching $b = \begin{cases} 0 & T > T_c \\ ? & T < T_c \end{cases}$	electric field $\langle \alpha \rangle = \begin{cases} 0 \\ ? \end{cases}$
probability density	?	?
thermodyn. free energy	?	?
heat capacity	?	?

### 23.4.1 CARL as a laser

Why is CARL a laser? What is the basic difference between CARL and an AOM or a moving Bragg mirror? CARL is essentially based on exponential self-amplification. This self-amplification is in fact observed in our switch-off experiment [416]<sub>DOI</sub>. But a laser is normally understood as a steady-state system. For CARL to find to a steady-state we have to insert friction forces.

Gordon rewrites the CARL as a common laser: He generalizes the linear stability analysis (previous Sec.) and retains the lowest-order nonlinearity. The Fokker-Planck equations read:

$$\begin{aligned} \frac{dB_n}{d\tau} &= \eta(aB_{n-1} + a^*B_{n+1}) - n^2DB_n \\ \frac{da}{d\tau} &= B_1 - \kappa a, \end{aligned} \quad (23.78)$$

with  $B_0 = 1$  and  $B_{-n} = B_n^*$ . Linearization means  $B_{n>1} = 0$ ,

$$\begin{aligned}\frac{dB_1}{d\tau} &= \imath a - DB_1 \\ \frac{da}{d\tau} &= B_1 - \kappa a\end{aligned}\quad (23.79)$$

or,

$$\begin{aligned}\frac{d^2a}{d\tau^2} + (\kappa + D)\frac{da}{d\tau} + (\kappa D - \imath)a &= 0 \\ \frac{d^2B_1}{d\tau^2} + (\kappa + D)\frac{dB_1}{d\tau} + (\kappa D - \imath)B_1 &= 0\end{aligned}\quad (23.80)$$

The determinant is,

$$\det \begin{pmatrix} -D - \lambda & \imath \\ 1 & -\kappa - \lambda \end{pmatrix} = (D + \lambda)(\kappa + \lambda) - \imath = 0 \quad (23.81)$$

Including the lowest-order nonlinear term means  $B_{n>2} = 0$ ,

$$\begin{aligned}\frac{dB_2}{d\tau} &= 2\imath a B_1 - 4DB_2 \\ \frac{dB_1}{d\tau} &= \imath a + \imath a^* B_2 - DB_1 \\ \frac{da}{d\tau} &= B_1 - \kappa a\end{aligned}\quad (23.82)$$

Assuming  $dB_2/d\tau = 0$ ,

$$\begin{aligned}\frac{dB_1}{d\tau} &= \imath a - \left(\frac{|a|^2}{2D} + D\right) B_1 \\ \frac{da}{d\tau} &= B_1 - \kappa a\end{aligned}\quad (23.83)$$

or,

$$\begin{aligned}\frac{d^2B_1}{d\tau^2} + (\kappa + D)\frac{dB_1}{d\tau} + (\kappa D - \imath)B_1 &= -\frac{1}{2D} \left(\frac{d}{d\tau} + \kappa\right) |a|^2 B_1 \\ &= -(K_1|a|^2 - K_2|a|^4) B_1 \\ \frac{d^2a}{d\tau^2} + (\kappa + D)\frac{da}{d\tau} + (\kappa D - \imath)a &= -\frac{|a|^2}{2D} \left(\frac{d}{d\tau} + \kappa\right) a\end{aligned}\quad (23.84)$$

substitute  $a(\tau) = A(\tau)e^{\lambda\tau}$  and Eq. (xx),

$$\begin{aligned}e^{\lambda\tau} \left(\frac{d^2}{d\tau^2} + 2\lambda\frac{d}{d\tau} + \lambda^2\right) A + e^{\lambda\tau} \left((\kappa + D)\frac{d}{d\tau} + (\kappa + D)\lambda\right) A - (\lambda^2 + D\lambda + \kappa\lambda)e^{\lambda\tau} A \\ = -\frac{|e^{\lambda\tau} A|^2}{2D} \left(e^{\lambda\tau}\frac{dA}{d\tau} + \lambda e^{\lambda\tau} A + \kappa e^{\lambda\tau} A\right)\end{aligned}\quad (23.85)$$

neglect  $d^2 A/d\tau^2$  and  $|A|^2 dA/d\tau$ ,

$$e^{\lambda\tau} 2\lambda \frac{dA}{d\tau} + e^{\lambda\tau} (\kappa + D) \frac{dA}{d\tau} = -\frac{|e^{\lambda\tau} A|^2}{2D} (\lambda e^{\lambda\tau} A + \kappa e^{\lambda\tau} A) \quad (23.86)$$

substitute back  $a(\tau) = A(\tau)e^{\lambda\tau}$ ,

$$\begin{aligned} \frac{da}{d\tau} &= \lambda a - \frac{\lambda + \kappa}{2D(2\lambda + \kappa + D)} |a|^2 a \\ &= \lambda a - C|a|^2 a \end{aligned} \quad (23.87)$$

or,

$$\frac{d|a|^2}{d\tau} = 2|a|^2 \operatorname{Re} \lambda - 2|a|^4 \operatorname{Re} C \quad (23.88)$$

in steady-state,

$$0 = \lambda a - C|a|^2 a . \quad (23.89)$$

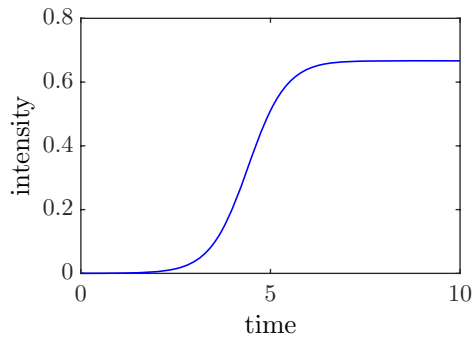


Figure 23.7: (code) Laser crossing the threshold.

According to A. Politi a general laser theory exists, there is no point in repeating this for CARL. The analogy is there and evident.

### 23.4.1.1 CARL as a ferromagnet

A similar treatment with  $a(\tau) = A(\tau)e^{\lambda\tau}$  and  $B_1(\tau) = \beta(\tau)e^{\lambda\tau}$  and  $d^2\beta/d\tau^2 = 0$  and  $|A|^2 d\beta/d\tau = 0$  and  $\beta d|A|^2/d\tau = 0$  results in,

$$\begin{aligned} \frac{dB_1}{d\tau} &= \lambda B_1 - \frac{2\lambda + \lambda^* + \kappa}{2D(2\lambda + \kappa + D)} |a|^2 B_1 \\ &= \lambda B_1 - \tilde{C}|a|^2 B_1 , \end{aligned} \quad (23.90)$$

i.e. the instability comes from the field and it drives the bunching.

### 23.4.2 Out-of-equilibrium thermodynamics

Strictly speaking the above analogy is flawed. In particular the analogy between CARL bunching and ferromagnetic ordering is not good. While the ferromagnetic ordering occurs as a thermodynamic phase transition, the CARL bunching is driven by a dissipative force, which triggers spatio-temporal instabilities. Therefore viscous CARL occurs far from thermodynamic equilibrium. This may point towards an interpretation of CARL bunching as a *dissipative structure* along the lines traced by Prigogine, who showed that *non-equilibrium may be a source of order*.

On the other hand, the laser itself is a system operating far from thermal equilibrium, since it requires a pump to emit steady-state radiation. Perhaps a comparison with *estruturas de Bénard* is better than with ferromagnets. Bénard structures occur as spontaneous breaking of translational symmetry, just like CARL. One could say that the periodicity of CARL is predefined by the pump laser wavelength, and thus not surprising. However, the size of the periodic structures is always fixed by boundary conditions in a more or less complicated way. For example, the size of the Bénard structures is fixed by the viscosity, the provided amount of heat, etc., the wavelength of surface waves can be calculated from first principles, i.e. the Navier-Stokes equations and the continuity equation for given boundary conditions. The symmetry breaking resides in the exact *place*, where the Bénard structure develops. It is the *phase*, which is broken, just like for CARL.

The Kuramoto model and the Weiss model of ferromagnetism are both mean field theories [632]. Despite the fundamental difference that ferromagnetism is a thermodynamic feature and Kuramoto a nonequilibrium phenomenon, they are far-reaching analogies. The role of temperature in ferromagnetism is played by external noise in Kuramoto. CARL is clearly a dissipative structure: *It survives only as long as energy is fed to the system*.

#### 23.4.2.1 Finite and infinite temperature reservoirs

The phase transition is ruled by a competition of dissipation and diffusion. If the reservoir has zero temperature  $\gamma_{fric} \neq 0$  but  $D = \sigma^2/\gamma_{fric} = 0$ , i.e. we have dissipation without diffusion. In this case, we do not expect a threshold behavior. The Lindtblad operator for coupling to a finite-temperature reservoir is something like  $\mathcal{L} \approx \kappa(\bar{n} + 1) \{...emission...\} + \kappa\bar{n} \{...absorption...\} + \eta \{...phase\ noise...\}$ , where  $\bar{n}$  is the mean photon number at thermal equilibrium with a given temperature  $T \propto \bar{n}/(\bar{n} + 1)$ . The interpretation in terms of dissipation without diffusion is correct according to A. Buchleitner. There are three kinds of noises: 0 temperature noise for  $\bar{n} \rightarrow 0$ ,  $\infty$  temperature noise for  $\bar{n} \approx \bar{n} + 1$  and phase noise. Thus for  $T = 0$  the energy flux goes only from the system to the reservoir. At  $T > 0$  entropy may go from the reservoir to the system. The system reaches its cooling limit when the temperatures of the system and the reservoir are balanced.

But how to explain Doppler cooling or cavity-cooling? The electromagnetic vacuum is an effective  $T = 0$  reservoir, but the cooling is nevertheless limited by the spontaneous decay width or the cavity linewidth, resp.. Why does coupling to a zero-temperature reservoir not cool down to zero? Apparently, the coupling is afflicted by vacuum noise. This permits coupling of degrees of freedom having different temperatures without reaching a temperature equilibrium. Examples are the limit of

cavity-cooling to the cavity decay width or simply Doppler-cooling by spontaneous emission.

Interprete damping as scattering into continuum!

## 23.5 Coherent properties of CARL

In Ref. [415] we have demonstrated collective interaction of atoms with light fields and how the application of friction via optical molasses can lead to stationary CARL radiation at a self-determined frequency. In the papers [583, 701] we have demonstrated that the molasses also lead to diffusion resulting in a threshold behavior and in atomic self-organization at finite temperatures. An interesting question is whether the temperature not only determines the collective behavior, but also the deviation from it. The temperature being related to the amount of random walk on top of the center-of-mass motion, we may wonder whether the viscous CARL radiation bears a signature of the atomic temperature not only in the self-determined CARL frequency, but also in the laser emission bandwidth. It is conceivable that the autocorrelation functions and the emission spectrum of the CARL are influenced by the fact that the atoms experience a random walk in momentum space due to the diffusion in the optical molasses.

In this subtext we will attempt an analytical approach, present numerical simulations and discuss how to access to the informations experimentally. The Fokker-Planck approach described in Refs. [583, 701] is particularly well adapted to calculating collective variables. In contrast the simulation of the Langevin equation conveniently gives access to the noise properties.

### 23.5.1 Analytical derivation of the coherence

Our starting point are the Langevin equations (23.13) [583, 701] in the adiabatic limit,  $\dot{\theta}_n = 0$ . The Langevin noise force is uncorrelated,

$$\langle \xi_n^*(t) \xi_m(t + \tau) \rangle \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \xi_n^*(t) \xi_m(t + \tau) d\tau = 2D_{\dot{\theta}} \delta_{mn} \delta(\tau) , \quad (23.91)$$

where the momentum diffusion coefficient  $D_{\dot{\theta}} = \gamma_{fr} \sigma^2$  is proportional to the atoms' equilibrium temperature, which is related to the Maxwell-Gaussian velocity spread by  $\sigma \equiv 2k\sqrt{k_B T/m}$ . In contrast, the trajectories of the atoms are not, because all atoms are motionally coupled by the fields, so that the noise imparted to one atom is sensed by all others. Therefore the relationship (23.92) certainly does not hold for the atomic positions,

$$\langle \theta_n^*(t) \theta_m(t + \tau) \rangle \approx \delta_{mn} \delta(\tau) . \quad (23.92)$$

#### 23.5.1.1 Single atom

So, let us first concentrate on a single atom coupled to the cavity fields. If its velocity only fluctuates a little around a mean value  $\omega_{ca}$ , we may write  $\theta(t) \equiv \omega_{ca}t + \varphi(t)$ . The randomized position has a Gaussian statistics leading to a Brownian motion described

by a Wiener-Levy stochastic process:  $\langle \varphi(t) \rangle = 0$  and  $\langle \varphi(t)\varphi(t+\tau) \rangle = D_\theta(2t+\tau-|\tau|)$  ([626], p. 344),

$$R_{\dot{\theta}}(\tau) = \langle [\omega_{ca} + \dot{\varphi}(t)][\omega_{ca} + \dot{\varphi}(t+\tau)] \rangle = \langle \dot{\varphi}(t)\dot{\varphi}(t+\tau) \rangle = 2D_\theta\delta(\tau) , \quad (23.93)$$

where  $D_\theta = \sigma^2/\gamma_{fr}$  is the position diffusion coefficient. Note that deterministic parts are removed from the function in order to satisfy  $\langle \dot{\varphi}(t) \rangle = 0$ . In that case the *spectral density of fluctuations of the atomic phase* is constant,

$$S_{\dot{\theta}}(f) = \int_{-\infty}^{\infty} R_{\dot{\theta}}(\tau)e^{-2\pi i f \tau} d\tau = 2D_\theta . \quad (23.94)$$

Note that  $S_{\dot{\theta}}(f) = f^2 S_\theta(f)$ . The *variance of the fluctuations* for white noise is or,

$$\sigma_{\dot{\theta}}^2(\tau) = \langle \dot{\varphi}(t)^2 \rangle = \frac{D_\theta}{\tau} . \quad (23.95)$$

Under the assumption  $\dot{\alpha}_- = i\omega_{ca}\alpha_-$  and introducing the abbreviation  $\alpha_0 \equiv -iU_0\alpha_+ / (\kappa + i\omega_{ca})$ , the first equation (23.13) takes the form  $\alpha_- = \alpha_0 e^{i\theta}$  such that the *autocorrelation function of the field amplitude* reads,

$$\begin{aligned} R_\alpha(\tau) &\equiv \langle \alpha_-^*(t)\alpha_-(t+\tau) \rangle \\ &= |\alpha_0|^2 \langle e^{i[\theta(t+\tau)-\theta(t)]} \rangle \\ &= |\alpha_0|^2 e^{i\omega_{ca}\tau} \langle e^{i[\varphi(t+\tau)-\varphi(t)]} \rangle = |\alpha_0|^2 e^{i\omega_{ca}\tau} \langle e^{i\tau\dot{\varphi}(t)} \rangle . \end{aligned} \quad (23.96)$$

In the case of a Gaussian distribution for the noise amplitude with  $\dot{\varphi}(t) = \dot{\varphi}(-t)$ , we have  $\langle \dot{\varphi}^{2k-1} \rangle / (2k-1)! = 0$  and  $\langle \dot{\varphi}^{2k} \rangle / (2k)! = \langle \frac{1}{2}\dot{\varphi}^2 \rangle^k / k!$  [171, ?, 225],

$$\begin{aligned} \langle e^{i\tau\dot{\varphi}(t)} \rangle &= \sum_k \frac{i^k \langle \tau^k \dot{\varphi}(t)^k \rangle}{k!} = \sum_k \frac{i^{2k} \langle \tau^{2k} \dot{\varphi}(t)^{2k} \rangle}{(2k)!} \\ &= \sum_k \frac{\langle -\frac{1}{2}\tau^2 \dot{\varphi}(t)^2 \rangle^k}{k!} = e^{-\frac{1}{2}\tau^2 \langle \dot{\varphi}(t)^2 \rangle} . \end{aligned} \quad (23.97)$$

Apparently, noise mainly affects the field's phase and not its amplitude. Note that the *first-order coherence* is just the normalized autocorrelation  $g^{(1)}(\tau) \equiv R_\alpha(\tau)/R_\alpha(0)$ ,

$$\begin{aligned} g^{(1)}(\tau) &= e^{i\omega_{ca}\tau} e^{-\omega_{ca}^2 \tau^2 \sigma_\theta^2 / 2} \\ &= e^{i\omega_{ca}\tau} e^{-D_\theta |\tau| / 2} . \end{aligned} \quad (23.98)$$

The *power spectral density* is a Lorentzian,

$$\begin{aligned} S_\alpha(\omega) &= |\alpha_0|^2 \int_{-\infty}^{\infty} R_\alpha(\tau) e^{-i\omega\tau} d\tau \\ &= \frac{|\alpha_0|^2 D_\theta^2}{(\omega - \omega_{ca})^2 + D_\theta^2} . \end{aligned} \quad (23.99)$$

The CARL *emission bandwidth* is thus  $\frac{1}{2}D_\theta$ . The above results show that the CARL laser bandwidth increases linearly with temperature and reduces with the friction force. In our experiment we have  $\gamma_{fr} = 5\kappa$  and  $\sigma = 10\kappa$ , so that  $D_\theta = \sigma^2/\gamma_{fr} = 20\kappa$ . The CARL bandwidth is extremely large as compared to the CARL frequency  $\omega_{ca} = 5\kappa$ . The reason is that we only considered a single atom. The impact of several atoms will partially compensate and reduce the linewidth.

### 23.5.1.2 Many atoms, hand-waving

In order to account for the combined effect of many atoms, we reconsider the Eq. (23.13). If  $\dot{\alpha}_- = i\omega_{ca}\alpha_-$ , we may write it like,

$$\begin{aligned}\alpha_- &= \alpha_0 \sum_m e^{i\theta_m}, \\ \dot{\theta}_n &= \frac{4\varepsilon i U_0 \alpha_+ \alpha_0}{\gamma_{fr}} \sum_m (e^{i\theta_m - i\theta_n} + e^{-i\theta_m + i\theta_n}) + \frac{\xi_n}{\gamma_{fr}}.\end{aligned}\quad (23.100)$$

The light mode  $\alpha_-$  appears to be a superposition of coherent waves having the same frequencies,  $\alpha_m(t) = \alpha_0 e^{i\omega_{ca}t + i\varphi_m(t)}$ , but interrupted by random phase jumps. We may thus try an analogous argumentation as for pressure broadening,

$$\begin{aligned}\langle \alpha_-^*(t) \alpha_-(t + \tau) \rangle &= |\alpha_0|^2 \int \sum_n e^{-i\omega_{ca}t - i\varphi_n(t)} \sum_m e^{i\omega_{ca}t + i\omega_{ca}\tau + i\varphi_n(t + \tau)} dt \\ &= |\alpha_0|^2 e^{i\omega_{ca}\tau} \sum_{n,m} \int e^{i\varphi_m(t + \tau) - i\varphi_n(t)} dt = N \langle \alpha_n^*(t) \alpha_m(t + \tau) \rangle \delta_{nm}.\end{aligned}$$

Cross-terms vanish, the autocorrelation function is just the sum of the single-atom components. However, while we may view the noise impact of the atoms as coming from a single atom, the rate of the phase jumps is much higher, than for a single atom. For one atom the probability density for encountering a coherent interval of length  $\tau$  is given by  $p_1(\tau)d\tau = \frac{1}{2}D_\theta e^{-D_\theta|\tau|/2}d\tau$  [440]. Thus,

$$\langle \alpha_1^*(t) \alpha_1(t + \tau) \rangle = |\alpha_0|^2 e^{i\omega_{ca}\tau} e^{-D_\theta|\tau|/2} = |\alpha_0|^2 e^{i\omega_{ca}\tau} \int_\tau^\infty p_1(\tau') d\tau'. \quad (23.101)$$

For  $N$  atoms we expect a probability density for encountering a coherent interval of length  $\tau$ ,

$$p_N(\tau)d\tau = p_1(\tau/N)d\tau = \frac{D_\theta}{2\sqrt{N}} e^{-D_\theta|\tau|/2\sqrt{N}} d\tau, \quad (23.102)$$

such that  $\int_0^\infty p_N(\tau') d\tau' = 1$ . However this remains to prove. Thus,

$$g_N^{(1)}(\tau) = e^{i\omega_{ca}\tau} \int_\tau^\infty p_N(\tau') d\tau' = e^{i\omega_{ca}\tau - D_\theta|\tau|/2\sqrt{N}}. \quad (23.103)$$

The second-order correlation function is,

$$g_N^{(2)}(\tau) = 1 + |g_N^{(1)}(\tau)|^2. \quad (23.104)$$

The laser bandwidth is accordingly reduced by,

$$D_N = \frac{D_\theta}{\sqrt{N}}. \quad (23.105)$$

Fig. 23.8 shows the dependencies of the correlation functions on  $N$  and  $T$ . For  $N = 10^6$  atoms the CARL bandwidth becomes  $\beta_N = 0.01\kappa$ , which is already well below any mechanical noise. The linewidth reduction with increasing atom numbers is quantitatively supported by numerical simulations (see below).

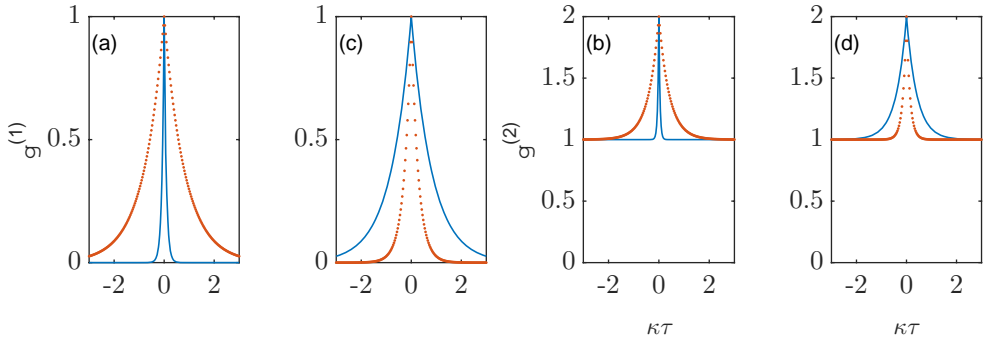


Figure 23.8: (code) First and second-order correlation functions. The solid and dotted lines in (a) and (b) are calculated for  $N = 1$  and  $N = 100$ , resp.. The solid and dotted lines in (c) and (d) are calculated for  $T = 100 \mu\text{K}$  and  $T = 300 \mu\text{K}$ , resp..

### 23.5.1.3 Many atoms, formal

In order to account for the combined effect of many atoms, we reconsider the Eq. (23.13). If  $\dot{\alpha}_- = i\omega_{ca}\alpha_-$ , we get,

$$\alpha_- = -\frac{iU_0\alpha_+}{\kappa + i\omega_{ca}} \sum_m e^{i\theta_m}, \quad (23.106)$$

$$\dot{\theta}_n = \frac{4\varepsilon U_0^2 \alpha_+^2}{\gamma_{fr}(\kappa + i\omega_{ca})} \sum_m (e^{i\theta_m - i\theta_n} + e^{-i\theta_m + i\theta_n}) + \frac{\xi_n}{\gamma_{fr}}.$$

The autocorrelation is then,

$$R_\alpha(\tau) \equiv \langle \alpha_-^*(t) \alpha_-(t+\tau) \rangle = \frac{U_0^2 \alpha_+^2}{\kappa^2 + \omega_{ca}^2} \sum_{n,m} \langle e^{i\theta_n(t+\tau) - i\theta_m(t)} \rangle \quad (23.107)$$

$$= |\alpha_0|^2 e^{i\omega_{ca}\tau} \sum_{n,m} \langle e^{i\varphi_n(t+\tau) - i\varphi_m(t)} \rangle = |\alpha_0|^2 e^{i\omega_{ca}\tau} \sum_{n,m,k} \frac{i^k}{k!} \langle [\varphi_n(t+\tau) - \varphi_m(t)]^k \rangle$$

$$= |\alpha_0|^2 e^{i\omega_{ca}\tau} \sum_{n,m,k} \frac{i^k}{k!} \sum_{j=0}^k (-1)^j \binom{k}{j} \langle \varphi_n(t+\tau)^j \varphi_m(t)^{k-j} \rangle.$$

The main role of cavity-induced interparticle correlations is to self-consistently establish a constant center-of-mass motion  $\omega_{ca}$ . We may, to first order, neglect the possibility that the coupling correlates the noise, since the noise is imprinted from the outside, i.e. the molasses. Therefore,  $\langle \varphi_n(t+\tau) \varphi_m(t) \rangle \propto \delta_{nm}$ ,

$$\langle \varphi_n(t+\tau)^j \varphi_m(t)^{k-j} \rangle = \sum_{\text{all pairs}} \langle \varphi_n(t+\tau)^2 \rangle^{j/2} \langle \varphi_m(t)^2 \rangle^{k/2 - j/2} \quad (23.108)$$

$$= \frac{j!}{2^{j/2}(j/2)!} \frac{(k-j)!}{2^{(k-j)/2}(k/2 - j/2)!} \langle \varphi_n(t+\tau)^2 \rangle^{j/2} \langle \varphi_m(t)^2 \rangle^{k/2 - j/2}$$

so that,

$$R_\alpha(\tau) = |\alpha_0|^2 e^{i\omega_{ca}\tau} \sum_{n,m,k} \frac{i^k}{k!} \sum_{j=0}^k \binom{k}{j} \frac{j!}{2^{j/2}(j/2)!} \frac{(k-j)!}{2^{(k-j)/2}(k/2 - j/2)!} \langle \varphi_n(t+\tau)^2 \rangle^{j/2} \langle \varphi_m(t)^2 \rangle^{k/2 - j/2} \quad (23.109)$$



where  $j$  and  $k$  are even,

$$\begin{aligned}
R_\alpha(\tau) &= |\alpha_0|^2 e^{i\omega_{ca}\tau} \sum_{n,m,k} \frac{i^k}{2^{k/2} (k/2)!} \sum_{j=0}^k \binom{k/2}{j/2} \langle \varphi_n(t+\tau)^2 \rangle^{j/2} \langle \varphi_m(t)^2 \rangle^{k/2-j/2} \\
&= |\alpha_0|^2 e^{i\omega_{ca}\tau} \sum_{n,m,k} \frac{1}{(k/2)!} \left( -\frac{1}{2} \langle \varphi_n(t+\tau)^2 \rangle - \frac{1}{2} \langle \varphi_m(t)^2 \rangle \right)^{k/2} \\
&= |\alpha_0|^2 e^{i\omega_{ca}\tau} \sum_n e^{-\frac{1}{2} \langle \varphi_n(t+\tau)^2 \rangle} \sum_m e^{-\frac{1}{2} \langle \varphi_m(t)^2 \rangle} = |\alpha_0|^2 N^2 e^{i\omega_{ca}\tau} e^{-\frac{1}{2} \langle \varphi_n(t+\tau)^2 \rangle} e^{-\frac{1}{2} \langle \varphi_n(t)^2 \rangle} .
\end{aligned} \tag{23.110}$$

#### 23.5.1.4 Memory effects

Relax adiabaticity,  $\dot{\alpha}_- \neq i\omega_{ca}\alpha_-$ , substitute  $\beta = e^{\kappa t}\alpha_-$ ,

$$\begin{aligned}
\dot{\theta} &= \frac{4\varepsilon i U_0 \alpha_+}{\gamma_{fr}} (\beta e^{-i\theta - \kappa t} - \beta^* e^{i\theta - \kappa t}) + \frac{\xi}{\gamma_{fr}} , \\
\beta &= -i U_0 \alpha_+ \int^t e^{i\theta + \kappa t'} dt' .
\end{aligned} \tag{23.111}$$

so that,

$$\begin{aligned}
R_\alpha(\tau) &\equiv \langle \alpha_-^*(t) \alpha_-(t+\tau) \rangle = \langle e^{-\kappa t} \beta^*(t) e^{-\kappa t - \kappa \tau} \beta(t+\tau) \rangle \\
&= e^{-\kappa \tau} \langle e^{-2\kappa t} \beta^*(t) \beta(t+\tau) \rangle \\
&= U_0^2 \alpha_+^2 e^{-\kappa \tau} \int \int^t \int^{t+\tau} e^{i\theta(t'') - i\theta(t') + \kappa t' + \kappa t'' - 2\kappa t} dt'' dt' dt \\
&= U_0^2 \alpha_+^2 e^{-\kappa \tau} \int \int^t \int^{t+\tau} e^{i\omega_{ca} t'' - i\omega_{ca} t' + i\varphi(t'') - i\varphi(t') + \kappa t' + \kappa t'' - 2\kappa t} dt'' dt' dt .
\end{aligned} \tag{23.112}$$

Using the representation of half the  $\delta$ -distribution  $\int^t e^{(i\omega_{ca} + \kappa)t'} dt' = \delta_{1/2} = \lim_{\kappa \rightarrow 0} \frac{1}{\kappa + i\omega_{ca}}$ .

#### 23.5.1.5 Schawlow-Townes limit for CARL

The ultimate limit for the spectral purity of a perfectly stable laser oscillator is the *Schawlow-Townes limit* [609]. The origin of this limitation is the discrete nature of the light field. Similarly to quantum projection noise, which is caused by the discretisation of atomic energy levels, the optical *shot-noise* registered in photodetectors arises from the discrete repartition of electromagnetic energy in photons. With a laser power  $P$ , a cavity bandwidth  $\kappa$  and an interrogation time  $\tau$ , the Allan variance [?] and the linewidth of a Schawlow-Townes limited laser are given by,

$$\begin{aligned}
\sigma_{ST}(\tau) &= \frac{1}{\omega/\kappa} \frac{1}{\sqrt{(P/\hbar\omega)\tau}} , \\
\beta &= \kappa^2 \frac{\hbar\omega}{P} .
\end{aligned} \tag{23.113}$$

In the case of CARL, using  $P = \delta\hbar\omega|\alpha_-|^2$  the variance is  $\sigma_{ST}^2(\tau) = \kappa/\tau\omega\delta|\alpha_-|^2 \approx 10^{-20} \text{ s}/\tau$ . The shot-noise which limits the CARL is not the one of the CARL light

itself, but the random momentum kicks imparted by molasses-cooled atoms. The CARL linewidth is  $\beta = \kappa^2 / \delta |\alpha_-|^2 = 10^{-14} \kappa$ .

The time-lap between two scattering events for a single atom be distributed according to  $p_1(\tau) d\tau = \gamma e^{-\gamma\tau} d\tau$ . What is the waiting time distribution for two atoms [611]? Schenzle related the waiting time distribution to the autocorrelation function  $g^{(2)}(\tau)$ .

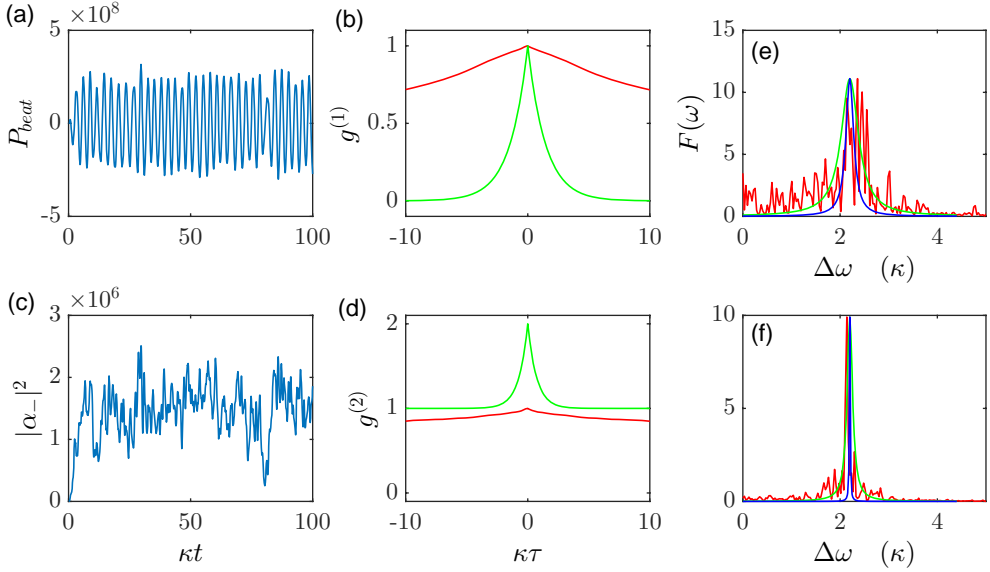


Figure 23.9: Simulated time-dependence of the (a) beat and the (b) intensity signals. Calculated (c) first and second-order correlation functions. The temperature was set to  $T = 100 \mu\text{K}$  and the atom number to  $N = 40$ . (e-f) Spectra of the CARL laser for (e) 4 and (f) 40 atoms. The total coupling constant  $NU_0$  has been held constant, only the number of atoms whose trajectories are simulated is varied.

Fig. 23.9(e-f) shows spectra of the CARL frequency obtained by Fourier-transforming the autocorrelation function of a Langevin-simulated trajectory of the CARL frequency. The width results from thermal fluctuations in the atomic motion induced by momentum diffusion in the molasses. It is clearly visible that the width is reduced when the atom number is increased, thus confirming Eq. (23.105).

## 23.5.2 Measuring the coherence properties

We may also attempt to verify the predictions in experiment. Our signals are the beams transmitted through the cavity mirrors.

### 23.5.2.1 Homodyne signal

Ideally in order to get the full information on the the first-order coherence, we should record both the in-phase and the quadrature component of the field  $\alpha_- = \text{Re} \alpha_- + i \text{Im} \alpha_-$  by homodyning it with the local oscillator  $\alpha_+$ . Thus we need to use both

ports of the beamsplitter: For the in-phase component we get,

$$\begin{aligned}
 P_{\text{hody}}^{(ph)} &\propto b^\dagger b - c^\dagger c & (23.114) \\
 &= |\alpha_+ \sqrt{\eta} + \alpha_- \sqrt{1-\eta}|^2 - |\alpha_+ \sqrt{1-\eta} - \alpha_- \sqrt{\eta}|^2 \\
 &= (1-2\eta)(|\alpha_-|^2 - |\alpha_+|^2) + 4\sqrt{\eta-\eta^2} \alpha_+ \text{Re } \alpha_- .
 \end{aligned}$$

For a 50% beamsplitter the offsets disappear,  $P_{\text{hody}}^{(ph)} \propto 2\alpha_+ \text{Re } \alpha_-$ , which means that the homodyne signal is insensitive to intensity noise in the individual ports. Similarly we obtain for the quadrature component,

$$\begin{aligned}
 P_{\text{hody}}^{(qu)} &\propto |\alpha_+ \sqrt{\eta} + i\alpha_- \sqrt{1-\eta}|^2 - |\alpha_+ \sqrt{1-\eta} - i\alpha_- \sqrt{\eta}|^2 & (23.115) \\
 &= -2\alpha_+ \text{Im } \alpha_- .
 \end{aligned}$$

By mounting a piezo on one of the mirrors in the homodyne loop, we can influence which quadrature component to map. Is there a way how to get  $\text{Im } \alpha_-$  and  $\text{Re } \alpha_-$  simultaneously?

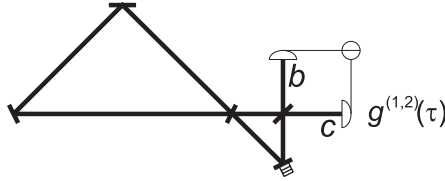


Figure 23.10: Homodyning the counterpropagating beams.

Knowing  $\alpha_-$  we can calculate the *first order coherence*,

$$g^{(1)}(\tau) \equiv \frac{\langle \alpha^*(t) \alpha(t+\tau) \rangle}{\langle \alpha^*(t) \alpha(t) \rangle} = \frac{\int \alpha^*(t) \alpha(t+\tau) dt}{\int \alpha(t)^2 dt} , \quad (23.116)$$

the *second-order coherence*,

$$\begin{aligned}
 g^{(2)}(\tau) &\equiv \frac{\langle \alpha^*(t) \alpha^*(t+\tau) \alpha(t+\tau) \alpha(t) \rangle}{\langle \alpha^*(t) \alpha(t) \rangle^2} & (23.117) \\
 &= \frac{\int P_-(t) P_-(t+\tau) dt}{\int P_-(t) dt} ,
 \end{aligned}$$

and the *emission spectrum* (power spectral density),

$$F(\omega) = \frac{1}{\pi} \text{Re} \int g^{(1)}(\tau) e^{i\omega\tau} d\tau . \quad (23.118)$$

All these quantities can be evaluated from numerical simulations of the Langevin equations.

### 23.5.2.2 Real Signals

What we record in experiment is the probe field power  $P_{probe}$  and only one quadrature component of the beat between the probe and the pump. The probe signal is simply,

$$P_- \propto |\alpha_-|^2 . \quad (23.119)$$

So it may be used directly for the intensity correlation function (23.117) analogous to *Hanbury-Brown-Twiss*.

The beat signal is obtained in a *Young* type experiment,

$$P_{beat} \propto |\alpha_+ \pm \alpha_-|^2 = |\alpha_+|^2 + |\alpha_-|^2 \pm 2\alpha_+ \text{Re } \alpha_- , \quad (23.120)$$

because we may assume  $\alpha_+$  real. Obviously, the beat signal oscillates between the limits  $\pm 2\alpha_+|\alpha_-|$ . Currently, we only use one port of the beamsplitter. Thus we miss information on the other quadrature phase. The question arises now, how to calculate the spectrum if only the real part of the field  $\text{Re } \alpha$  is known. The interesting quantity is  $|g^{(1)}(\tau)|$ , because it contains the information on the photon statistics. This function is smooth (it does not oscillate) and should in our case describe an exponential decay (23.98). Fortunately, from numerical calculation it seems that  $|g^{(1)}(\tau)|$  is just the convolution of  $\langle \text{Re } \alpha(t) \text{Re } \alpha(t + \tau) \rangle / \langle \text{Re}^2 \alpha(t) \rangle$ , so that we may recover the informations. For the spectrum, which is calculated from the complex quantity  $g^{(1)}(\tau)$  the question is more delicate. It comes down to asking if,

$$F(\omega) \propto \text{Re} \int \langle \text{Re } \alpha(t) \text{Re } \alpha(t + \tau) \rangle e^{i\omega\tau} d\tau \quad (23.121)$$

gives the correct spectrum (23.118)?

### 23.5.2.3 Preliminary experimental observations

Technical noise may overrule the thermal noise just like in ordinary lasers. This situation may change if atom numbers are low, so that we have bad statistics, or if the collective force is strong enough to correlate the noise.

The spectral width may also be limited by the finite time window  $t \in [-\frac{1}{2}t_0, \frac{1}{2}t_0]$ , which is taken for computing the spectrum. Even a perfect harmonic oscillation  $\alpha_-(t) = \alpha_- e^{i\omega_{ca}t}$  will then have a finite bandwidth,

$$\begin{aligned} F_{a_-}(\omega) &= F[\alpha_- e^{i\omega_{ca}t}] \star F[\chi_{[-t_0/2, t_0/2]}(t)] \\ &= \alpha_- \delta(\omega - \omega_{ca}) \star \sqrt{\frac{2}{\pi}} \frac{\sin \frac{1}{2}\omega t_0}{\omega} \\ &= \alpha_- \sqrt{\frac{2}{\pi}} \frac{\sin \frac{1}{2}(\omega - \omega_{ca})t_0}{(\omega - \omega_{ca})} . \end{aligned} \quad (23.122)$$

The spectrum  $S_{\alpha_-}(\omega) = |F_{a_-}(\omega)|^2$  has a bandwidth of  $\beta = 5.6/t_0$ . For example an oscillation observed for a period 100 times longer than the cavity decay time,  $t_0 = 100/\kappa$ , the bandwidth will be  $\beta = 0.056\kappa$ . Simulations are based on the Langevin equation.

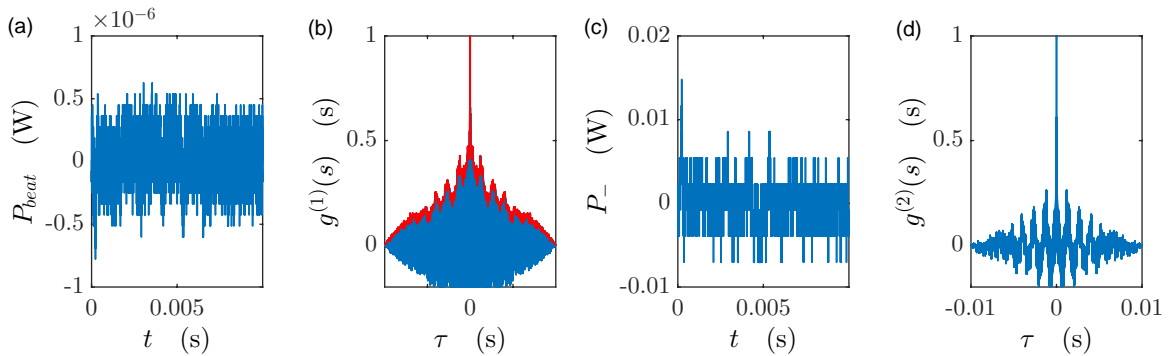


Figure 23.11: (code) Measured trajectories (a) and (b) and correlation functions (c) and (d) of the CARL laser. The coupling constant was  $NU_0 = -0.1$ .

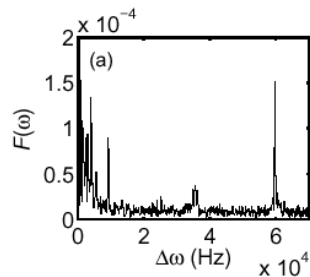


Figure 23.12: Spectrum of the CARL calculated from the first-order correlation function in Fig. 23.11(c). The coupling constant was  $NU_0 = -0.1\kappa$ .

## 23.5.3 Exercises

### 23.5.3.1 Ex: Autocorrelation functions

### 23.5.3.2 Ex: Signal to noise ratio of Bloch oscillations

You want to evaluate the stability of a noisy periodic signal. How many noisy oscillations do you have to observe in order to evaluate the oscillation period with a given S/N ratio [739].

## 23.6 Further reading

J. Javaloyes et al., *Reduced Model for the Description of Radiation-Matter Interaction Including Atomic Recoil* [\[DOI\]](#)

J. Javaloyes et al., *Self-Generated Cooperative Light Emission Induced by Atomic Recoil* [\[DOI\]](#)

- T. Griesser et al., *A Vlasov approach to bunching and selfordering of particles in optical resonators* [\[DOI\]](#)



Part V

Atom Optics





## Chapter 24

# Manipulation of atomic gases

The field of *atom optics* deals with the motion of atoms and its control by technical tools. At high velocities with no external forces, the atoms follow straight paths, similar to light beams in *classical optics*. At low speeds, they propagate as waves, similarly to wave optics in Maxwell's theory of *electrodynamics*. The term *atom optics* emphasizes the analogy and the duality in the behavior of microscopic particles.

The *duality principle* is one of the fundamental ideas of quantum mechanics. The appearance of an object as a wave or as a particle depends on the situation in which it is observed. While the wave nature of light was well established in classical physics since a long time, Louis de Broglie was the first in 1924 to apply the duality principle also to massive particles and to predict that particles, under certain conditions, behave like waves whose wavelengths increase as their velocity decreases. Each particle (or sample of particles) is delocalized along a distance corresponding to the 'de Broglie wavelength'. This feature of the matter was soon discovered experimentally in electron beams and is still used today in commercial devices, for example in electron microscopes.

The laser was discovered in 1956. In a laser, light particles are forced to oscillate synchronously, that is, coherently. By analogy, we can raise the question whether a similar phenomenon can occur with massive particles, and whether it is possible to construct an *atom laser*. Such a device would emit coherent matter waves just as the laser emits coherent light. When a gas is cooled to very low temperatures, the Broglie waves of the atoms become very long and, if the gas is sufficiently dense, eventually overlap. If the gas consists of a single species of bosonic particles with all atoms being in the same quantum state, their Broglie waves interfere constructively thus and form a huge wave of coherent matter. This matter wave is described by a single wavefunction exhibiting long range order and having a single phase. If this wavefunction is formed inside a trap, all atoms accumulate in its ground state. Thus, we obtain a pure quantum state of many bodies in the kinetic degree of freedom <sup>1</sup>. The transition of a gas from individual atoms to a degenerate mesoscopic many-body quantum state occurs as a phase transition named *Bose-Einstein condensation* (BEC) as a homage to Bose and Einstein who predicted the effect already in 1924 [97, 222].

The course begins in this chapter with a presentation of the most important experimental techniques for cooling, trapping, manipulating and detecting atomic gases. The knowledge of these techniques will allow for a better understanding of how it is possible to generate and analyze all the effects mentioned above. Chp. 26.9 introduces

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<sup>1</sup>In particular, for very cold atoms whose internal excitation occurs on a very different energy scale, the corresponding degree freedom is frozen and does not influence the kinetics.

the phenomenon of Bose-Einstein condensation and the following chapters focus on the thermodynamic, superfluid, coherent and dielectric properties of condensates.

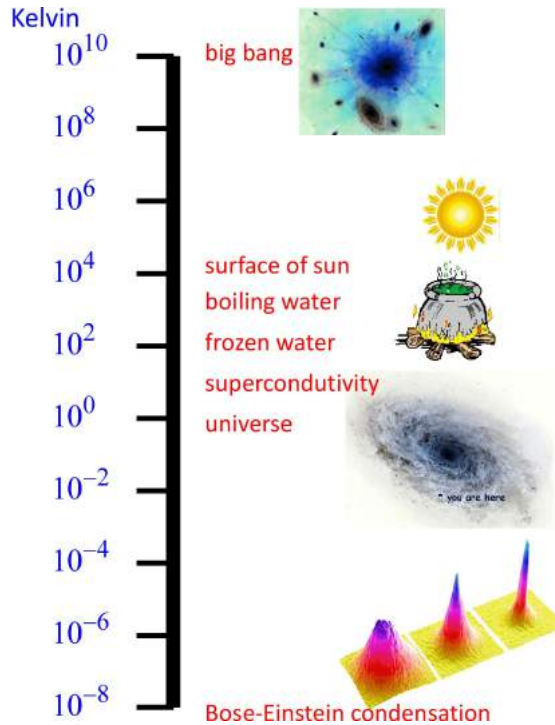


Figure 24.1: Temperature scale.

The incomparable success of atomic optics has been rewarded with 20 nobel prizes in the last 25 years (Dehmelt, Paul, Ramsey, Cohen-Tannoudji, Chu, Phillips, Cornell, Wieman, Ketterle, Hänsch, Glauber, Hall, Wineland, Haroche, Ahskin) plus several indirectly related noble prizes (De Gennes, Leggett, Thouless, Haldane, Kosterlitz). For review articles on BEC see [535, 166, 152, 268, 591, 652], [390] or check in internet sites <http://amo.phy.gasou.edu/bec.html> and <http://jila.edu/bec.html>.

In this chapter we review the basic techniques of *Atomic Optics*, emphasizing the cooling, trapping and measurement of cold atomic gases. See also ([watch talk](#)) and ([watch talk](#)).

## 24.1 The atomic motion

### 24.1.1 The atom as a matter wave

We have already emphasized that atomic optics deals with the motion of atoms in a gas, that is, we are interested only in the external degrees of freedom of the atoms. To describe the motion of a free massive particle in one dimension, we write the

Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} . \quad (24.1)$$

Therefore, the general solution of the stationary Schrödinger equation,

$$\hat{H}\psi(x) = E\psi(x) , \quad (24.2)$$

is,

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{with} \quad k = \sqrt{\frac{2mE}{\hbar^2}} . \quad (24.3)$$

Note, that the wavefunctions  $e^{ikx}$  are not quadratically integrable. On the other hand, they do not represent real physical systems. In practice, we need to consider wavepackets or specify a finite volume for the particle.

Note also that the eigenvalue spectrum of is continuous. To warrant the interpretation of the wavefunction as a probability density we will require quadratic integrability,  $\int |\psi|^2 d^3r = 1$ . This means that the wavefunction can not be infinite in a finite volume, but it can be infinite in an infinitely small volume.

The description of the atomic motion by a wave equation emphasizes the fact that microscopic particles have wave properties with each atom corresponding to a velocity-dependent *de Broglie wave*,

$$\boxed{\lambda_{dB} = \frac{\hbar}{p}} , \quad (24.4)$$

which describes the coherence length of the atom.

#### 24.1.1.1 Characteristic velocities

The behavior of an atom described by the Schrödinger equation depends very much on its kinetic energy. At high velocities (or short de Broglie waves), it will behave like a classical particle with a well-defined trajectory. At low velocities (or long de Broglie waves), it will propagate like a wave and exhibit phenomena such as diffraction and interference. Therefore, it is important to highlight some characteristic velocity regimes.

Most optical cooling techniques are based on the removal of kinetic energy upon light scattering on electronic transitions. It is, therefore, interesting to compare the kinetic energy (or temperature) of an ensemble of atoms with the width  $\Gamma$  of the transition. The *Doppler limit* is given by (see Exc. 24.1.4.1),

$$k_B T_D = \frac{\hbar}{2} \Gamma . \quad (24.5)$$

We can also compare the kinetic energy with the energy transferred to an atom by the absorption of a single photon. The *photonic recoil* energy is given by,

$$k_B T_{rec} = \frac{\hbar^2 k^2}{2m} . \quad (24.6)$$

Atomic clouds with temperatures around  $T \simeq T_D = 10..1000 \mu\text{K}$  are called *cold*. Clouds with temperatures around and below  $T \lesssim T_{rec} = 0.1..10 \mu\text{K}$  are called *ultra-cold*.

In most atomic optical experiments we do not work with individual atoms (or ions), but with relatively dilute ensembles of atoms, called *clouds*. In general, clouds can not be described by a single wavefunction. Either we describe every atom by a separate and independent wavefunction (which only works when the atoms do not interact), or we describe the cloud by probability distributions (such as the 'density matrix'). Let us now consider a thermal cloud. The *Maxwell-Boltzmann distribution* of velocities is,

$$g(\mathbf{v}) = \sqrt{\frac{m}{2\pi k_B T}}^3 e^{-m\mathbf{v}^2/2k_B T} . \quad (24.7)$$

This distribution is normalized,  $\int g(\mathbf{v})d^3\mathbf{v} = \int_0^\infty 4\pi v^2 g(v)dv = 1$ . Average velocity is now

$$\bar{v} = \int v g(v)dv = \sqrt{\frac{k_B T}{m}} . \quad (24.8)$$

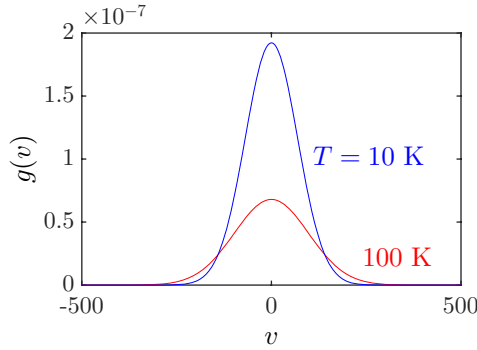


Figure 24.2: (code) Maxwell-Boltzmann distribution.

We define the *thermal de Broglie wavelength* of an atomic ensemble as,

$$\lambda_{therm} \equiv \frac{h}{m\bar{v}} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}} . \quad (24.9)$$

It represents an average over the de Broglie wavelengths of all atoms of the sample. When a dense gas is sufficiently dense, so that this quantity exceeds the average distance between atoms,

$$\rho \equiv n\lambda_{therm}^3 > 1 , \quad (24.10)$$

where  $n$  is the atomic density, we enter a new regime, where the *Maxwell-Boltzmann law* ceases to be valid. Since  $\lambda_{therm} \propto T^{-1/2}$ , this regime corresponds to low temperatures. The quantity  $\rho$  is called *phase space density*. A phase space density approaching 1 means an increased probability of finding *more than one atom per elementary phase space cell*. We then enter the regime of quantum degeneracy, where the Boltzmann

statistics must be replaced by the Bose-Einstein statistics, in the case of bosons, or the Fermi-Dirac statistics, in the case of fermions. We will deepen the discussion of quantum statistics of ideal gases in Chp. 25.3. From the condition  $n\lambda_{therm}^3 \simeq 1$ , we obtain

$$k_B T_c = \frac{1}{m} \left( \frac{2\pi\hbar}{\lambda_{therm}} \right)^2 = \frac{(2\pi\hbar)^2 n^{2/3}}{m} . \quad (24.11)$$

### 24.1.2 Localized atoms

To avoid perturbative influence of the environment on the atoms, they are often trapped in potentials, which suspend them in a volume distant from massive walls. The Hamiltonian of a trapped atoms is,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) . \quad (24.12)$$

As the wavefunction is now localized, the spectrum of possible energies organizes into discrete levels, and the atoms are allocated in populations of these levels.

Often, a 3D potential can be written in the form,

$$U(x, y, z) = U_x(x) + U_y(y) + U_z(z) . \quad (24.13)$$

This is the case, for example, of a rectangular well characterized by  $U_x(x) = U_y(y) = U_z(z) = U_0/3$  inside the well. The relationship (24.13) also holds for a harmonic potential,

$$U(\mathbf{r}) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) . \quad (24.14)$$

In these cases, a product ansatz for the wavefunction is generally useful,

$$\psi(\mathbf{r}) = \psi_x(x)\psi_y(y)\psi_z(z) , \quad (24.15)$$

since its insertion into the Schrödinger equation,

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) + U_x(x) + U_y(y) + U_z(z) \right] \psi_x(x)\psi_y(y)\psi_z(z) = E\psi_x(x)\psi_y(y)\psi_z(z) , \quad (24.16)$$

separates it into three independent one-dimensional equations,

$$-\frac{\hbar^2}{2m} \frac{\psi_x''(x)}{\psi_x(x)} + U_x(x) = const. \equiv E_x , \quad (24.17)$$

and similarly for  $y$  and  $z$ . Since  $E = E_x + E_y + E_z$ , we can have the same energy for different combinations of  $E_x$ ,  $E_y$  and  $E_z$ . That is, multidimensional systems are often degenerate.

### 24.1.3 Density-of-states of a trapping potential

The way an atomic cloud accommodates itself inside a trapping potential is governed by the density of available states. To calculate this density, we consider the Hamiltonian  $H(\mathbf{r}, \mathbf{p}) = \frac{\hbar^2 \mathbf{k}^2}{2m} + U(\mathbf{r})$ . For a cylindrical harmonic oscillator we write,

$$U(\mathbf{r}) = \frac{m}{2} \omega_r^2 r^2 + \frac{m}{2} \omega_z^2 z^2 \quad \text{where} \quad r^2 = x^2 + y^2 , \quad (24.18)$$

or  $U(\mathbf{x}) = \frac{m}{2}\omega_r^2\rho^2$ , where  $\rho^2 = x^2 + y^2 + \lambda^2 z^2$  with  $\lambda = \omega_z/\omega_r$ . We define  $\bar{\omega} = (\omega_r^2\omega_z)^{1/3} = \lambda^{1/3}\omega_r$ . The single-particle levels of this Hamiltonian are,  $\epsilon_{n_x n_y n_z} = \hbar\omega_x n_x + \hbar\omega_y n_y + \hbar\omega_z n_z$ , where the  $n_j$  are integer numbers.

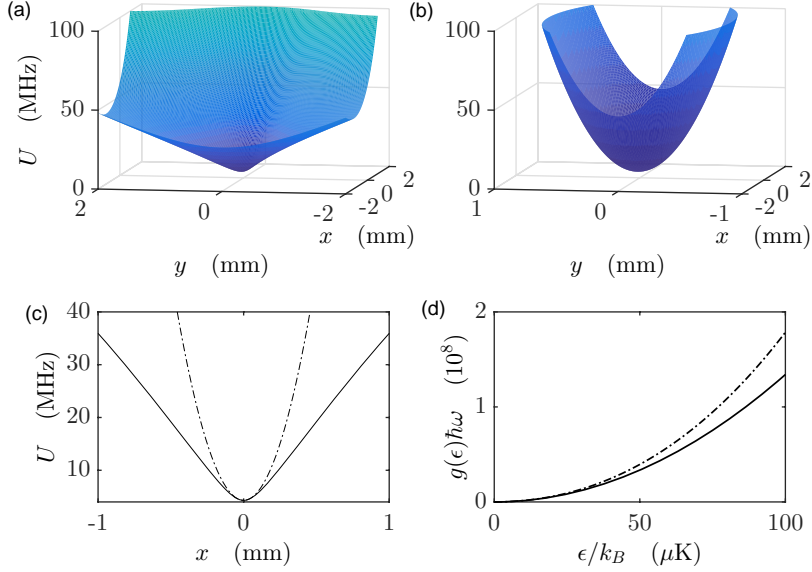


Figure 24.3: (code) (a) The figure shows two dimensions of a Ioffe-Pritchard type magnetic trapping potential (characterized by being approximately linear at large distances from the center and harmonic near the center). (b) Harmonic approximation (most experimentally feasible potentials are approximately harmonic near the center). (c) One-dimensional cut through the potential of (a,b). (d) Density of states for a harmonic (dotted line) and a Ioffe-Pritchard type potential (solid line).

We now introduce the *density of states*  $\eta(\epsilon)$  for an arbitrary potential via,

$$\int \eta(\epsilon) d\epsilon \equiv \frac{1}{(2\pi)^3} \int d^3r d^3k = \frac{(2m)^{3/2}}{(2\pi)^2 \hbar^3} \int d^3r \int d\epsilon \sqrt{\epsilon - U(\mathbf{r})}. \quad (24.19)$$

For the cylindrical harmonic trap defined in (24.18), we find with a little help from Dr. Bronstein [107],

$$\begin{aligned} \eta(\epsilon) &= \frac{(2m)^{3/2}}{(2\pi)^2 \hbar^3} \int d^3r \sqrt{\epsilon - \frac{m}{2}\omega_r^2\rho^2} \\ &= \frac{1}{(2\pi)^2} \frac{8\epsilon^2}{(\hbar\bar{\omega})^3} \int_{-1}^1 d\tilde{x} \int_{-\sqrt{1-\tilde{x}^2}}^{\sqrt{1-\tilde{x}^2}} d\tilde{y} \int_{-\sqrt{1-\tilde{x}^2-\tilde{y}^2}}^{\sqrt{1-\tilde{x}^2-\tilde{y}^2}} d\tilde{z} \sqrt{1 - \tilde{x}^2 - \tilde{y}^2 - \tilde{z}^2}. \end{aligned} \quad (24.20)$$

The resolution of the integral gives,

$$\eta(\epsilon) = \frac{\epsilon^2}{2(\hbar\bar{\omega})^3} \quad (\text{harmonic potential}). \quad (24.21)$$

Another example is the box potential. In this case we can simply obtain,

$$\eta(\epsilon) = \frac{(2m)^{3/2}}{(2\pi)^2 \hbar^3} \int_V d^3r \sqrt{\epsilon} = \frac{(2m)^{3/2}}{(2\pi)^2 \hbar^3} V \sqrt{\epsilon} \quad (\text{box potential}) . \quad (24.22)$$

A generalization is discussed in the Exc. 24.1.4.2.

## 24.1.4 Exercises

### 24.1.4.1 Ex: Fundamental temperature limits

Calculate the Doppler limit, the recoil limit, and the threshold to quantum degeneracy for an atomic cloud of density  $n = 10^{14} \text{ cm}^{-3}$  for the sodium  $D2$  transition ( $\lambda = 590 \text{ nm}$ ,  $\Gamma/2\pi = 10 \text{ MHz}$ ) and the rubidium  $D2$  transition ( $\lambda = 780 \text{ nm}$ ,  $\Gamma/2\pi = 6 \text{ MHz}$ ).

### 24.1.4.2 Ex: Density of states for non-harmonic potentials

Calculate the density of states for non-harmonic potentials,  $\hat{H} = \frac{\hbar^2 k^2}{2m} + \left| \frac{x}{2\bar{x}} \right|^p + \left| \frac{y}{2\bar{y}} \right|^l + \left| \frac{z}{2\bar{z}} \right|^q$  using Ref. [37]. Apply the result to a quadrupolar potential.

## 24.2 Optical cooling

As discussed in Sec. 18.2, the force exerted by a light field on an atom can be of two types: a dissipative force arising called *radiation pressure*, which is often used for optical cooling purposes, and a conservative *dipolar force* which often serves for the engineering of optical trapping potentials. Both applications of optical forces will be detailed in the following sections.

### 24.2.1 Optical molasses

In the *Doppler cooling* model, we treat the phenomenology of optical forces quantitatively by considering the amplitude, phase and frequency of a classical field interacting with the dipole of an atomic transition in a two-level atom. From Eq. (18.24) and previous definitions of  $\Omega$  and  $\Omega_{sat}$ , and with the intensity  $I \propto E_0^2$ , we can write the *saturation parameter*,

$$s = \frac{I}{I_{sat}} = \frac{\Omega^2}{\Omega_{sat}^2} = \frac{\Omega^2}{\Gamma^2/2} , \quad (24.23)$$

and

$$\mathbf{F}_{rp} = \frac{\hbar \mathbf{k} \Gamma}{2} \frac{s}{(2\Delta/\Gamma)^2 + 1 + s} . \quad (24.24)$$

Now, if we consider an atom propagating in  $+z$  direction with the velocity  $v_z$  counterpropagating to a light wave detuned by  $\Delta$  from the resonance, the total detuning will be

$$\Delta \longrightarrow \Delta + kv_z . \quad (24.25)$$



where the term  $kv_z$  is the Doppler shift. The force  $F_-$  acting on the atom will be in the direction opposite to the motion. In general,

$$\mathbf{F}_{\pm} = \pm \frac{\hbar \mathbf{k} \Gamma}{2} \frac{s}{(2(\Delta \mp kv_z)/\Gamma)^2 + 1 + s} . \quad (24.26)$$

Supposing now, that we have two light fields propagating in directions  $\pm z$ , the total force will be  $\mathbf{F} = \mathbf{F}_+ + \mathbf{F}_-$ . If  $kv_z$  is small compared to  $\Gamma$  and  $\Delta$ , we find through a Taylor expansion,

$$F_z \simeq 4\hbar ks \frac{kv_z(2\Delta/\Gamma)}{[1 + s + (2\Delta/\Gamma)^2]^2} . \quad (24.27)$$

This expression shows that, if the detuning  $\Delta$  is negative (that is, on the red side of the resonance), then the cooling force will oppose the motion and be proportional to the atomic velocity. Fig. 24.4 shows this restoring dissipative force as a function of  $v_z$  at a detuning  $\Delta = -\Gamma$  with  $I = I_{sat}/2$ . The one-dimensional motion of the atom, subject to a restoring force which is proportional to the atomic velocity, is that of a damped harmonic oscillator. The proportionality factor,

$$\alpha_d = s \frac{-4k^2(2\Delta/\Gamma)}{1 + s + (2\Delta/\Gamma)^2} \quad (24.28)$$

is just the *friction coefficient*.

However, the atom will not cool down indefinitely. At some point, the Doppler cooling rate will be balanced by the heating rate coming from the momentum fluctuations of the atom absorbing and remitting photons. The *Doppler cooling limit* is given by,

$$k_B T = \hbar \frac{\Gamma}{2} . \quad (24.29)$$

This limit is generally, for alkaline atoms, on the order of dozens of micro-Kelvin. In the early years of cooling and trapping, the Doppler limit was thought to be a real physical barrier. But in 1988, several groups have shown that, in fact, atoms could be cooled well below the Doppler limit. The effect arises in atoms, whose ground state exhibits a hyperfine structure. We will show simplified one-dimensional models for sub-Doppler cooling in the next section. Resolve the Excs. 24.2.5.1 and 24.2.5.2.

## 24.2.2 Sub-Doppler cooling

It turns out that atoms with a hyperfine structure in the ground state can be cooled below the Doppler limit (24.5). To explain this unexpected observation, models involving a slow motion of the atoms in polarization gradients of a standing light wave have been invoked. The phenomenon is now known as *polarization gradient cooling*.

Two principal mechanisms for cooling atoms to temperatures below the Doppler limit are based on spatial polarization gradients. These two mechanisms, however, invoke very different physical processes and are distinct by the spatial dependence of the light polarization. A key point is that these sub-Doppler mechanisms only work on atoms with multiple ground state levels. Two parameters, the friction coefficient and the capture velocity, determine the importance of these cooling processes. In this section we compare the expressions for these quantities in the sub-Doppler regime to those found by the conventional one-dimensional Doppler cooling model for optical molasses.

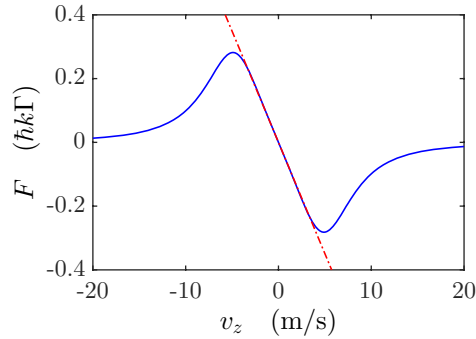


Figure 24.4: (code) Doppler force due to one-dimensional radiative pressure as a function of atomic velocity along the  $z$ -axis for red detuning  $\Delta = -\Gamma$  at a light intensity of  $I = 2I_{sat}$ . The solid line shows the exact expression for the restoring force [Eq. (24.26)]. The broken line shows the approximate linear expression of the velocity dependence according to Eq. (24.27).

### 24.2.2.1 Lin $\perp$ lin molasses

In the first case, two counterpropagating light waves with orthogonal linear polarizations form a standing wave. This configuration is familiarly called lin-perp-lin. Fig. 24.5 illustrates the change of polarization every period of  $\lambda/8$  from linear to circular to linear again, but rotated by  $90^\circ$ , and so on [169]. Along the same distance, the light-atom coupling produces a periodic energy shift (light-shift) of the ground state Zeeman levels. To illustrate the cooling mechanism, we assume the simplest case, a transition  $J_g = \frac{1}{2} \rightarrow J_e = \frac{3}{2}$ . As shown in Fig. 24.5 an atom moving through the region  $z \simeq \lambda/8$ , where the polarization is  $\sigma_-$ , will see its population pumped to  $J_g = -\frac{1}{2}$ . In addition, the Clebsch-Gordan coefficients that control the dipolar coupling of the  $J_e = \frac{3}{2}$  require that the  $J_g = -\frac{1}{2}$  couples to  $\sigma_-$  with a force three times larger than the  $J_g = +\frac{1}{2}$  does. The difference of the coupling forces leads to the light-shift between the two fundamental states shown in Fig. 24.5. As the atom continues to move toward  $+z$ , the relative coupling forces are reversed near  $3\lambda/8$ , where the polarization is essentially  $\sigma_+$ . Thus, the relative energy levels of the two hyperfine fundamental states oscillate 'out of phase' when the atom moves through the standing wave.

The fundamental idea is that the optical pumping rate, which always redistributes population to the lower hyperfine level, delays the light-shift of the atom moving through the field. The result is a 'Sisyphus effect', where the atom spends most of its time in sub-levels climbing a potential hill and thus converting kinetic energy into potential energy. This accumulated potential energy is subsequently dissipated by spontaneous emission to the electromagnetic modes of the vacuum. Simultaneously, the spontaneous emission transfers the population back to the lower one of two ground state levels. The lower diagram of Fig. 24.5 illustrates the phase delay of optical pumping. For this cooling mechanism to work, the optical pumping time, which is controlled by the intensity of the light, must be sufficiently slow to give the atom enough time to climb a noticeable part of the light-shift potential. This time essentially depends on the speed of the atom. As the atom is moving slowly, having

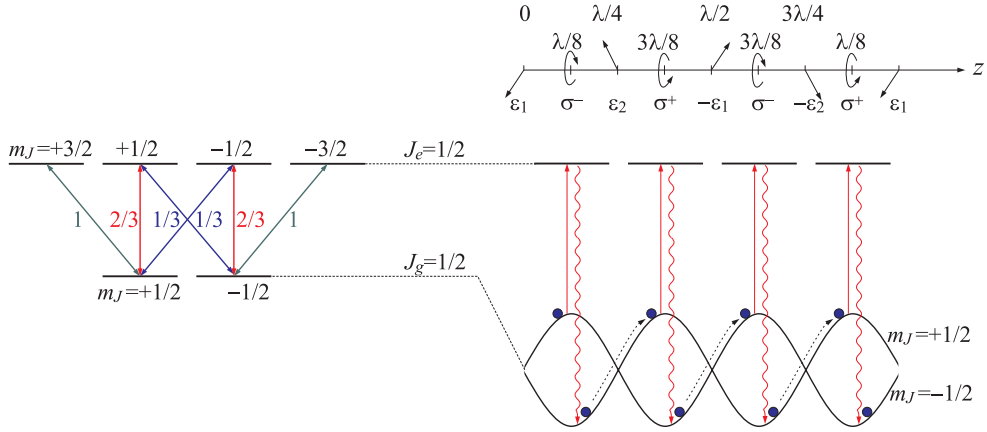


Figure 24.5: The upper line shows, how the polarization changes as a function of position (in units of a wavelength) for the 'lin-perp-lin' standing wave configuration. The figure below shows a simplified picture of the Sisyphus cooling mechanism for an atom with two levels,  $J_g \leftrightarrow J_e$ .

previously been cooled by the Doppler mechanism, the light field must be weak in order to decrease the optical pumping rate. Interestingly, this physical picture combines the conservative dipole optical force, whose spatial integral gives rise to the mounts and valleys of the potential on which the atom moves, and the irreversible dissipation of energy by spontaneous emission, which is necessary for any type of cooling.

We can obtain simple expressions for the friction coefficient and the capture velocity after some definitions. As in the Doppler cooling model we define the friction coefficient  $\alpha_{lpl}$  as the proportionality constant between the force  $F$  and the atomic velocity  $v$ ,

$$F = -\alpha_{lpl}v . \tag{24.30}$$

We assume that the light field is tuned to the red of the transition  $J_g - J_e$ ,

$$\Delta = \omega - \omega_0 , \tag{24.31}$$

and we denote the light-shifts of the levels  $J_g = \pm \frac{1}{2}$  as  $\Delta_{\pm}$ , respectively. At the position  $z = \lambda/8$ , we find  $\Delta_- = 3\Delta_+$  and at  $z = 3\lambda/8$ ,  $\Delta_+ = 3\Delta_-$ . As the applied field is tuned to red, all  $\Delta_{\pm}$  have negative values. Now, for the cooling mechanism to be efficient, the optical pumping time  $\tau_p$  should be similar to the time needed for an atom with velocity  $v$  to move from the bottom to the top of the potential,  $\frac{\lambda/4}{v}$ ,

$$\tau_p = \frac{\lambda/4}{v} \tag{24.32}$$

or

$$\Gamma' \simeq kv , \tag{24.33}$$

where  $\Gamma' = 1/\tau_p$  and  $\lambda/4 \simeq 1/k$ . Now, the energy  $W$  dissipated during a cycle of escalation and spontaneous emission is essentially the average energy difference between

the light-shifted ground states,  $\Delta_{ls} \equiv \Delta_+ + \Delta_-$ , that is  $W \simeq -\hbar\Delta_{ls}$ . Therefore, the rate for energy dissipation is,

$$\frac{dW}{dt} = \Gamma' \hbar \Delta_{ls} . \quad (24.34)$$

At the same time, every temporal energy change of a system can always be expressed as  $\frac{dW}{dt} = \mathbf{F} \cdot \mathbf{v}$ . Therefore, in this one-dimensional model, considering Eq. (24.31), we can write,

$$\frac{dW}{dt} = -\alpha_{lpl} v^2 = -\Gamma' \hbar \Delta_{ls} , \quad (24.35)$$

such that with (24.33),

$$\alpha_{lpl} = -\frac{\Gamma' \hbar \Delta_{ls}}{v^2} \simeq -k v \frac{\hbar \Delta_{ls}}{v^2} \simeq -\frac{\hbar k^2 \Delta_{ls}}{\Gamma'} . \quad (24.36)$$

Note that since  $\Delta < 0$ ,  $\alpha_{lpl}$  is a positive quantity. Also note, that for large detunings, ( $\Delta \gg \Gamma$ ) Eq. (18.23) gives,

$$\frac{U}{\hbar} = \frac{\Delta_{ls}}{4} = \frac{\Omega^2}{4\Delta} . \quad (24.37)$$

It is also true that for light-shifts, which are large compared to the natural width of ground state ( $\Delta_{ls} \gg \Gamma'$ ), and for large red detunings ( $\Delta \gtrsim 4\Gamma$ ),

$$\frac{\Gamma}{\Gamma'} \simeq \frac{\Delta^2}{4\Omega^2} . \quad (24.38)$$

Therefore, the sub-Doppler friction coefficient can also be written,

$$\alpha_{lpl} = -\frac{\hbar k^2 \Delta}{4\Gamma} \quad (24.39)$$

Eq. (24.39) makes two remarkable predictions: Firstly, in the 'lin-perp-lin' configuration the sub-Doppler friction coefficient can be a large number in comparison to  $\alpha_d$ . Note that from Eq. (24.28), with  $I \lesssim I_{sat}$  and  $\Delta \gg \Gamma$ ,

$$\alpha_d \simeq \hbar k^2 \left( \frac{\Gamma}{\Delta} \right)^3 , \quad (24.40)$$

and

$$\frac{\alpha_{lpl}}{\alpha_d} \simeq \left( \frac{\Delta}{\Gamma} \right)^4 . \quad (24.41)$$

Secondly,  $\alpha_{lpl}$  is independent of the intensity of the applied field. This last result is different from the friction coefficient, which is proportional to the field intensity up to until saturation (see Eq. (24.28)). However, although  $\alpha_{lpl}$  seems impressive, the range of atomic velocities where it can operate is constrained by the condition,

$$\Gamma' \simeq k v . \quad (24.42)$$

The ratio of the capture velocities for sub-Doppler versus Doppler cooling is therefore only,

$$\frac{v_{lpl}}{v_d} \simeq \frac{4\Delta_{ls}}{\Delta} . \quad (24.43)$$

Fig. 24.6 graphically illustrates the comparison between the Doppler and the 'lin-perp-lin' sub-Doppler cooling mechanisms. The dramatic difference of the capture ranges is evident. Note also that the slopes of the curves give the friction coefficients and that, within the capture range, the slope is much steeper for the sub-Doppler mechanism.

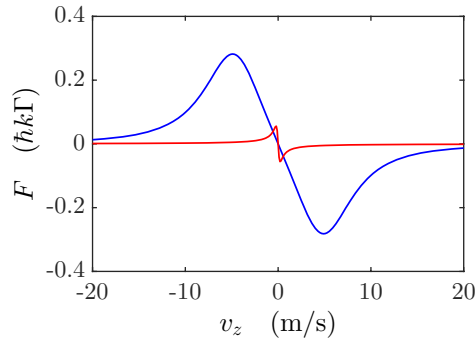


Figure 24.6: (code) Comparison of slopes, amplitudes, and capture ranges for Doppler and Sisyphus cooling.

#### 24.2.2.2 $\sigma^+ - \sigma^-$ molasses

The second mechanism operates with two counterpropagating light beams, which are circularly polarized in opposite directions. When the two counterpropagating beams have the same amplitude, the resulting polarization is always linear and orthogonal to the propagation axis, but the tip of the polarization vector traces a helix with a periodicity of  $\lambda$  [see Fig. 24.7(b)]. The physics of this sub-Doppler mechanism *does not involve hill-climbing nor spontaneous emission*, but an imbalance of the photon scattering rates by the two counterpropagating light waves as the atom moves along the  $z$ -axis. This imbalance leads to a velocity-dependent force counteracting the atomic displacement. The essential factor leading to the different scattering rates is the creation of a population orientation along the  $z$ -axis between the sub-levels of the atomic ground state. The more populated sub-levels scatter more photons. Now, considering the energy level diagram (see Fig. 24.5) and the symmetry of the Clebsch-Gordan coefficients, it is evident that transitions  $J_g = \frac{1}{2} \leftrightarrow J_e = \frac{3}{2}$  coupled by linearly polarized light can not produce an orientation of the population in the ground state. In fact, the simplest system exhibiting this effect is  $J_g = 1 \leftrightarrow J_e = 2$ . A measure for this orientation is the magnitude of the matrix element  $\langle J_z \rangle$  between the sublevels  $J_{g_z} = \pm 1$ . For an atom at rest at the position  $z = 0$  interacting with the light polarized along the  $y$ -direction, the light-shifts  $\Delta_0$  and  $\Delta_{\pm}$  of the three sub-levels of the ground state would be,

$$\Delta_{+1} = \Delta_{-1} = \frac{3}{4}\Delta_0, \quad (24.44)$$

and the stationary populations would be  $4/17$ ,  $4/17$  e  $9/17$ , respectively. Obviously, linearly polarized light does not produce a stationary orientation,  $\langle J_z \rangle_s = 0$ . But when the atom begins to move along the  $z$ -axis with velocity  $v$ , it sees a linear polarization

precessing about the axis of propagation at an angle  $\varphi = kz = -kvt$ . This precession gives rise to a new term in the Hamiltonian,  $V = kvJ_z$ . Furthermore, when we transform to a rotating coordinate system, the eigenfunctions of the Hamiltonian of the atom moving in this new 'inertial' system become linear combinations of the basis functions of the resting atom. The expectation value of the stationary orientation operator  $J_z$ , is now zero in the inertial system [169],

$$\langle J_z \rangle = \frac{40 \hbar kv}{17 \Delta_0} = \hbar(\Pi_+ - \Pi_-) . \tag{24.45}$$

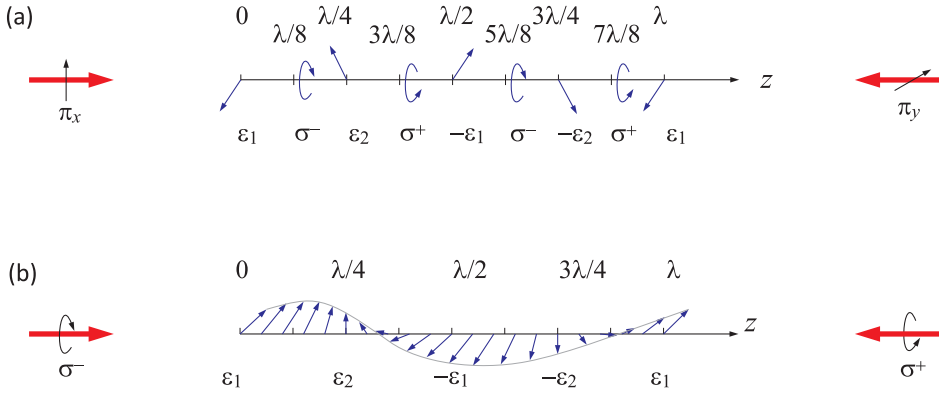


Figure 24.7: Polarization as a function of position (in units of a wavelength) for the  $\sigma^+ - \sigma^-$  standing wave configuration.

Note that, as the expectation value of the orientation is nonzero only when the atom moves. In Eq. (24.45) we denote the populations of the sub-levels  $|\pm \rangle$  as  $\Pi_{\pm}$ , and we interpret nonzero matrix elements as a direct measure of the population difference between the ground state levels  $|\pm \rangle$ . Note that, since  $\Delta_0$  is negative (red tuning), the Eq. (24.45) tells us, that the population  $\Pi_-$  is larger than  $\Pi_+$ . Now, when an atom traveling in  $+z$  direction is exposed to two light waves with polarizations  $\sigma_{\mp}$  propagating in the  $\mp z$  directions, the preponderance of population in the state  $|-\rangle$  will result in a higher scattering rate from the wave propagating in  $-z$  direction. Therefore, the atom will be subject to a total force opposite to its movement and proportional to its velocity. The differential scattering rate is,

$$\frac{40}{17} \frac{kv}{\Delta_0} \Gamma' . \tag{24.46}$$

With a quantized momentum of  $\hbar k$  transferred at each scattering event, the total force is,

$$F = \frac{40}{17} \frac{\hbar k^2 v \Gamma'}{\Delta_0} . \tag{24.47}$$

The friction coefficient  $\alpha_{cp}$  is,

$$\alpha_{cp} = -\frac{40}{17} \hbar k^2 \frac{\Gamma'}{\Delta_0} , \tag{24.48}$$

which is a positive quantity, since  $\Delta_0$  is negative for red detuning. Comparing  $\alpha_{cp}$  with  $\alpha_{lpl}$  we see, that  $\alpha_{cp}$  must be much smaller, because we always assumed that the light shifts  $\Delta$  are much larger than the linewidths  $\Gamma'$ . However, the heating rate due to fluctuations of the recoil is also much lower. Thus, the minimum temperatures that can be reached with the two sub-Doppler mechanisms are comparable.

Although the Doppler cooling mechanism also depends on an imbalance of scattering from counterpropagating light waves, in this case the imbalance comes from the fact that the Doppler shift experienced by the moving atoms leads to different probabilities for photon scattering. For the sub-Doppler mechanism the scattering probabilities from the two light waves are the same, but the ground state populations are not. The state with the largest population suffers the highest scattering rate.

## 24.2.3 Raman cooling

### 24.2.3.1 Optical cooling of confined particles

It is also possible to cool ions confined in a trap [725]. The direction of their motion and their velocity change periodically with the secular frequencies  $\zeta_r$  und  $\zeta_z$ . For optical cooling it is sufficient to irradiate a single red-detuned running-wave light field: In a real ion trap the cylindrical symmetry cannot be realized with absolute precision so that we get different secular frequencies  $\zeta_x \neq \zeta_y \neq \zeta_z$  and a coupling of the degrees of freedom for all directions of space. The cooling of the ionic motion in a single direction results in a cooling of the motion in the other directions.

In the rest system of an ion oscillating in a harmonic trap the Doppler-shift of the laser frequency changes periodically:  $\mathbf{v}(t) = \mathbf{v}_0 \cos \zeta_{r,z} t$ . The ion absorbs therefore in its rest system the light on a width of sidebands whose distance and strength depend on the oscillation frequency and amplitude. The absorption profile of a transition in such a harmonically vibrating ion follows as a convolution of the Lorentz profile  $\mathcal{L}_\Gamma$ , describing the naturally broadened resonance, with a function  $\mathcal{S}$ , describing the splitting of the absorption profile into sidebands [357]:

$$\mathcal{A}(\Delta) = (\mathcal{L}_\Gamma \star \mathcal{S})(\Delta) \quad , \quad \mathcal{S}(\Delta) = \sum_n \mathcal{J}_n(\mathbf{k} \cdot \mathbf{v}_0 / \zeta_{r,z})^2 \delta(\Delta - n\zeta_{r,z}) . \quad (24.49)$$

$\mathcal{J}_n$  denotes the Bessel function of  $n^{th}$  order. In essence, the system is governed by three time-constants: The natural decay width of the cooling transition  $\Gamma$  is a measure for the innerratomic time scale, since it determines the average duration of absorption-emissions cycles. The secular frequencies  $\zeta_{r,z}$  determine the time scales for changes in the external degrees of freedom, i.e. for changes of the ion's location and velocity. The Doppler-shift  $k v_0$  of the resonance frequency in the return point of the ion motion finally, is a measure for the kinetic energy of the ion.

The relative importance of these three characteristic frequencies reveal the state of the ion in the trap. The modulation index  $\mathbf{k v}_0 / \zeta_{r,z}$  decides on the hight and the number of sidebands in the excitation spectrum. The better the ion has been cooled, the smaller the modulation index and the smaller the hight and number of sidebands. The kinetic energy of the ion is,

$$E_{kin} = \frac{1}{2} m v_0^2 = \frac{1}{2} m \zeta_{r,z}^2 x_0^2 . \quad (24.50)$$

The modulation index  $\mathbf{k}\mathbf{v}_0/\zeta_{r,z} = kx_0 = 2\pi x_0/\lambda$  is also called *Lamb-Dicke parameter*. By cooling the der Lamb-Dicke parameter is so much reduced and the ion is so well localized that its motional sidebands are smaller than the wavelength of the exciting light. It then is in the so-called Lamb-Dicke regime  $x_0 \ll \lambda$  [?] and has so small motional sidebands that they do not contribute to the line shape and do not influence the line width. Therefore the linear Doppler effect vanishes.

The quantity  $\zeta_{r,z}/\Gamma$  defines the *resolution* of the sidebands. If the resolution is poor, we talk about weak confinement, else about strong confinement. Therefore the same ion can be weakly confined with respect to an allowed transition and strongly confined with respect to a forbidden transition. The cooling processes in the two cases of strong and weak trapping must be described differently. At weak confinement the oscillation frequency  $\zeta_{r,z}$  is so slow that many absorption-emission cycles with the time constant  $\Gamma^{-1}$  can occur during one oscillation period. Cooling process and cooling limit are approximately the same as for free particles and are described by Doppler cooling.

### 24.2.3.2 Raman sideband cooling

In the case of strong confinement for the description of the cooling process we must consider the quantization of the motional energy in the harmonic potential. The two levels coupled by the narrow transition split into vibrational sublevels  $|n_{r,z}\rangle$ , which are populated in thermal equilibrium according to the Bose-Einstein distribution and have the kinetic energies  $E_{kin}$ ,

$$n_{r,z} = \frac{1}{e^{\hbar\zeta_{r,z}/k_B T} - 1} \quad \text{and} \quad E_{kin} = \hbar\zeta_{r,z}(n_{r,z} + \frac{1}{2}) . \quad (24.51)$$

To perform the so-called optical cooling *sideband cooling* [725] the laser is tuned to the first lower sideband. The laser light is then scattered in a Raman-Anti-Stokes process at the excited electronic state with a vibrational quantumnumber lower by 1  $|e, n_{r,z} - 1\rangle$ . The subsequent spontaneous decay occurs most probably to the same vibrational substate of the ground state  $|g, n_{r,z} - 1\rangle$ . The net effect of such a scattering process therefore is a transition to the next lower vibrational quantum number. The zero point energy of the ion in the trapping potential cannot be underscored by cooling,  $E_{kin} > \frac{1}{2}\hbar\zeta_{r,z}$  (for the Yb<sup>+</sup> ion it is  $E_{kin} > 2$  neV). However, the uncertainty of the kinetic energy, and the temperature  $T$  given by (24.51) have no lower limit [197].

At every absorption process, free particles carry away the momentum of the photons  $\hbar k$ . The recoil of a free Yb<sup>+</sup> ion corresponds to the frequency shift  $\varepsilon/2\pi = 5.3$  kHz. On a narrow transition, it yields a resonance at the frequency  $\varepsilon$ . For trapped ions, this is not the case, because the momentum is absorbed by the whole trap (see analogy to the *Mößbauer effect*).

### 24.2.3.3 Stimulated Raman sideband cooling

We may use two lasers detuned far from resonance to couple two vibrational states. However, additional dissipation by optical pumping is still required.

Numerous schemes have been tested to cool neutral atoms in optical lattices. For the schemes to work, the ion should be already in the Lamb-Dicke regime. Otherwise,



transitions with transfer of higher vibrational quantum numbers  $n_{r,z}$  are possible during spontaneous emission. The Lamb-Dicke limit is set by  $kr < 1$ , or,

$$\langle n \rangle = \frac{m\omega_{trap}}{2\hbar k^2}. \quad (24.52)$$

This means that higher trap frequencies ease the required temperature at which side-band cooling can start to work.

### 24.2.4 Adiabatic cooling of an optical lattice

Adiabatic cooling by [385] in 1D. Defining the lattice constant  $Q_0$ , the Boltzmann factor  $f_B \equiv e^{-\hbar\omega/k_B T}$ , the initial thermal population  $\pi_n = (1 - f_B)f_B^n$ , the recoil energy  $E_{rec} \equiv \frac{\hbar^2 k^2}{2m}$ ,

$$\frac{k_B T}{2} = \sum_n \frac{\pi_n}{\hbar Q_0} \int_{(n+1)\pi\hbar Q_0}^{(n+1)\pi\hbar Q_0 + 2\pi\hbar Q_0} \frac{p^2}{2m} dp = 2 \sum_n \frac{\pi_n}{\hbar Q_0} \int_n^{n+1} \frac{p^2}{2m} dp \quad (24.53)$$

$$= 2E_{rec} \left(\frac{Q_0}{k}\right)^2 \sum_{n=0}^{\infty} \pi_n \frac{3n^2 + 3n + 1}{24} = E_{rec} \left(\frac{Q_0}{k}\right)^2 \frac{1 + 4f_B + f_B^2}{12(1 - f_B)^2}. \quad (24.54)$$

Furthermore,

$$f_B = \frac{\bar{n}}{1 + \bar{n}} \iff \bar{n} = \frac{f_B}{1 - f_B}.$$

### 24.2.5 Exercises

#### 24.2.5.1 Ex: Optical molasses

Optical molasses are created (in one dimension) by two beams counterpropagating lasers tuned to red of an atomic transition. Each of the laser beams exerts on the atoms the radiative pressure force  $F_{\pm} = \hbar k \frac{\Gamma}{2} \frac{s}{[2(\Delta \pm kv)/\Gamma]^2 + 1 + s}$ .  $\Delta$  is the detuning of the laser,  $v$  is the velocity of an atom.

a. Show that for small velocities ( $|kv| \ll \Gamma$  and  $\Delta \leq \Gamma$ ) the optical molasses can be understood as a friction force and calculate the friction coefficient.

b. Heating processes caused by spontaneous emission limit the minimum temperature that can be reached in optical molasses. Calculate the laser tuning, where the temperature reaches its minimum value and specify the cooling limit.

**Help:** Suppose a one-dimensional molasses and assume, that the spontaneous emission only happens along this dimension. The heating rate follows from the scattering rate  $R$  through  $\left(\frac{dE}{dt}\right)_{heat} = \frac{d}{dt} \frac{\langle p^2 \rangle}{2m} = \frac{\hbar^2 k^2}{2m} 2R$ , the cooling rate follows from  $\left(\frac{dE}{dt}\right)_{cool} = Fv$ .

#### 24.2.5.2 Ex: Atomic fountain

In atomic fountains atoms are accelerated upward by a 'moving optical molasses'. After the molasses has been switched off, they perform a ballistic flight in the Earth gravitational field. The moving molasses is generated by two pairs of counterpropagating laser beams intersecting at right angle and oriented both at an angle of  $45^\circ$

with respect to gravity. The upgoing beams are tuned to the blue, and the counter-propagating downgoing beams have the same detuning to the red side of the atomic resonance ( $\lambda = 780$  nm). Supposing that the resonator is close to the position of the molasses and has with negligible length, what should be the detuning in order to achieve 1 s time period between the two passages of the atoms through the microwave resonator?

## 24.3 Optical and magneto-optical traps

### 24.3.1 The magneto-optical trap

An apparently fatal obstacle to the confinement of particles by optical forces is Earnshaw's optical theorem. This theorem states that, if a force is proportional to the light intensity, its divergence must be zero because the divergence of the Poynting vector expressing the directional flux of intensity is zero inside a volume without sources nor sinks of radiation. The absence of divergence precludes the possibility of a restoring force to the interior at all places of a closed surface [23]. However, Earnshaw's optical theorem can be bypassed by a clever trick. The internal degrees of freedom of the atom (i.e., its electronic energy levels) can change the proportionality between the force and the Poynting vector in a position-dependent manner, such that the optical Earnshaw's theorem does not apply. Spatial confinement is then possible using the radiative pressure force generated by counterpropagating light beams. The most common trap configuration is based on a radial magnetic field gradient produced by a quadrupolar field and three pairs of counterpropagating circularly polarized laser beams tuned to the red of an atomic transition and intersecting at right angles at the point where the field is zero. This *magneto-optical trap (MOT)* uses the position-dependent Zeeman shift of the electronic levels as the atom moves in the radially increasing magnetic field. The use of circularly polarized light which is red-detuned by about  $\Gamma$  results in a spatially varying transition probability, whose effect is to produce a restoring force that pulls the atom back to the origin. To understand bet-

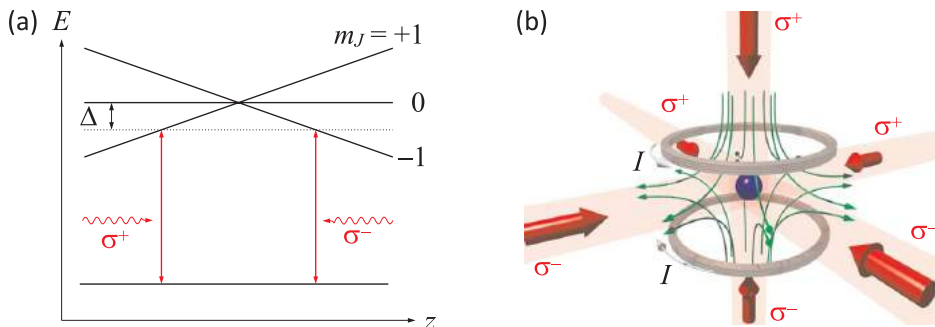


Figure 24.8: Left: Diagram of the energy level shift in an MOT, when an atom moves out of the center of the trap. A restoring force is observed around the indicated resonance positions. Right: Scheme of a typical MOT set up showing the six laser beams and the current-carrying coils in anti-Helmholtz configuration producing the quadrupolar magnetic field.

ter how the trapping scheme works, we consider a two-level atom with a transition

$J = 0 \rightarrow J = 1$  moving along the  $z$ -direction. We apply a magnetic field  $B(z)$  growing linearly with the distance from the origin. The Zeeman shifts of the electronic levels depend on the position,

$$\Delta_B = \frac{\mu_B g_F m_F}{\hbar} \frac{dB}{dz} z \equiv \partial \omega_{zeem} z, \quad (24.55)$$

see Fig. 24.8. We also apply counterpropagating laser beams along the directions  $\pm z$  with circular polarizations of opposite signs and tuned to the red of the atomic transition. It is clear from Fig. 24.8 that an atom moving in  $\pm z$  direction will scatter  $\sigma_{\mp}$  type photons at a faster rate than  $\sigma_{\pm}$  type photons, because the Zeeman effect will pull the  $\Delta m_J = \mp 1$  transition closer to the laser frequency. The expression for the radiation pressure force extends Eq. (24.26) to include the Doppler effect  $kv_z$  and the Zeeman effect,

$$F_{\pm z} = -\frac{\hbar k}{2} \Gamma \frac{2\Omega^2}{4(\Delta \pm kv_z \pm \partial \omega_{zeem} z)^2 + 2\Omega^2 + \Gamma^2}. \quad (24.56)$$

The atom will, therefore, feel a restoring force which pushes it back to the origin. If the laser beams are red-detuned by an amount  $\Delta = -\Gamma$ , the Doppler shift of the atomic motion introduces velocity-depending term to the restoring force, such that for small displacements and velocities the total restoring force can be expressed by the sum of a term which is linear in the velocity and a term which is linear in the displacement,

$$F_{MOT} = F_{1z} + F_{2z} = -\alpha \dot{z} - \kappa z. \quad (24.57)$$

From Eq. (24.57) we can derive the equation of motion of a damped harmonic oscillator with mass  $m$ ,

$$\ddot{z} + \frac{2\alpha}{m} \dot{z} + \frac{\kappa}{m} z = 0. \quad (24.58)$$

The damping constant  $\alpha$  and the spring constant  $\kappa$  can be written compactly in terms of atomic parameters and the field as,

$$\kappa = \frac{16\hbar k \Gamma \Omega^2 \Delta \partial_z \omega_{zeem}}{4\Delta^2 + 2 \cdot 6\Omega^2 + \Gamma^2}. \quad (24.59)$$

and

$$\alpha = \kappa \frac{k}{\partial_z \omega_{zeem}}. \quad (24.60)$$

Typical conditions for MOT are  $\Omega = \Gamma/2$ ,  $\Delta = -\Gamma$ . For typical MOTs,

$$\alpha \simeq 2 \cdot 10^{-22} \text{ Ns/m} \quad \text{and} \quad \kappa \simeq 3.7 \cdot 10^{-19} \text{ N/m}. \quad (24.61)$$

We can also estimate the curvature of the MOT,

$$\omega = \sqrt{\frac{\kappa}{m}} \simeq (2\pi) \cdot 200 \text{ Hz}. \quad (24.62)$$

Solve

Exc.

24.3.3.1

and

24.3.3.2.

MOTs are realized with current-carrying coils in anti-Helmholtz configuration which generates a quadrupolar geometry potential. Near the center, the magnetic field and its absolute value are well approximated by,

$$\mathbf{B} = q \begin{pmatrix} x \\ y \\ -2z \end{pmatrix} \quad \text{and} \quad |\mathbf{B}| = qB\sqrt{r^2 + 4z^2}, \quad (24.63)$$

with  $r^2 = x^2 + y^2$  and the gradient  $q \equiv \partial_r B$  is a constant, which depends only on the geometry of the coils and the current in them. Thus, the extension of the above results to three dimensions is simple if we consider the fact that the gradient of the quadrupolar field in the  $z$ -direction is twice the gradient in the radial directions  $x$  and  $y$ , such that  $\kappa_z = 2\kappa_x = 2\kappa_y$ . The damping term, which proportional to the velocity, implies that the kinetic energy  $E$  is dissipated from the atom (or a cloud of atoms) as,

$$E/E_0 = e^{-2\alpha t/m}, \quad (24.64)$$

where  $m$  is the atomic mass and  $E_0$  the kinetic energy at the beginning of the cooling process. Therefore, the dissipative force term cools the atomic cloud and, at the same time, combines with the position-dependent term to confine it. The time constant for the damping,

$$\tau = \frac{m}{2\alpha} \quad (24.65)$$

is typically dozens of microseconds. It is important to keep in mind that a MOT is anisotropic, since the restoring force is proportional to the anisotropic field gradients. Because of its dissipative non-conservative nature, it is more accurate to characterize a MOT by the maximum capture rate, rather than by a 'potential depth'.

In early experiments MOTs were loaded from a decelerated atomic beam. Later it was shown, that the low-velocity tail of the Maxwell-Boltzmann distribution provides a sufficient amount of atoms that can be captured by a MOT, so that it can be loaded directly from an atomic vapor at room temperature. Now many groups in the world use these assemblies for applications ranging from precision spectroscopy to the optical control of reactive collisions; the MOT has become the working horse of atom optics.

#### 24.3.1.1 Density in a MOT

A typical MOT captures up to a billion atoms in a volume of a few  $1 \text{ mm}^3$  resulting in densities of  $\sim 10^{10} \text{ cm}^{-3}$ . Although a MOT works as a versatile and robust 'reaction cell' for many applications, the frequencies of the light beams must be tuned close to atomic transitions, which bears the disadvantage that a considerable fraction of



Figure 24.9: Picture of a strontium MOT operated at 461 nm. The atomic cloud, which consists of about  $10^6$  atoms at 10 mK temperature is visible as a diffuse spot located inside a three-mirror ring cavity (courtesy: Camila Beli and Michelle Moreno).

atoms remains in excited states. This fact is at the origin of two processes limiting the density of a MOT: (1) losses of trapped atoms by collisions and (2) repulsive forces between the atoms caused by reabsorption of photons scattered within the cloud. Collisional losses arise from two sources: (i) hot atoms of the residual gas inside the chamber can elastically collide with cold atoms and kick them out of the MOT, and (ii) cold atoms in excited states can undergo inelastic binary collisions. 'Photon-induced repulsion' or *radiation trapping* arises when a trapped atom spontaneously emits a photon, which is then reabsorbed by other atoms. If the optical density of the cloud is high, it can take a long time for the photon to find its way out <sup>2</sup>. Since any photon exchange between two atoms will increase their relative momentum by  $2\hbar k$ , this leads to a repulsive force, which is proportional to the absorption cross section for the incident light beam. When this repulsive force balances the confining force exerted by the MOT, any increase in the number of trapped atoms augments its size, but its density.

### 24.3.1.2 Dark SPOT

In order to overcome the 'radiation trapping' effect, the atoms can be optically pumped into a 'dark' hyperfine level of the ground state that does not interact with the MOT light. In a conventional MOT one usually employs an auxiliary light beam called 'repumper', copropagating with the MOT beams, but tuned to another transition between hyperfine levels of the ground and excited states. The repumper recycles the population leaking out of the (not perfectly) cyclic MOT transition. As an example, Fig. 24.10 shows the MOT and repumper transitions for sodium.

In contrast to this conventional MOT, the scheme known as the *dark spontaneous force optical trap* (dark SPOT), passes the repumping beam through a glass plate the center of which is obstructed by a small circular disk. The shadow of this disk is projected into the center of the trap in such a way that the atoms in the center are not repumped back into the cyclic transition, but spend most of their time ( $\sim 99\%$ ) in 'dark' hyperfine levels. While the cooling and confinement force continue to operate on the periphery of MOT, its center does not feel any radiation pressure. Dark SPOTs are able to increase the density of a trapped cloud by almost *two orders* of magnitude.

## 24.3.2 Optical dipole traps

When temporal variations are to be applied to a confinement potential, magnetic fields are not the best choice, because they are slow and of limited spatial resolution. On the other side, laser beams can be varied quickly and in localized well. The dipole force exerted by a far-detuned laser beam can be derived from the gradient of the Rabi frequency  $\mathbf{F} = -\nabla(\mathbf{d} \cdot \mathbf{E})$ . Hence, it can be derived from an optical potential, which can be used for trapping. The force may be attractive (toward the intensity maximum) or repulsive.

Compared to MOTs, optical traps (*far off-resonance optical trap*, FORT) are tuned far away from resonances, where the population in excited states is insignificant and spontaneous forces are absent. Note from Eq. (18.21), that spontaneous forces fall off

<sup>2</sup>E.g. a photon at the center of the sun will take thousands of years to get out.

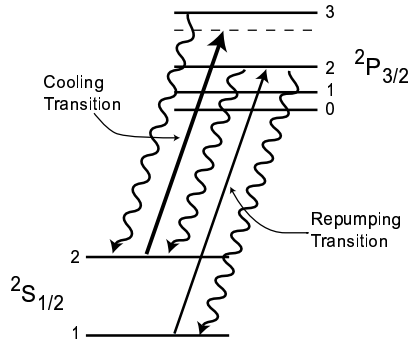


Figure 24.10: Hyperfine structure in sodium atoms showing the usual cooling, pumping, and repumping transitions.

with the square of the detuning while the potential derived from the dipolar force only decreases linearly with the detuning. The off-resonant optical density is negligible, so that radiation trapping is not an issue. The most simple FORT consists of a single focussed, linearly polarized gaussian laser beam tuned far to the red of an atomic resonance. For large detunings and strong field gradients the Eqs. (18.23) and Eqs. (18.24) become [287]<sup>3</sup>,

$$U(\mathbf{r}) \simeq \frac{\hbar\Omega(\mathbf{r})^2}{4\Delta} = \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} I(\mathbf{r}) \quad \text{and} \quad \hbar\gamma_{\text{scat}}(\mathbf{r}) \simeq \sigma_a(\Delta) \frac{I(\mathbf{r})}{\omega} = \frac{3\pi c^2}{2\omega_0^3} \left(\frac{\Gamma}{\Delta}\right)^2 I(\mathbf{r}), \quad (24.66)$$

using the Rabi frequency  $\hbar\Omega = d_{12}E$ , the dipole moment  $d = \sqrt{3\pi\epsilon_0\hbar\Gamma/k^3}$ , and the intensity  $I = \frac{\epsilon_0}{2}c|E|^2$ . This shows that the potential becomes directly proportional to the light intensity and inversely proportional to the detuning. Therefore, at large detuning but very high intensity, the depth of the FORT can be maintained, although the atoms do not absorb photons. Important advantages of FORTs as compared to MOTs are: (1) high densities ( $\sim 10^{12} \text{ cm}^{-3}$ ) and (2) a well-defined polarization axis along which the atoms can be aligned or oriented (polarization of the spins).

Since lasers beams can easily be manipulated in position, intensity, and frequency, they can realize a large wide variety of possible geometries. For example, with a focused laser beam, one may influence the local density of a condensate and stir it around by moving the position of the laser beam. Strongly focussed laser beams are often used for transporting or manipulating microscopic objects in arrangements called *optical tweezers*. And with standing light waves, it is possible to form periodic optical lattices in one, two or three dimensions (see Sec. 27.4.2).

### 24.3.2.1 Spin relaxation

When the atomic ground state has a hyperfine structure, another relaxation mechanism can be observed: Near-resonance Raman scattering can induce transitions between hyperfine states causing a population redistribution of between Zeeman sub-

<sup>3</sup>Jürgen Bosse claims that the dipole trap formula given in [287] is wrong!

states called *spin relaxation*. In magnetic traps, this can lead to losses, because not all Zeeman substates are trapped.

The rate of an arbitrary scattering process starting from an initial state  $|F, m\rangle$  through several possible excited states  $|F'_j, m'_j\rangle$  to a final state  $|F''m''\rangle$  is, according to the formula of Kramers-Heisenberg [485],

$$\gamma_{Fm \rightarrow F'm'} \propto \left| \sum_j \frac{\alpha_{Fm \rightarrow F'm'}^{(F'_j m'_j)}}{\Delta_{F'_j m'_j}} \right|^2. \quad (24.67)$$

Far from resonance the scattering decreases as  $\Delta^2$  for Rayleigh scattering,  $Fm = F'm'$ . Raman scattering,  $Fm \neq F'm'$ , is further suppressed by destructive interference of the different scattering paths.

In the case of rubidium, we calculate,

$$\gamma_{spin} = \frac{3c^2\omega^4}{8\pi} \frac{70}{81} \Gamma^2 \left| \left( \frac{1}{\omega_{D1}} \right)^3 \frac{1}{\Delta_{D1}} - \left( \frac{1}{\omega_{D2}} \right)^3 \frac{1}{\Delta_{D2}} \right|^2 \frac{I_0}{\hbar\omega}. \quad (24.68)$$

### 24.3.2.2 Potential of a Gaussian beam

The *far-off resonance optical trap* (FORT) is an example of an optical trap based on dipole forces [287]. The intensity distribution of a gaussian beam with a diameter of  $w_0$  at its waist is <sup>4</sup>,

$$I(\mathbf{r}) = \frac{2P}{\pi w_0^2} e^{(-2x^2 - 2y^2)/w_0^2} e^{-z^2/z_R^2}, \quad (24.69)$$

where  $P_{cav}$  is the total power of the beam and  $z_R \equiv \pi w_0^2/\lambda_{dip}$  the *Rayleigh length* at a given wavelength  $\lambda_{dip}$ . The dipolar potential is given by (24.66). Using the potential depth,

$$U_0 \equiv \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} \frac{2P}{\pi w_0^2} < 0, \quad (24.70)$$

we can approach the potential near its center, that is, near the optical axis,  $r \ll \frac{1}{2}w_0$ , and within the range of the Rayleigh length,  $z \ll \pi w_0^2/\lambda$ , by a harmonic potential <sup>5</sup>,

$$\begin{aligned} U(\mathbf{r}) &\simeq U_0 e^{(-2x^2 - 2y^2)/w_0^2} e^{-z^2/z_R^2} \simeq U_0 \left( 1 - \frac{2x^2 + 2y^2}{w_0^2} - \frac{z^2}{z_R^2} \right) \\ &\equiv U_0 + \frac{m}{2} \omega_r^2 r^2 + \frac{m}{2} \omega_z^2 z^2 \equiv k_B T \left( \frac{U_0}{k_B T} + \frac{r^2}{2\bar{r}^2} + \frac{z^2}{2\bar{z}^2} \right). \end{aligned} \quad (24.71)$$

This leads to the equivalences,

$$\boxed{\begin{aligned} \omega_r &= \frac{2}{w_0} \sqrt{\frac{U_0}{m}} & \text{and} & & \omega_z &= \frac{\sqrt{2}}{z_R} \sqrt{\frac{U_0}{m}} \\ \bar{r} &= \frac{w_0}{2} \sqrt{\frac{k_B T}{U_0}} & \text{and} & & \bar{z} &= \frac{z_R}{\sqrt{2}} \sqrt{\frac{k_B T}{U_0}} \end{aligned}}. \quad (24.72)$$

<sup>4</sup>See script on *Electrodynamics* (2020).

<sup>5</sup>The diameter of a Gaussian beam can be characterized in several ways,

$$\bar{r}_{1/\sqrt{e}\text{-radius}} = \frac{\bar{r}_{1/e^2\text{-radius}}}{\sqrt{2}} = \sqrt{2} \bar{r}_{1/e^2\text{-radius}} = \frac{\bar{r}_{1/2\text{-radius}}}{2 \ln 2},$$

and  $\bar{r}_{\text{-rms}} \equiv \bar{r}_{1/\sqrt{e}\text{-diam}}$  and  $\bar{r}_{\text{-hwhm}} \equiv \bar{r}_{1/2\text{-diam}}$  and  $\bar{r}_{\text{-diam}} = 2\bar{r}_{\text{-radius}}$ .

Solve Excs. 24.3.3.3 and 24.3.3.4.

**Example 110 (Dipole trap for rubidium):** The formulas (24.66) hold for a two-level system. In case of the  $D1$ - and  $D2$ -lines of rubidium, we must consider all contributions weighted by the respective detunings,

$$U_0 \equiv \sigma_0 \frac{\hbar\Gamma}{4} \left( \frac{1}{\Delta_{D1}} + \frac{g_{D2}/g_{D1}}{\Delta_{D2}} \right) \frac{I_0}{\hbar\omega} \simeq \frac{3\hbar\pi c^2}{2\omega^2} \frac{\Gamma}{\Delta} \frac{I_0}{\hbar\omega},$$

where  $g_{D2}/g_{D1} = 2$ .

Similarly, the spontaneous emission rate is,

$$\gamma_{sct} \simeq \frac{\pi c^2 \Gamma^2}{2\omega^2} \left( \frac{1}{\Delta_{D1}^2} + \frac{g_{D2}/g_{D1}}{\Delta_{D2}^2} \right) \frac{I_0}{\hbar\omega}.$$

The spontaneous emission rate decays faster with detuning than the potential depth. Thus, heating can be avoided by working at large detunings and providing higher laser intensities. Defining the recoil temperature by,

$$T_{rec} = \frac{\hbar^2 k^2}{k_B m},$$

the *heating rate* is [287],

$$\dot{T} = \frac{1}{3} T_{rec} \gamma_{sct} = \frac{\hbar^2 k^2}{3mk_B} \gamma_{sct}.$$

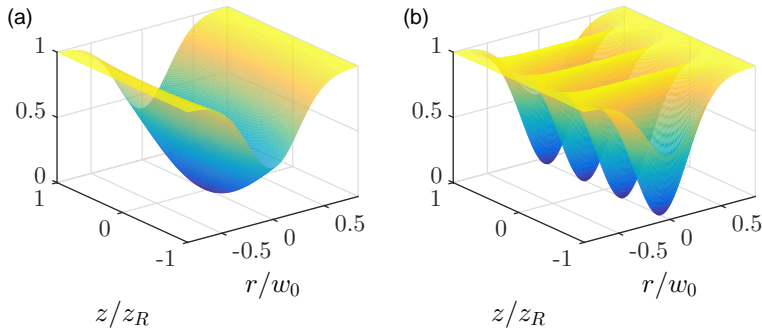


Figure 24.11: (code) (left) Dipole potential created by a Gaussian beam. (right) Dipole potential created by a stationary light wave.

### 24.3.2.3 Trapping in standing light waves

If both counterpropagating modes are pumped at different powers,  $P_{\pm}$ , the intensity distribution is,

$$I(\mathbf{r}) = \frac{2}{\pi w_0^2} e^{(-2x^2 - 2y^2)/w_0^2} e^{-z^2/z_R^2} \left| \sqrt{P_+} e^{ikz} + \sqrt{P_-} e^{-ikz} \right|^2. \quad (24.73)$$



The potential depth is,

$$U_0 = \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} \frac{2(\sqrt{P_+} + \sqrt{P_-})^2}{\pi w_0^2} < 0. \quad (24.74)$$

Therefore, within the Rayleigh length, the potential is,

$$U(\mathbf{r}) \simeq U_0 e^{(-2x^2 - 2y^2)/w_0^2} \frac{P_+ + P_- + 2\sqrt{P_+ P_-} \cos kz}{P_+ + P_- + 2\sqrt{P_+ P_-}}. \quad (24.75)$$

Letting the powers be equal,

$$U(\mathbf{r}) \xrightarrow{P_+ = P_-} U_0 e^{(-2x^2 - 2y^2)/w_0^2} \sin^2 \frac{kz}{2} \quad (24.76)$$

$$\xrightarrow{x, y \ll k^{-1}, w_0} U_0 \left( 1 - \frac{2x^2 + 2y^2}{w_0^2} - \frac{k^2 z^2}{4} \right).$$

This leads to the identities,

$$\left. \begin{aligned} \omega_r &= \frac{2}{w_0} \sqrt{\frac{U_0}{m}} & \text{and} & & \omega_z &= k \sqrt{\frac{U_0}{2m}} \\ \bar{r} &= \frac{w_0}{2} \sqrt{\frac{k_B T}{U_0}} & \text{and} & & \bar{z} &= \frac{\sqrt{2}}{k} \end{aligned} \right\} \quad (24.77)$$

Solve the Excs. 24.3.3.5 and 24.3.3.6.

### 24.3.3 Exercises

#### 24.3.3.1 Ex: Linearization of the MOT

Derive the friction coefficient and the spring constant for a MOT.

#### 24.3.3.2 Ex: Design of a Zeeman slower

In this exercise we will design a 'decreasing field *Zeeman slower*' for strontium (see also Exc. 14.4.6.3).

a. Calculate the mean velocity of atoms in a strontium gas heated to  $500^\circ\text{C}$ . What is the Doppler shift for an atom moving at this velocity at the cooling transition at  $\lambda = 461 \text{ nm}$  (linewidth  $30.5 \text{ MHz}$ )?

b. Assuming you want to decelerate a fraction of 20% of the atoms flying in a

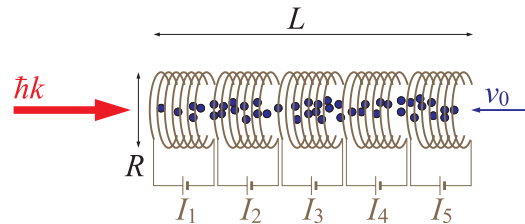


Figure 24.12: Design of a Zeeman slower.

particular direction, to what frequency should a counterpropagating laser (intensity  $I = 20 \text{ mW/cm}^2$ ) be tuned in order to slow down the atoms?

c. Suppose the strontium atoms were always in resonance with the counterpropagating laser light while being decelerated. What would be the evolution of their Doppler shift along their trajectory (supposed to be on a straight line antiparallel to the laser beam).

d. In order to maintain the laser always in resonance we need to compensate for the diminishing Doppler shift along the atomic trajectory. This can be done exploiting the Zeeman shift induced by a magnetic field. We will now design a magnetic field generating an appropriate Zeeman shift. For simplicity, let us assume 5 identical radial solenoids distributed over  $L = 30 \text{ cm}$  as sketched in Fig. 24.12, the only adjustable parameters being the currents in all solenoids, which need to be optimized such as to compensate the Doppler shift along the atom's trajectory.

e. Simulate the 1D trajectory of an atom cooled by the Zeeman slower.

### 24.3.3.3 Ex: Dipole trap near an intercombination line

a. Strontium has a strong transition ( $\Gamma_{461} = (2\pi) 30.5 \text{ kHz}$ ) at 461 nm and a weak intercombination resonance ( $\Gamma_{689} = (2\pi) 7.6 \text{ kHz}$ ) at 689 nm. A Gaussian laser beam with the power  $P = 10 \text{ mW}$  focused to a waist of  $w_0 = 100 \mu\text{m}$  is tuned  $\Delta_{689} = -(2\pi) 10 \text{ GHz}$  below the intercombination transition. Calculate the potential depth and the vibration frequencies for atoms trapped by this laser beam considering both resonances. What is the scattering rate on the two transitions.

b. Suppose that the trapped atomic cloud consists of  $N = 10^8$  atoms at the temperature  $T = 10 \mu\text{K}$ . Calculate the atomic density  $n_0$  in the center of the cloud.

### 24.3.3.4 Ex: Dipole trap with a focused beam

a. Calculate the vibration frequencies of  $^{87}\text{Rb}$  atoms confined in an optical trap consisting of a focused laser beam with the power  $P = 10 \text{ W}$  and the beam diameter  $w_0 = 100 \mu\text{m}$ . The laser beam is tuned 5 nm to the red side of the rubidium  $D1$  resonance located at  $\lambda = 795 \text{ nm}$ .

b. Assume that the trapped atomic cloud consists of  $N = 10^8$  atoms at the temperature  $T = 100 \mu\text{K}$ . Calculate the atomic density  $n_0$  in the center of the cloud.

c. The cross section for elastic collisions is  $\sigma = 10^{-12} \text{ cm}^2$ . How many times do atoms meet on average?

### 24.3.3.5 Ex: Optical lattice

A laser beam with wavelength  $\lambda_{dip} = 1064 \text{ nm}$ , power  $P = 2 \text{ W}$ , and diameter  $w_0 = 50 \mu\text{m}$  is subdivided into three retroreflected beams intersecting at right angles. With this configuration we form a cubic optical lattice for strontium atoms, whose relevant transition lies at  $\lambda_{Sr} = 461 \text{ nm}$  and has a decay width of  $\Gamma_{Sr} = (2\pi) 32 \text{ MHz}$ . Calculate the potential depth and the secular frequencies.

### 24.3.3.6 Ex: Ring shaped optical potential

An interesting system is the 1D array of annular optical potentials realized in a standing wave formed by red-detuned Gaussian beam and a counterpropagating blue-detuned donut-mode. In general, the tight longitudinal confinement freezes out the

axial motion by *quantum confinement*. It can be readily shown [730] that in the far-off resonance case and if the potential is approximate by a harmonic potential around its minimum the eigenenergy spectrum is given by,

$$E_{pq} = U_0 + \hbar\omega(q + \frac{1}{2}) + \frac{\hbar^2 p^2}{2mR_0^2} .$$

It thus reproduces the ro-vibrational spectrum of a 2D artificial molecule and gives rise to two normal motions. In its ground state, we have the atom optical analog of a 2D rigid rotator. Gravity plays formally the same role as static electric fields for molecules. Such systems might be interesting for investigating the selection rules for transitions between ro-vibrational states involving conservation of total angular momentum of light and atoms and yield insight into the concept of orbital angular momentum of light fields.

### 24.3.3.7 Ex: Time-averaged trap

For sufficiently fast periodic displacements of a far-detuned laser beam it is possible to engineer effective more complicated trapping potential. What are the conditions for modulation speed? Simulate the effective trapping potential generated by a vibrating laser beam.

## 24.4 Magnetic traps

Purely magnetic traps are widely used in atom optics, where they served, e.g., for the first realizations of Bose-Einstein condensation (BEC). The most important feature that distinguishes magnetic traps is, that they do not need light to confine atoms. Hence, they are free of heating effects caused by photonic absorption, which turned out to be necessary condition for reaching BEC. Magnetic traps rely on the interaction of atomic spins with magnetic fields and gradients designed to contain the atoms. Depending on the sign of  $U$  and  $\mathbf{F}$ , atoms in states whose energy increases or decreases with the magnetic field are called 'low-field seekers' or 'high-field seekers', respectively. One might think, that it should be possible to trap atoms in any of these states, generating either a magnetic field minimum or a maximum. Unfortunately, only low-field seekers can be trapped in static magnetic fields, because in free space magnetic fields can not form maxima. Even though low-field seekers are not in the energetically lowest hyperfine levels, they can still be trapped because the rate of spontaneous emission through the magnetic dipole is  $\sim 10^{-10} \text{ s}^{-1}$ , and hence completely negligible. However, spin changing collisions can induce losses and limit the maximum densities. Solve Exc. 24.4.6.1.

The most basic static magnetic trap for neutral atoms is generated by a pair of current-carrying coils in anti-Helmholtz configuration (similar to the geometry used for a MOT), producing an axially symmetric quadrupolar magnetic field. Since this field configuration always has a central point, where the magnetic field disappears, non-adiabatic Majorana transitions can occur when the atom passes through the zero point. The transitions transfers population from a low-field seeking state to a high-field seeker, which consecutively is expelled from the trap. This problem can

be overcome by using a different magnetic field geometries. One example is the so-called *magnetic bottle* also called the *Ioffe-Pritchard trap*, where the minimum field amplitude has a finite value different from zero. Other methods to eliminate the zero-field point are time-varying potentials, such as the time-orbiting potential (TOP) trap, or the application of an 'optical plug', which consist in an intense dipolar optical laser beam, tuned to the blue of an atomic transition, focused into the center of a quadrupole trap where the magnetic field is zero, and repelling the atoms from this area.

### 24.4.1 Quadrupolar traps and Majorana spin-flips

The most basic static magnetic trap for neutral atoms is generated by a pair of current-carrying coils in anti-Helmholtz configuration producing an axially symmetric quadrupolar magnetic field, as shown in Fig. 24.13.

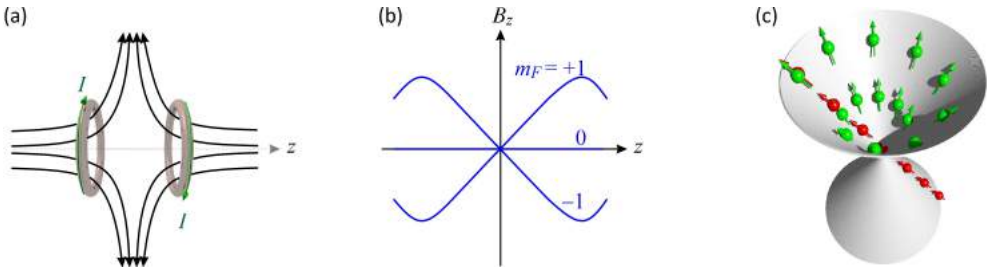


Figure 24.13: (a) Quadrupolar magnetic trap generated by a pair of current-carrying wires in anti-Helmholtz configuration. (b) Ground state energy levels of  $^{23}\text{Na}$ ,  $^2S_{1/2}$ ,  $F = 1$  as a function of axial distance from the trap center. (c) Illustration of Majorana spin-flips: The red atom passes through the hole, while the green one moves adiabatically avoiding the hole.

Close to the trap center an expansion of the magnetic field generated by anti-Helmholtz coils yields,

$$\mathbf{B} = \begin{pmatrix} x \\ y \\ -2z \end{pmatrix} \partial_r B, \tag{24.78}$$

where the field gradient  $\partial_r B$  along radial direction  $r^2 \equiv x^2 + y^2$  in the trap center depends on the applied current and the geometry of the coils. However, the 1:2 aspect ratio is generic for all quadrupolar potentials, as we will see in Exc. 24.4.6.2. We easily verify that,

$$\nabla \cdot \mathbf{B} = 0 \quad \text{but} \quad \nabla |\mathbf{B}| = \frac{\partial_r B}{\sqrt{r^2 + 4z^2}} \begin{pmatrix} x \\ y \\ 4z \end{pmatrix}. \tag{24.79}$$

Thus, the quadrupolar magnetic potential is linear in the spatial coordinates,

$$U(\mathbf{r}) = -|\mu||\mathbf{B}| = \mu_B g_J m_J \partial_r B \sqrt{r^2 + 4z^2}, \tag{24.80}$$

where  $2\partial_r B = \partial_z B$ .

To calculate the *rms*-radius  $\bar{r}$  of a cloud of temperature  $T$  confined to this potential, we set,

$$k_B T \equiv U(\bar{r}, 0) = \mu_B \bar{r} \partial_r B, \quad (24.81)$$

and obtain the density distribution,

$$n(\mathbf{r}) = n_0 e^{-U(\mathbf{r})/k_B T} = n_0 e^{-\sqrt{r^2+4z^2}/\bar{r}}. \quad (24.82)$$

Normalization requires,

$$\begin{aligned} N &= \int_{R^3} n(\mathbf{r}) d^3 r = n_0 \int_{-\infty}^{\infty} \int_0^{\infty} e^{-\sqrt{r^2+4z^2}/\bar{r}} 2\pi r dr dz \\ &= n_0 2\pi \bar{r}^2 \int_{-\infty}^{\infty} \int_{2|z|/\bar{r}}^{\infty} \xi e^{-\xi} d\xi dz = n_0 2\pi \bar{r}^2 \int_{-\infty}^{\infty} e^{-\frac{2|z|}{\bar{r}}} \left(1 + \frac{2|z|}{\bar{r}}\right) dz \\ &= n_0 2\pi \bar{r}^3 \int_0^{\infty} e^{-\zeta} (1 + \zeta) d\zeta = n_0 4\pi \bar{r}^3. \end{aligned} \quad (24.83)$$

Therefore, the effective volume is,  $V_{eff} = 4\pi \bar{r}^3$ . In application example is discussed in Exc. 24.4.6.3.

### 24.4.1.1 Majorana spin-flips

The quadrupolar trap is the simplest one that can be technically realized. Unfortunately, this trap is not stable because of the phenomenon of *Majorana spin-flips*, which expel atoms from the trapped cloud. Since this field configuration always has a central point, where the magnetic field disappears, non-adiabatic Majorana transitions can occur when the atom passes through the zero point [see Fig. 24.13(c)]. The disappearance of the field leaves the atoms disoriented, that is, ready to reorient their spins. The transitions transfer population from a low-field seeking state to a high-field seeker, which consecutively is expelled from the trap. This problem is particularly severe for hydrogen, where it can induce a so-called *relaxation explosion* [334].

From (24.81) we get the *rms*-radius,

$$\bar{r} = \frac{k_B T}{\mu_B \partial_r B}. \quad (24.84)$$

The average velocity of an atom is,

$$\bar{v} = \sqrt{\frac{k_B T}{m}}. \quad (24.85)$$

In order for the atomic motion in the magnetic potential to be adiabatic [so that Eq. (24.80) applies], the *local Larmor frequency*,

$$\omega_{Larmor}(\mathbf{r}) = \frac{\mu_B}{\hbar} \sqrt{r^2 + 4z^2} \partial_r B \quad (24.86)$$

must be faster, than any change the atom might experience due to its motion with velocity  $\mathbf{v}$ . I.e. we need [544],

$$\omega_{Larmor}(\mathbf{r}) > \frac{\mathbf{v} \cdot \nabla |\mathbf{B}|}{|\mathbf{B}|}. \quad (24.87)$$

This can not be satisfied within a volume located at the trap center. This ellipsoidal volume is delimited by  $\mathbf{r}_{sf}$  given by the condition,

$$\omega_{Larmor}(\mathbf{r}_{sf}) \equiv \frac{\mathbf{v} \cdot \nabla |\mathbf{B}|}{|\mathbf{B}|}. \quad (24.88)$$

For our quadrupole trap,

$$\frac{\mathbf{v} \cdot \nabla |\mathbf{B}|}{|\mathbf{B}|} = \frac{\mathbf{v} \cdot \frac{\partial_r B}{\sqrt{r_{sf}^2 + 4z_{sf}^2}}}{\partial_r B \sqrt{r_{sf}^2 + 4z_{sf}^2}} \begin{pmatrix} x_{sf} \\ y_{sf} \\ 4z_{sf} \end{pmatrix} = \frac{x_{sf}v_x + y_{sf}v_y + 4z_{sf}v_z}{r_{sf}^2 + 4z_{sf}^2}. \quad (24.89)$$

Considering for simplicity only radial motion,  $\mathbf{v} = v\hat{\mathbf{e}}_r$ , then by equating (24.86) and (24.88),

$$\frac{\mu_B}{\hbar} r_{sf} \partial_r B = \omega_{Larmor}(r_{sf}) = \frac{v}{r_{sf}}, \quad (24.90)$$

that is, the spin-flip volume is on the order of,

$$r_{sf} = \sqrt{\frac{\hbar v}{\mu_B \partial_r B}}. \quad (24.91)$$

Let us now estimate the spin relaxation rate from the flow of atoms through the volume,

$$\frac{1}{\tau_{sf}} = N \frac{r_{sf}^3}{V_{eff}} \frac{\bar{v}}{r_{sf}}, \quad (24.92)$$

where  $r_{sf}^3/V_{eff}$  is simply the fraction of the cloud's volume overlapping with the spin-flip volume. Then,

$$\begin{aligned} \frac{1}{\tau_{sf}} &= \frac{N}{4\pi\bar{r}^3} r_{sf}^2 \bar{v} = \frac{N}{4\pi \left( \frac{k_B T}{\mu_B \partial_r B} \right)^3} \frac{\hbar \bar{v}}{\mu_B \partial_r B} \\ &= \frac{N\hbar}{4\pi(k_B T)^3} (\mu_B \partial_r B)^2 \frac{k_B T}{m} = \frac{N\hbar(\mu_B \partial_r B)^2}{4\pi m (k_B T)^2}. \end{aligned} \quad (24.93)$$

That is, the problem gets worse when the cloud is cooled to low temperatures.

### 24.4.2 Magnetic Ioffe-type traps

The spin-flip problem can be overcome by using a different magnetic field geometries. One example is the so-called *magnetic bottle*, also called the *Ioffe-Pritchard trap* illustrated in Fig. 24.14(a), where the minimum field amplitude has a finite value different from zero. Other methods to eliminate the zero-field point are time-varying potentials, such as the time-orbiting potential (TOP) trap illustrated in Fig. 24.14(b) and discussed in Exc. 24.4.6.4 [227, 307], or the application of an 'optical plug', which consist in an intense dipolar optical laser beam, tuned to the blue of an atomic transition, focused into the center of a quadrupole trap where the magnetic field is zero, and repelling the atoms from this area (see Fig. 24.22). The advantage of Ioffe-Pritchard-type traps is that they are always harmonic sufficiently close to the trap center, which simplifies the theoretical treatment in many respects, as shown in Exc. 24.4.6.5.

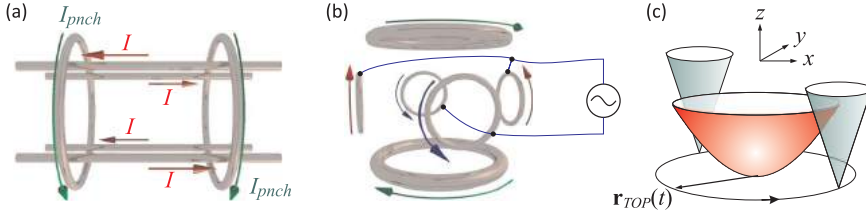


Figure 24.14: (a) Magnetic trap in Ioffe-Pritchard configuration. (b) Time-Orbiting Potential (TOP) trap. (c) Death-circle in a TOP trap.

Close to the trap center Ioffe-Pritchard-type traps are described by,

$$U(\mathbf{r}) = \mu_B g_F m_F \sqrt{B_0^2 + (r \partial_r B)^2 + (z \partial_z B)^2}, \quad (24.94)$$

and this magnetic trapping potential can be harmonically approximated by,

$$\begin{aligned} U(\mathbf{r}) &\simeq \mu_B g_F m_F \left( B_0 + \frac{(r \partial_r B)^2}{2B_0} + \frac{(z \partial_z B)^2}{2B_0} \right) \\ &\equiv const + \frac{m}{2} \omega_r^2 r^2 + \frac{m}{2} \omega_z^2 z^2 \equiv k_B T \left( const + \frac{r^2}{2\bar{r}^2} + \frac{z^2}{2\bar{z}^2} \right), \end{aligned} \quad (24.95)$$

where the *rms*-radius  $\bar{r} = \omega_r^{-1} \sqrt{k_B T / m}$  follow from the normalization of the density  $n(\mathbf{r}) = n_0 e^{-U(\mathbf{r})/k_B T}$  to the number of atoms,

$$N = \int n(\mathbf{r}) d^3 r = n_0 \int_0^\infty e^{-r^2/2\bar{r}^2} 2\pi dr \int_{-\infty}^\infty e^{-z^2/2\bar{z}^2} dz = n_0 (2\pi)^{3/2} \bar{r}^2 \bar{z} \equiv n_0 V_{eff}. \quad (24.96)$$

The trap frequencies can be calculated as,

$$\omega_{r,z} = \sqrt{\frac{\mu_B (\partial_r B_{r,z})^2}{m B_0}}. \quad (24.97)$$

The Earth's gravitational field deforms the trapping potential and, in the case of a harmonic potential, causes a gravitational sag without changing the secular frequencies of the potential. Assuming the potential to be given by,

$$U = \frac{m}{2} \omega_r^2 r^2 + \frac{m}{2} \omega_z^2 z^2 - mgz = \frac{m}{2} \omega_r^2 r^2 + \frac{m}{2} \omega_z^2 (z - g/\omega_z^2)^2 - \frac{m}{2} g^2/\omega_z^2, \quad (24.98)$$

the atoms sag to a height of  $g/\omega_z^2$ . In time-dependent traps, gravity causes a more complex behavior [302]. Important works have been done by [133, 546, 229, 291, 2, 172, 425, ?, 192]. We study the impact of gravitation in Exc. 24.4.6.6.

#### 24.4.2.1 Characterization of Ioffe-type traps

The 'time-of-flight' density distribution is,

$$r_{TOF} = \sqrt{\bar{r}^2 + \bar{v}^2 t_{TOF}^2} = \sqrt{\frac{k_B T}{m}} \sqrt{\frac{1}{\omega_r^2} + t_{TOF}^2} \simeq t_{TOF} \sqrt{\frac{k_B T}{m}}. \quad (24.99)$$

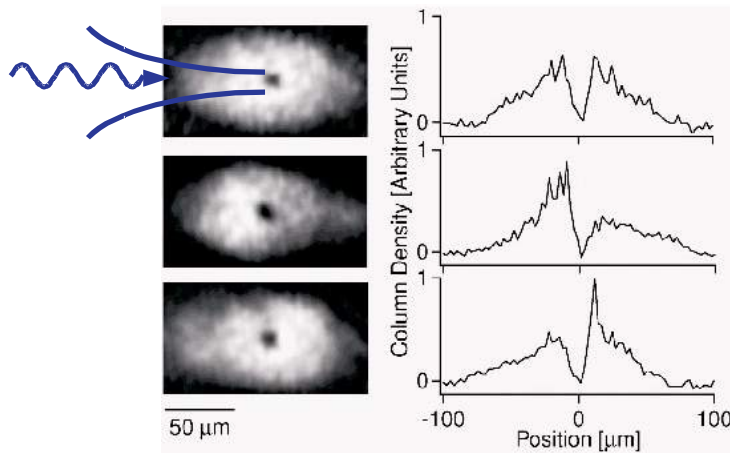


Figure 24.15: Creation of a repulsive hole by light tuned to the blue of an atomic transition.

The *phase space density* is,

$$\rho = n_0 \lambda_{dB}^3 = \frac{N}{(2\pi)^{3/2} \bar{r}^2 \bar{z}} \left( \frac{2\pi \hbar^2}{mk_B T} \right)^{3/2} = N \omega_r^2 \omega_z \left( \frac{\hbar}{k_B T} \right)^3 = \zeta(3) \left( \frac{T_c}{T} \right)^3. \quad (24.100)$$

where  $\zeta(3) = 1.202$  is,

$$k_B T_c = \hbar \left( \frac{N \omega_r^2 \omega_z}{\zeta(3)} \right)^{1/3} \quad (24.101)$$

is the critical temperature. The *maximum collision rate* is,

$$\gamma_{coll} = n_0 \sigma \bar{v} = n_0 4\pi a_s^2 \sqrt{\frac{k_B T}{m}}. \quad (24.102)$$

The average collision rate can be obtained from,

$$\bar{\gamma}_{coll} N = \frac{1}{N} \int \gamma_{coll}(\mathbf{r}) n(\mathbf{r}) d^3 r = \frac{\int \sigma \bar{v} n^2(\mathbf{r}) d^3 \mathbf{r}}{\int n(\mathbf{r}) d^3 r}. \quad (24.103)$$

### 24.4.3 Radiative coupling and evaporative cooling

As we saw in the last section, optical cooling becomes ineffective when the density of the gas is high. Hence, we need another dissipation mechanism to cool trapped atoms. A method called *evaporation* has been proposed by Hess [332] for spin-polarized hydrogen ( $H\uparrow$ ) and was observed by Masuhara et al. [462]. Later, evaporation was used on alkali metals [2, 544, 174]. A detailed review of the subject was published by Ketterle and van Druten [389].

Another collision-based cooling mechanism is *sympathetic cooling*. The technique was originally used in ion traps. Later it was applied to neutral atoms confined in magnetic traps. The idea is to get the cloud under study into thermal contact with a cold buffer gas. In some cases, the buffer gas may be optically or evaporatively cooled.





Figure 24.16: The basic idea of evaporation consists in removing hot particles from the sample.

Sympathetic cooling has been used in magnetic traps to create double condensates [514] and to cool fermions until the regime of quantum degeneracy [183].

#### 24.4.4 Evaporative cooling

Evaporation always occurs when energetic particles abandon a system with finite bonding energy, removing more than their share of average energy per particle. Here, we consider the case of a finite-sized trapping potential, that is, the potential has an edge or a beak through which hot atoms, with sufficient kinetic energy to reach that region, may leave the trap. In the ideal case, this will lead to a complete truncation of the hot tail of the equilibrium Maxwell-Boltzmann velocity distribution. If the remaining system finds back to thermal equilibrium, it will do at a lower temperature. The redistribution of kinetic energy between atoms leading to *thermalization* occurs through elastic collisions.

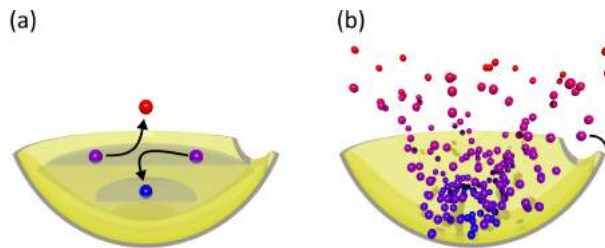


Figure 24.17: Principle of (a) rethermalization due to elastic collisions and (b) evaporation.

### 24.4.4.1 Truncating the Boltzmann distribution

Let us first explain how the truncation leads to colder temperatures.

The objective is to calculate the Boltzmann distribution in a particular trap for a given atom number  $N$  and temperature  $T$ . The first step is to obtain the density-of-states. For an isotropic harmonic trap  $\varepsilon = \frac{p^2}{2m} + V(r)$  with  $V(r) = \frac{m}{2}\omega^2 r^2$ , it is,

$$\eta(\varepsilon)d\varepsilon = \frac{1}{(2\pi)^3} \int_V d^3r d^3k = \frac{2\pi(2m)^{3/2}}{h^3} \int_V \sqrt{\varepsilon - V(r)} d^3r d\varepsilon = \frac{\varepsilon^2 d\varepsilon}{2(\hbar\omega)^3}. \quad (24.104)$$

The atom density is,

$$n(\varepsilon) = e^{(\mu-\varepsilon)/k_B T} = Z e^{-\varepsilon/k_B T}. \quad (24.105)$$

From these expression we obtain the atom number,

$$N = \int_0^\infty n(\varepsilon)\eta(\varepsilon)d\varepsilon = \int_0^\infty e^{(\mu-\varepsilon)/k_B T} \frac{\varepsilon^2}{2(\hbar\omega)^3} d\varepsilon = Z \frac{(k_B T)^3}{(\hbar\omega)^3}, \quad (24.106)$$

which we may now use to calibrate the fugacity via

$$Z = N \frac{(\hbar\omega)^3}{(k_B T)^3}, \quad (24.107)$$

which finally allows us to calculate the total energy,

$$E = \int_0^\infty \varepsilon n(\varepsilon)\eta(\varepsilon)d\varepsilon = \int_0^\infty \varepsilon e^{(\mu-\varepsilon)/k_B T} \frac{\varepsilon^2}{2(\hbar\omega)^3} d\varepsilon = 3Z \frac{(k_B T)^4}{(\hbar\omega)^3} = 3N k_B T. \quad (24.108)$$

The evaporation consists in truncating the distribution function  $n(\varepsilon)$  at some energy  $\hbar\omega_{rf}$ . We get with  $\beta \equiv (k_B T)^{-1}$ ,

$$\tilde{N} = \int_0^{\hbar\omega_{rf}} n(\varepsilon)\eta(\varepsilon)d\varepsilon = N \left( 1 - \frac{2 + 2\beta\hbar\omega_{rf} + (\beta\hbar\omega_{rf})^2}{2e^{\beta\hbar\omega_{rf}}} \right) \quad (24.109)$$

and

$$\tilde{E} = \int_0^{\hbar\omega_{rf}} \varepsilon n(\varepsilon)\eta(\varepsilon)d\varepsilon = E \left( 1 - \frac{6 + 6\beta\hbar\omega_{rf} + 3(\beta\hbar\omega_{rf})^2 + (\beta\hbar\omega_{rf})^3}{6e^{\beta\hbar\omega_{rf}}} \right). \quad (24.110)$$

As the truncation removes the hottest atoms from the cloud, we loose atom number and energy. Assuming the existence of some rethermalization mechanism, we may now use the new values for  $N$  and  $T$  to calculate the new equilibrium Boltzmann distribution starting all over from Eq. (24.105),

$$N \longleftarrow \tilde{N} \quad \text{and} \quad T \longleftarrow \frac{\tilde{E}}{3Nk_B} \quad (24.111)$$

Repeating this over and over the temperature will gradually reduce. The cooling process can be speed up by readjusting the truncation frequency to the actual temperature. This is called forced evaporation (see Fig. 24.18).

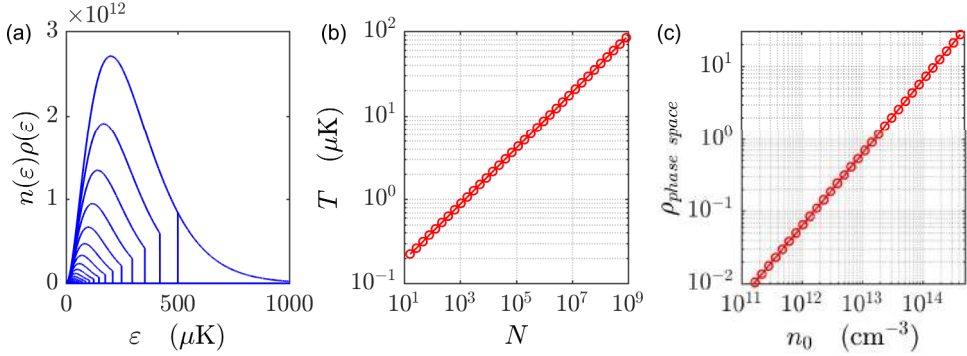


Figure 24.18: (code) (a) Forced evaporation by truncating the Boltzmann distribution over and over again. (b) Evolution of the temperature and (c) of the phase space density with number of remaining atoms.

#### 24.4.4.2 Rethermalization

As already mentioned, rethermalization occurs due to elastic collisions. It needs more or less three collisions per atom to rethermalize a cloud [497, 735], so that the collision rate determines the speed of the evaporation process. A large collision rate is desirable to keep the evaporation process faster than trap loss processes. Evaporation ramps between several seconds and a minute are typical.

The maximum rate of elastic collisions between trapped atoms (in the trap center) is,

$$\gamma_{\text{coll}} = n_0 \sigma_{el} \bar{v} \sqrt{2} \propto \rho^3 N^{2/3}, \quad (24.112)$$

where  $n_0$  is the peak density,

$$\sigma_{el} = 8\pi a_s^2, \quad (24.113)$$

is the cross-section for elastic collisions and,  $\bar{v}$  being the average thermal velocity of the cloud,  $\sqrt{2}\bar{v}$  is the average relative velocity between two of its atoms [388]. This formula gives the average collision rate at the *center of the cloud*, where the density is highest. To calculate the total collision rate, we need to integrate over the entire volume of the cloud,

$$\bar{\gamma}_{\text{coll}} = \frac{1}{N} \int \gamma_{\text{coll}}(\mathbf{r}) n(\mathbf{r}) d^3r = \frac{\int \sigma_{el} \bar{v} n^2(\mathbf{r}) d^3r}{\int n(\mathbf{r}) d^3r}. \quad (24.114)$$

For harmonic potential we find an average rate reduced by  $2\sqrt{2}$ , for linear potentials by 8. We verify this in Exc. 24.4.6.7. Finally, the rate for collision events is two times smaller, as it involves two atoms at a time.

Obviously, the evaporation process slows down when the cloud cools more, unless the edge of the potential is lowered, such that the hotter atoms of the colder cloud can be evaporated. By continually lowering the edge of the potential, while the atomic cloud keeps on rethermalizing (this procedure is called *forced evaporation*) very low temperatures in the nano-Kelvin regime can be achieved, and the phase space density can be increased by many orders of magnitude (between a MOT and a BEC there are 6 orders of magnitude) up to the threshold of Bose-Einstein condensation. Of course,

this is only possible by sacrificing many hot atoms. Even with a well optimized evaporation ramp (i.e., a controlled lowering of the potential edge), usually only some 0.1% of the atoms reach the condensation phase after about 500 collisions per atom.

Two aspects should be mentioned regarding the optimization of the evaporation ramp. The first aspect is, that elastic collisions with atoms from the residual background vapor of the vacuum chamber limit the lifetime of the trap. Therefore, the evaporation must be sufficiently fast, which requires either a high rate of elastic collisions or a good vacuum. A compromise must be found between a slow but efficient evaporative cooling and a minimization of the losses, which come into play when the evaporation takes too long. The second aspect is, that the dimensionality of the evaporation surface determines the effectiveness of the cooling. In the first demonstration of evaporation,  $\text{H}\uparrow$  atoms of a hot cloud were ejected over a saddle point. The saddle was located a small region away from the trap center, and only atoms with sufficient kinetic energy *along a certain direction*,  $E_z > U_{edge}$ , could leave the trap. In such cases, evaporation is called one-dimensional. Even though ergodic redistribution due to anharmonicities of the potential will drive, sooner or later, all the atoms to this region, this effect becomes less pronounced when the cloud cools down, because the atoms accumulate at the bottom of the approximately harmonic (and therefore separable) potential. This fact has inhibited efficient evaporation of  $\text{H}\uparrow$  below 120  $\mu\text{K}$  [248].

A second evaporative technique has been demonstrated in traps called *time-orbiting potential* (TOP) [544]. It is a feature of TOP traps to display a spatial region called a 'death-circle', where passing atoms are ejected from the trap. This fatal circle can act as a 2-dimensional evaporation surface, provided the radius of the circle is large enough [307]. However, under the influence of gravity the dimensionality is further reduced to 1D [388].

The most successful evaporation technique implemented so far is based on a radiative coupling of confined and free states. We discuss this technique in the following sections. Publications on *evaporative cooling* are [442, 483, 544, 562, 63, 477, 497, 228, 231, 320, 519, 332, 462, 174, 389, 734, 308, 457, 210, 334]. See ([152], Sec. 3.1.4) for an overview.

### 24.4.4.3 Adiabatic decompression

The condition for *adiabatic decompression* of a trapping potential is,

$$\frac{|\dot{\omega}_{trap}|}{\omega_{trap}} \ll \omega_{trap} . \quad (24.115)$$

The population of the quantized levels should not change under adiabatic decompression,  $e^{\hbar\omega_i/k_B T_i} = e^{\hbar\omega_f/k_B T_f}$ , and the phase space density remains unchanged,  $n_i \lambda_{dB,i} = n_f \lambda_{dB,f}$ . If this is true, then the temperature and density change as,

$$\frac{\omega_f}{\omega_i} = \frac{T_f}{T_i} = \left( \frac{n_f}{n_i} \right)^{3/2} . \quad (24.116)$$

Solve Exc. 24.4.6.8.

#### 24.4.4.4 Radiative coupling of internal state

The most successful evaporation technique implemented so far is based on a radiative coupling of confined and free states. We discuss this technique in the following sections. See ([152], Sec. 3.1.4) for an overview.

The radiative coupling technique originates from an idea proposed by Pritchard et al. [308], who have already had some experience with radiofrequency spectroscopy in magnetically trapped neutral atoms [457, 320]. The spatial dependence of the Zeeman splitting is an intrinsic feature of magnetic traps. Irradiation of a radio wave at a certain frequency couples trapped and untrapped Zeeman substates at a well-defined distance from the trap center. This gives rise to a 3D evaporation surface, where the passing atoms can undergo

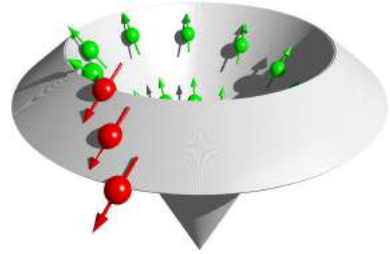


Figure 24.19: Illustration of evaporative truncation.

Landau-Zener transitions and be expelled from the trap. The technical advantages of this technique are substantial: The magnetic trapping potential does not have to be manipulated, for example, by the creation of a nozzle, and the potential edges can be easily controlled by the radiofrequency. If evaporation is forced via a continuous reduction of the radiofrequency and if the evaporation ramp is optimized, the density will increase as well as the collision rate. Rethermalization will accelerate and initiate a self-accelerated evaporation process (*run-away evaporation*). Rf-evaporation was first demonstrated by Ketterle and colleagues [174]. Solve Exc. 24.4.6.9.

#### 24.4.4.5 Adiabatic and diabatic limits of rf-induced evaporation

Rf-induced evaporation can be described within the formalism of the dressed atom [142], where the different states  $m_F$  of an atom with spin  $F$  are coupled to an rf-field <sup>6</sup>, which we assume to be linearly polarized:

$$B(t) = B\hat{\mathbf{e}}_{rf} \cos \omega t . \quad (24.117)$$

The element of the coupling matrix between the levels,  $|F, m_F\rangle$  and  $|F, m_F \pm 1\rangle$  is,

$$\Omega = \frac{\mu_B g}{4\hbar} |\mathbf{B}_{rf} \times \hat{\mathbf{e}}_B| \sqrt{F(F+1) - m_F(m_F \pm 1)} , \quad (24.118)$$

where  $g$  is the atomic  $g$ -factor and  $\hat{\mathbf{e}}_B$  the orientation of the local static magnetic field.

The adiabatic potentials  $U(r)$  are obtained through the eigenvalues of the atomic states dressed by the local magnetic field  $B(r)$ . In the dressed atom picture, we consider the total energy of the atom plus the field of  $N$  radiofrequency photons. Without coupling, this simply means that  $N\hbar\omega$  is added to the atomic Zeeman energies, resulting in a Zeeman pattern being vertically shifted by  $N\hbar\omega$  for  $N = 0, \pm 1, \dots$ . At positions where the rf-field is in resonance, curves with  $\Delta N = 1$  intersect. Here, the coupling develops an *avoided crossing*, which determines the pattern of adiabatic energy levels [see Fig. 24.20(b)].

<sup>6</sup>Alternatively, a *microwave* frequency may be used to couple *different hyperfine levels*.

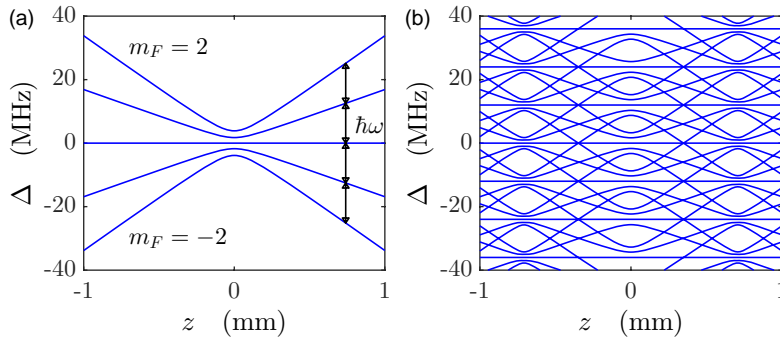


Figure 24.20: (code) (Left) Potentials due to the Zeeman structure of an atom in the ground state with  $F = 1$ . (Right) Adiabatic potentials resulting from the coupling of Zeeman levels via radiofrequency radiation being resonant with the difference of Zeeman levels at the position 0.7.

A slowly moving atom remains on the curve of an *adiabatic potential*. As an example, let us assume an atom in the hyperfine state  $|F, F\rangle$  moving away from the center of the trap. When it comes close to resonance, the rf-field blends this state with other  $m_F$ -states, from the  $|F, F - 1\rangle$  down to the  $|F, -F\rangle$  state, which changes the slope of the potential curve. Beyond the resonance point, the atomic state is adiabatically transformed into an untrapped high-field seeking state, and the atom is repelled from the trap. Thus, while passing the avoided crossing, the atom has emitted  $2F$  rf-photons in a stimulated manner and inverted the orientation of both the electron and the nuclear spin.

In this way the radiofrequency generates an adiabatic potential surface with a depth of approximately  $|m_F|\hbar(\omega - \omega_0)$ , where  $\omega_0$  is the resonant rf-frequency at the center of the trap. The evaporation process corresponds, then, to the removal of the most energetic atoms out of the trap.

For this adiabatic picture to be valid, an adiabaticity condition must be fulfilled. This condition requires that the energy difference at the avoided crossover be larger than the energy uncertainty related to the limited time that an atom with velocity  $v$  spends in the resonance region. For a two-level system coupled by a matrix element  $V_{12}$  and an atom moving with velocity  $v$  along the  $z$ -axis, the transition probability  $P$  between the adiabatic curves is given by the *Landau-Zener formula* [588],

$$P = 1 - e^{-\xi} \quad \text{with} \quad \xi = \frac{2\pi|V_{12}|^2}{\hbar g \mu_B \partial_z B v}. \quad (24.119)$$

The Landau-Zener theory is strictly valid only for a two-level system, which we use here only for a qualitative discussion of two following limiting cases.

For a weak rf-field,  $\xi \ll 1$ ,  $P$  is much smaller than 1, i.e., the atoms remain predominantly on the diabatic surface shown in Fig. 24.20(a). The probability for a *spin flip* transition is,  $P \approx \xi$ , which describes the diabatic limit of rf-induced evaporative cooling: The atomic energy levels are almost unperturbed, the atoms often spill across the resonance surface, and only after  $1/P$  oscillations, they spin-flip from the hyperfine state  $|F, F\rangle$  to the  $|F, F - 1\rangle$ .

The adiabatic limit is clearly the ideal situation for evaporative cooling. However, the evaporation process in a trap (with oscillation time  $T_{osc}$ ) saturates at a lower rf-power. The condition for saturation is  $P \approx T_{osc}/\tau_{el}$ , where  $\tau_{el}$  is the average time between two collisions. This means that an energetic atom is evaporated before it collides again.

Only the component of the magnetic field of the rf-radiation which is *perpendicular* to the magnetic trapping field induces spin-flips. In certain geometries of the confinement potential, for example the quadrupole trap, the magnetic field covers the entire solid angle. Consequently, there are two points where the trapping field and the rf-field are parallel and the elements of the transition matrix consequently zero. Within an area around these points, the coupling is diabatic. In practice however, the rf-transition can be sufficiently saturated that this area is small and does not strongly affect the evaporation efficiency.

Note also that gravitation deforms the equipotential surfaces of the confinement potential, which can reduce the evaporation efficiency [388]. Solve Exc. 24.4.6.10.

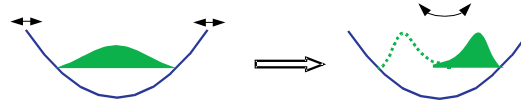


Figure 24.21: Effective potential due to a rapid modulation of the trap's location.

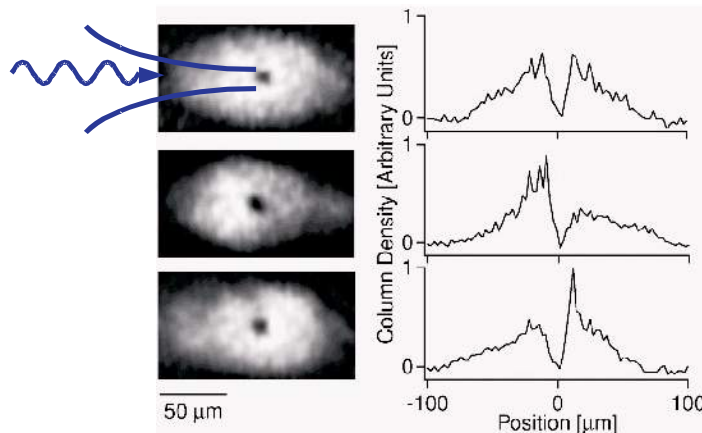


Figure 24.22: Creation of a repulsive hole by light tuned to the blue of an atomic transition.

### 24.4.5 Sympathetic cooling

The efficiency of evaporative cooling depends on the rate of interatomic collisions. However, there are atomic species with unfavorable, that is, small or even negative scattering lengths. Also, while at low temperatures only *s*-wave collisions occur (higher partial waves being frozen behind the centrifugal barrier), such collisions are prohibited for fermionic gases. Fermions or species with unfavorable scattering lengths

can not be cooled by evaporation. There is, however, another technique called *sympathetic cooling* by thermal contact with another species. The additional species is, in general, actively cooled (e.g., by evaporation), while the species of interest is passively cooled via elastic collisions with atoms of the additional species. Of course, for this scheme to work the *interspecies scattering length* and the mass ratio must be adequate to ensure adequate thermal coupling.

Following [512] the transfer of kinetic energy between two colliding atoms is reduced by a factor depending on their mass difference,

$$\xi = \frac{4m_1m_2}{(m_1 + m_2)^2} . \quad (24.120)$$

Around  $3/\xi$  collisions per atom on average are required for complete thermalization of a gas. For example, for the Rb-Li mixture, we have  $3/\xi = 12.4$ . The collision rate is,

$$\Gamma_{coll} = \sigma_{12}\bar{v} \int n_1(\mathbf{r})n_2(\mathbf{r})d^3r , \quad (24.121)$$

where the average thermal velocity is,

$$\bar{v} = \sqrt{\frac{8k_B}{\pi} \left( \frac{T_1}{m_1} + \frac{T_2}{m_2} \right)} . \quad (24.122)$$

The instantaneous temperature is calculated by,

$$\gamma_{therm} = -\frac{1}{\Delta T} \frac{d\Delta T}{dt} , \quad (24.123)$$

or via simulations:  $\Delta T(t + dt) = \Delta T(t) - \Delta T(t)\gamma_{therm}dt$ . Following [182] the rethermalization rate is connected to the collision rate via,

$$\boxed{\gamma_{therm} = \frac{\xi}{3} \left( \frac{\Delta E_{1 \rightarrow 2}}{N_1 k_B \Delta T} + \frac{\Delta E_{2 \rightarrow 1}}{N_2 k_B \Delta T} \right) = \frac{\xi}{3} \left( \frac{\Gamma_{coll}}{N_1} + \frac{\Gamma_{coll}}{N_2} \right)} . \quad (24.124)$$

Analytic solutions can be derived for harmonic traps. This will be studied in Excs. 24.4.6.11 and Exc. 24.4.6.12.

## 24.4.6 Exercises

### 24.4.6.1 Ex: Lack of trapping potentials for strong field seekers

Show that it is not possible to create magnetic trapping potentials for atoms in low-field seeking Zeeman states.

### 24.4.6.2 Ex: Quadrupolar potential

Show that for a quadrupolar trap always holds  $2\partial_r B_{qua} = \partial_z B_{qua}$ .



**24.4.6.3 Ex: Magnetic quadrupole trap**

- a. Consider  $^{87}\text{Rb}$  atoms confined in a magnetic trap with  $\mathbf{B}(x, y, z) = x \hat{y} - 2z \hat{x} \times 200 \text{ G/cm}$ . The atoms are in the state  $|F = 1, m_F = -1\rangle$  with the  $g$ -factor  $g_F = 1/2$ . Check whether it is reasonable to assume constant vibration frequencies for such traps.
- b. Assume that the trapped atomic cloud consists of  $N = 10^8$  atoms at temperature  $T = 100 \text{ K}$ . Calculate the atomic density  $n_0$  at the center of the cloud.
- c. The cross section for elastic collisions is  $\sigma = 10^{-12} \text{ cm}^2$ . How many times do atoms meet in the middle of the trap?

**24.4.6.4 Ex: TOP trap**

The TOP trap (time-orbiting potential) was the first design to allow for Bose-Einstein condensation in 1995. It consists of the superposition of a quadrupolar magnetic field, with the radial and axial gradients  $2\partial_r B_{qua} = \partial_z B_{qua}$ , and a homogeneous magnetic field  $B_{top}$  rotating in the symmetry plane of the quadrupole field. Atoms which oscillate with an amplitude beyond a given radius  $r_d$ , called the 'circle of death', undergo Majorana transitions and are expelled from the trap.

- a. Calculate the radius of the death circle.
- b. Plot the time-averaged 'effective' trapping potential.

**24.4.6.5 Ex: Harmonic trap**

Calculate the vibration frequencies of  $^{87}\text{Rb}$  atoms trapped in a harmonic trap, when the atoms are in the  $|F = 1, m_F = -1\rangle$  hyperfine level of the ground state.

**24.4.6.6 Ex: Gravitational sag in a trap**

Consider (a) a quadrupolar trap and (b) an isotropic harmonic trap. What is the gradient, respectively the curvature of the trapping potential required to suspend a cloud of rubidium subject to gravitation? What is the sag of the cloud in the potential due to gravitation?

**24.4.6.7 Ex: Mean collision rate**

Assuming that the peak collision rate  $\gamma_{coll}$  is known, calculate the average collision rate (a) in a quadrupolar and (b) in a harmonic trap.

**24.4.6.8 Ex: Adiabatic compression**

How does temperature change upon adiabatic compression of (a) a quadrupole trap and (b) a harmonic trap. How do density, phase space density, and elastic collision rate vary. **Help:** Define the compression for quadrupole trap as  $\eta \equiv \partial_r B_{r,final} / \partial_r B_{r,initial}$  and for harmonic trap as  $\eta \equiv \omega_{r,final} / \omega_{r,initial}$ .

**24.4.6.9 Ex: RF-antenna for radiative coupling**

Calculate the Rabi frequency that can be generated by an rf-antenna consisting of a single square loop with side length  $L = 2 \text{ cm}$  on a cloud of trapped  $^{87}\text{Rb}$  atoms

located in the center of the loop on transitions between magnetic sublevels of the  $F = 1$  ground state hyperfine structure. Assume the antenna to carry an ac-current with  $I = 1$  A amplitude.

#### 24.4.6.10 Ex: Landau-Zener transitions

Consider a rubidium-88 cloud in its ground state  $^2S_{1/2}$ ,  $F = 1$ ,  $m_F = -1$  confined in an isotropic quadrupolar potential with the gradient 200 G/cm. To initiate an efficient radiofrequency evaporation, you want atoms crossing the region where the radiofrequency couples the Zeeman states to make a transition to the untrapped Zeeman state  $m_F = 0$  with 95% probability. What is the amplitude of the required magnetic field.

#### 24.4.6.11 Ex: Damping in mixtures of species

From Eq. (24.124) derive the interspecies thermalization rate for harmonic potentials.

#### 24.4.6.12 Ex: Damping in mixtures of species

Describe the damping in mixtures of species, and show how to use a measurement of the damping time for a determination of the interspecies scattering length.

## 24.5 Other traps

### 24.5.1 Ion traps

The electric charge of ions allow for their efficient manipulation and control by electric and magnetic fields exploiting the Coulomb-Lorentz force. In fact, the control is so good, that it is possible to isolate and store individual ions or even arrays of quantum entangled ions and to perform coherent operations on them, which qualifies them as quantum registers. Two different types of traps have been investigated. In *Penning traps* [541], electrically charged particles are subjected to a radially attractive quadrupolar electrostatic field superimposed to an axial magnetostatic field forcing the particles into closed circular orbitals <sup>7</sup>. In the so-called *radiofrequency trap* or *Paul trap* – *Wolfgang Paul* received the Nobel Prize in 1989 together with Hans Dehmelt and Norman Ramsey – charged particles subjected to an alternating electric field with quadrupolar symmetry. Hyperboloidal electrode configurations produce saddle-shaped potentials, as shown in Fig. 24.24, which are, at any instant of time, parabolically repulsive in the one direction (axial or radial) and parabolically attractive in the other (radial or axial). The alternating electric field causes a periodic reorientation of the Coulomb force, which leads to a time-averaged parabolic quasi-potential  $\Phi(\mathbf{r}, t)$ . In this potential the particles perform harmonic oscillations at characteristic frequencies, which are independent of the oscillation amplitude [536]:

$$\Phi(r, z) = \Phi_0(t)(r^2 - 2z^2) \quad , \quad r^2 = x^2 + y^2 \quad , \quad (24.125)$$

<sup>7</sup>Note that purely electrostatic fields do not lend themselves to trapping, since the necessary condition for the existence of minima in a potential,  $\partial_i \partial_j \phi < 0$ , does not obey the Laplace equation.

where the polarity is alternated at a radiofrequency  $\Omega_a$ ,

$$\Phi_0(t) = \Phi_{dc} + \Phi_{ac} \cos(\Omega_a t) . \quad (24.126)$$

$\Phi_{dc}$  denotes the amplitude of the *dc* part of the voltage,  $\Phi_{ac}$  the amplitude of the *ac* part. The potential  $\Phi(r, z, t)$  exerts, in the temporal average, a central force on the ion, if the radiofrequency field satisfies specific conditions.

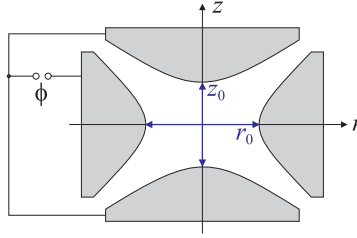


Figure 24.23: Geometry of the Paul trap.

### 24.5.1.1 Evaluation of the stability diagram

Paul traps do not have to have perfect quadrupolar geometry. To determine the secular frequencies of the pseudo-potential for an arbitrary geometry, we expand the potential around the position  $\mathbf{r}_0$  of the potential minimum, which depends on the geometry of the electrodes and the applied voltages,

$$\begin{aligned} \Phi(\mathbf{r}) &= \Phi_a + (\mathbf{r} - \mathbf{r}_0) \nabla \Phi(\mathbf{r}_0) + \frac{1}{2} [(\mathbf{r} - \mathbf{r}_0) \nabla]^2 \Phi(\mathbf{r}_0) + \dots \\ &\equiv \Phi_a [1 + b_r (r - r_0)^2 + b_z (z - z_0)^2] . \end{aligned} \quad (24.127)$$

In the last step, we assume that the potential has an almost cylindrical shape. For a given geometry, the curvatures  $b_{z,r}$  can be extracted from numerical simulations. From the continuity equation, we find  $b_z = -2b_r$ . The polarity of the electrodes is modulated with frequency  $\Omega$ ,

$$\Phi(\mathbf{r}, t) = \Phi(\mathbf{r})(\zeta - \cos \Omega t) . \quad (24.128)$$

The equations of motion are derived from  $m\ddot{\mathbf{r}} = -e\nabla\phi(\mathbf{r}, t)$ ,

$$m\ddot{r}_j + 2e\Phi_a b_j (\zeta - \cos \Omega t) r_j = 0 . \quad (24.129)$$

Introducing the parameters  $a$  and  $q$ ,

$$a_z = \frac{8e\phi_a b_z \zeta}{m\Omega^2} = -2a_r \quad \text{and} \quad q_z = \frac{4e\Phi_a b_z}{m\Omega^2} = -2q_r , \quad (24.130)$$

we arrive at the so-called *Mathieu equation* [472, 237],

$$\ddot{r}_j + \frac{1}{4}\Omega^2 (a_j - 2q_j \zeta \cos \Omega t) r_j = 0 . \quad (24.131)$$

These equations predict stable orbits, provided that the parameters  $a$  and  $q$  are within the so-called stability diagram shown in Fig. 24.25.

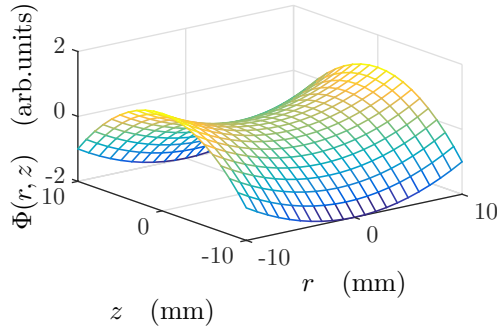


Figure 24.24: (code) Two-dimensional illustration of time-dependent potential: at each instant of time the potential has the form of a saddle. The potential rotates around the vertical axis at an appropriate pace.

According to these equations, the ion goes through oscillatory motions that are defined by the trap parameters  $a_i$  and  $q_i$ . For the motion of the ion to be finite, its oscillation amplitude may not exceed the boundaries defined by the electrodes. This condition imposes an allowed regime for the trap parameters called *stability diagram* [472].

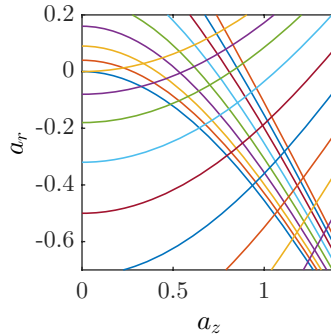


Figure 24.25: (code) Stability diagram.

In the limit  $|a_i|, q_i \ll 1$  the ion travels only a short distance  $s \ll r_0$  during one modulation period  $\Omega_a$ . Then the ion undergoes a slow periodic motion called *macro-motion* within the trapping potential with the secular frequency  $\zeta_i$ . This motion is modulated by a rapid oscillation called *micromotion*, which is excited by the modulation field  $\Omega_a$ . Without *dc* voltage applied between the ring and the endcaps,  $a_i = 0$ , the motion of the ion is described by the following simple equation:

$$r_i(t) = r_i^0 \left(1 - \frac{1}{2}q_i \cos \Omega_a t\right) \cos \zeta_i t \quad , \quad \zeta_i = \frac{1}{\sqrt{8}}q_i \Omega_a \quad , \quad i = r, z \quad . \quad (24.132)$$

The orbit of the ion is confined to the inner region of the trap, if its kinetic energy is less than  $m\zeta_r^2 r_0^2 + M\zeta_z^2 z_0^2$ . Since the trap is, at any instant of time, focusing in some directions and defocusing others, it is not a conservative potential. The oscillatory

motion (disregarding micromotion) of the ion, however suggests a model, where the trap is described by a pseudo-potential [237, ?] whose depth is,

$$D_z = \frac{q_z}{8} eV_{ac} = 2D_r \quad \text{if} \quad a_i = 0. \quad (24.133)$$

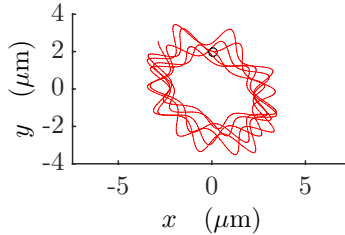


Figure 24.26: (code) Simulated micro- and macromotion of an ion.

Other geometries, deviating from the perfect quadrupole, are possible for the electrodes. These traps are also well described by equation (24.125), as long as the ion is near the trap center. For example, higher order multipolar traps have been used for trapping ion clouds [710], as well as Paul-Straubl traps [618] and storage rings [704]. Particularly important for the storage of arrays of cooled ions with applications in quantum computing is the *linear Paul trap* [560, 240, 559], where immobilized ions are aligned on a linear chain. The advantage of the linear trap, as compared to other traps designed for many ions, is the easier optical access to individual ions by focused laser beams and the possibility of canceling the micromotion.

## 24.5.2 Micromotion

The motion of an ion in a Paul trap is a superposition of two vibrations with the respective oscillation frequencies  $\Omega_a$  (modulation frequency) and  $\zeta_{r,z}$  (secular frequencies for radial and axial direction vibrations). For an ion in thermal equilibrium (i.e., without active cooling), the mean kinetic energies of the micro- and macromotion are equal [76].

The macromotion can be reduced by cooling, in contrast to the micromotion, which is constantly excited by the modulation of the applied electric field [136]. On the other hand, the amplitude of the micromotion decreases with the distance of the ion from the trap center and, in the minimum of the pseudo potential, disappears completely. Therefore, to suppress the micromotion, it is imperative to cool the macromotion and push the ion to the trap center, if necessary, using additional static electric fields. Since the frequency of the micromotion is much higher than that of the macromotion, the dynamic sidebands can be resolved on a sufficiently narrow optical transition. When the modulation frequency  $\Omega_a$  is very high, the secular frequencies of the macromotion are also high, so that even large optical transitions are able to resolve the macromotional sidebands. This is called the *strong coupling* regime.

Because of Coulomb repulsion, only a single atom can be at the center of a Paul trap, such that it is difficult to zero micromovement. One solution is to use a linear trap, where the center is smeared out over a straight line. Solve Exc. 24.5.4.1.

**Example 111 (Numerical calculation of the electric field created by a charged surface):** To calculate the trapping potential for a charged particle held on top of a planar microtrap structure, we proceed as follows. The energy of a charge in an electric field is  $H = -e\Phi$ . The electrostatic potential is given by Coulomb's law,

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_n \int_{V_n} \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' - \frac{1}{4\pi} \sum_n \int_{S_n} \Phi_n \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{f}' + \frac{1}{4\pi} \sum_n \int_{S_n} \frac{E(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{f}' ,$$

where  $\phi_n$  is the voltage applied to the  $n$ -th boundary. In practice, electric fields are generated by electrodes set to specific voltages. Using the Dirichlet boundary conditions, we only retain the second term. Furthermore, to account for the planar geometry of the chip electrodes, we only consider surface boundaries in the  $y' = 0$  plane,

$$\Phi(\mathbf{r}) = -\frac{1}{4\pi} \sum_n \Phi_n \int_{S_n} \frac{y dx' dz'}{\sqrt{(x - x')^2 + y^2 + (z - z')^2}^3} .$$

This implies that the field lines cross the chip surface orthogonally, which in reality is only true if the chip electrodes cover the whole area. Therefore, we

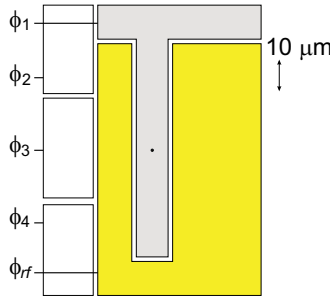


Figure 24.27: Possible design for a microchip ion trap.  $\Phi_n$  are static potentials except for  $\Phi_0$ , which is alternates sign with radio frequency.

only consider small gaps between the electrodes. We digitize the integral by dividing every electrode  $\Phi_n$  into a number of identical surface elements  $\Delta f_m$ ,

$$\Phi(\mathbf{r}) = -\frac{1}{4\pi} \sum_{n,m} \Phi_n \frac{y \Delta f_m}{\sqrt{(x - x_m)^2 + y^2 + (z - z_m)^2}^3} .$$

This formula can easily be evaluated numerically. A concrete example for a microchip ion trap is shown in Fig. 24.27.

**Example 112 (Numerical calculation of the magnetic field created by a current wire):** Current-carrying wires may exert Lorentz forces on the ions. The magnetostatic field is given by the Biot-Savart law,

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int_V \frac{(\mathbf{r} - \mathbf{r}') \times \mathbf{j}}{|\mathbf{r} - \mathbf{r}'|^3} dV' .$$

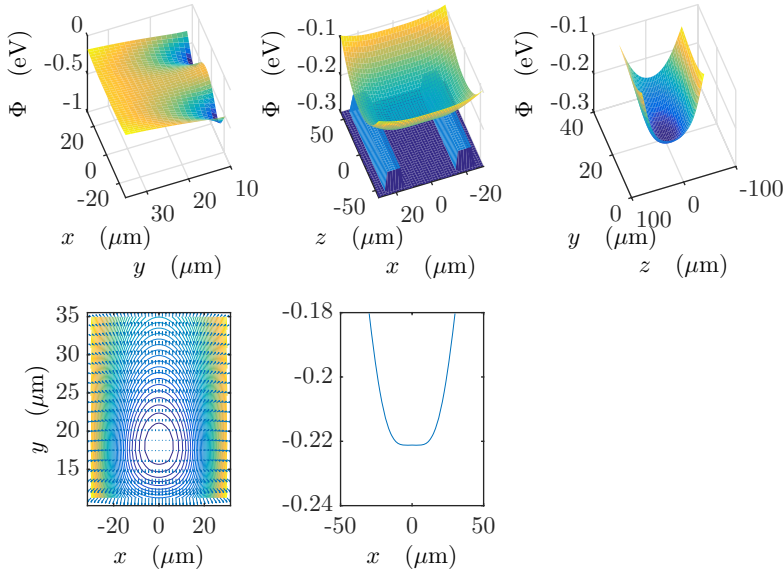


Figure 24.28: (code) Two-dimensional cuts through the electric potential generated by the microchip shown in Fig. 24.27 for  $\Phi_{rf} = 100$  V and  $\Phi_j = 0$ .

In practice magnetic fields are created by current-carrying wires. Those can be parametrized by one-dimensional currents,  $\mathbf{j} = I\delta^2 ds$ , so that,

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0 I}{4\pi} \int_C \frac{d\mathbf{s}' \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3}$$

$$|\mathbf{B}(\mathbf{r})| = \frac{\mu_0 I}{4\pi} \sum_n \frac{\sqrt{ds_{y,n}^2(z - z_n)^2 + ds_{z,n}^2(x - x_n)^2 + ds_{x,n}^2(y - y_n)^2}}{\sqrt{(x - x_n)^2 + (y - y_n)^2 + (z - z_n)^2}^3}.$$

can immediately be numerically solved.

### 24.5.2.1 Electronic detection of ions

The presence of ions in the trap can be probed through the damping that they induce a coupled electronic resonance circuit [709, 713].

## 24.5.3 QUEST

Homonuclear atoms and dimers do not have a permanent electrical dipole moment, but they may have a permanent magnetic dipole moment. Therefore, homonuclear dimers must be confined by magnetic field gradients, or else an electric dipole moment must be *induced* by an oscillating electromagnetic field. In the optical regime, this was demonstrated with the quasi-electrostatic trap (*QUEST*).

In contrast, heteronuclear dimers are polar molecules with a permanent electric dipole moment, which can be quite large if the molecules are deeply bound. According to Earnshaw's theorem, there is no static magnetic field maximum in free space. Thus, no 'high-field seeking' state can be trapped. In principle, QUEST-type dipolar optical

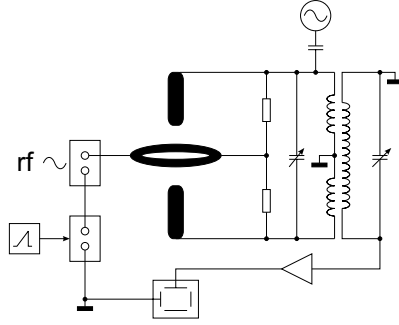


Figure 24.29: Resonance circuit for electronic ion detection. The trap is operated by a radiofrequency, while a DC voltage is scanned across the stability diagram. Simultaneously, an oscillating field is tuned near one of the trap’s secular frequencies. When the stability point is such, that the secular frequency coincides with the frequency of the oscillating field, the motion of the ions is parametrically excited and the resonance circuit is damped. This damping is detected by a narrow-band amplifier.

traps can also be used for heteronuclear dimers. The problem is, however, that in contrast to homonuclear molecules, transitions between the vibrational ground state levels are possible. Thus, the light generating the QUEST also induces transitions leading to a redistribution of the population over all vibrational states.

Very far from resonance,

$$U_{dip}(\mathbf{r}) = -\alpha_{stat} \frac{I(\mathbf{r})}{2\epsilon_0 c} . \tag{24.134}$$

Loosely bound homonuclear molecules are subject to the sum of the restoring forces exerted by magnetic traps on the individual atoms,  $\mu_m = 2\mu_a$  and  $d_m = 2d_a$ . This is also true for heteronuclear molecules as long as the trapping potential is much weaker than the binding energy.

**Example 113 (Permanent electric dipole moment of LiRb ):** The interaction energy of two dipoles is,

$$\hat{H}_{int} = \frac{1}{4\pi\epsilon_0} \frac{\mathbf{p}_1 \cdot \mathbf{p}_2 - 3(\mathbf{p}_1 \cdot \hat{\mathbf{r}})(\mathbf{p}_2 \cdot \hat{\mathbf{r}})}{r^3} .$$

Thus, two identical dipoles with 1 Debye =  $10^{-27}/2.998 \text{ Cm} = 10^{-19}/c \text{ Cm}^2/\text{s} = 39.36 \text{ ea}_B$  parallel oriented at a distance  $r = 1 \mu\text{m}$  have the energy,

$$\hat{H}_{int} = \frac{1}{4\pi\epsilon_0} \frac{p^2}{r^3} \approx h \times 1.5 \text{ MHz} \approx k_B \times 73 \mu\text{K} .$$

For example, LiRb has an electrical dipole moment of between -2 and -4.2 Debye depending on the vibrational state of the molecule.

### 24.5.4 Exercises



### 24.5.4.1 Ex: Coulomb repulsion in linear Paul trap

Coulombian repulsion prevents that two ions confined in a linear Paul trap be simultaneously in the ground state. Determine the spatial extent of the ground state and the depth of the potential in the pseudo-potential approximation. What is the equilibrium distance of the ions?

### 24.5.4.2 Ex: Motion of ions in a surface Paul trap

Programs on the motion of ions in a surface Paul trap.

## 24.6 Analysing techniques

To analyze the kinetic state of an atomic gas and, for example, to identify the presence of a Bose-Einstein condensate, it is necessary to measure its spatial or momentum distributions. However, the only way to gather information from the atoms is to throw some kind of particles into them and to detect, where these particles are scattered. The most suitable particle to penetrate an ultra-high vacuum chamber surely is the *photon*. Therefore, apart from few exceptions where electron beams are used, all information on ultra-cold gases has been obtained so far through their reactions to incident laser beams [339, 124, 18, 369, 278].

### 24.6.1 Time-of-flight imaging

The most common imaging techniques measure the absorption of a laser beam by an atomic cloud after a *time-of-flight* or the dispersion of a laser beam induced by trapped cloud. The amplitude  $E_0$  of a light wave traversing an atomic cloud of diameter  $L$  and characterized by the refractive index  $\eta$  is modified by a factor  $e^{i\omega L\eta/c}$ . For an inhomogeneous cloud, we have,

$$\mathcal{E} = \mathcal{E}_0 e^{i\omega L/c} \exp\left(i\frac{\omega}{c} \int_{-\infty}^{\infty} (\eta(\mathbf{r}) - 1) dz\right). \quad (24.135)$$

We can approximate the refractive index by the atomic susceptibility,

$$\eta = \sqrt{1 + \chi} \simeq 1 + \frac{\chi}{2} \quad \text{with} \quad \chi = -\frac{4\pi n(\mathbf{r})}{k^3(2\Delta/\Gamma + i)}. \quad (24.136)$$

where  $n(\mathbf{r})$  is the density distribution of the cloud. The imaginary part of the susceptibility is related to the *absorption coefficient*  $\alpha$  and the real part to the *dispersion coefficient*  $\delta$ ,

$$\text{Im } \chi = \frac{\alpha}{\omega/c} \quad \text{and} \quad \text{Re } \chi = \frac{2\delta}{\omega/c}. \quad (24.137)$$

Now, the absorption and dispersion coefficients can be related to the optical cross-section  $\sigma(\Delta)$  defined in (1.102) [440], where  $\Delta$  is the detuning of light frequency from an atomic resonance, whose linewidth is  $\Gamma$ . This result is called the *optical theorem*,

$$\alpha = n\sigma(\Delta) \quad \text{and} \quad \delta = n\sigma(\Delta)\frac{\Delta}{\Gamma}, \quad (24.138)$$

Finally, we obtain the *Lambert-Beer law*,

$$\mathcal{E} = \mathcal{E}_0 e^{i\omega L/c} \exp \left[ i\sigma(\Delta) \left( \frac{i}{2} - \frac{\Delta}{\Gamma} \right) \int_{-\infty}^{\infty} n(\mathbf{r}) dz \right] \equiv \mathcal{E}_0 e^{i\omega L/c} e^{-b/2} e^{i\varphi}. \quad (24.139)$$

For the intensity,  $I \propto |E|^2$ , we get,

$$\frac{I}{I_0} = \exp \left[ -\sigma(\Delta) \int_{-\infty}^{\infty} n(\mathbf{r}) dz \right] \equiv e^{-b}. \quad (24.140)$$

The *absorption*  $b$  describes the loss of intensity for the laser beam due to scattering by the (disordered) atoms. It is strong near resonance, but diminished quadratically with the detuning  $\Delta$ . The scattering is necessarily accompanied by radiation pressure accelerating and heating the atoms. The *dispersion*  $\varphi$  describes the refraction of the laser beam by the atomic density distribution (which for this purpose can be considered as continuous) [153, 243]. It disappears in resonance and diminishes slowly with increased detuning ( $\propto \Delta$ ). It is connected to the dipole force and, thus, does not heat the atomic cloud. The coefficient  $\varphi$  describes the phase shift of the electromagnetic wave transmitted through the atomic cloud.

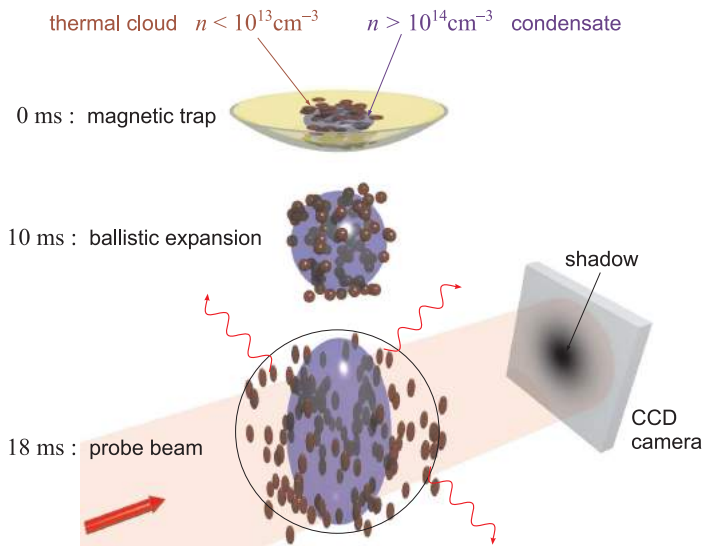


Figure 24.30: Sequence of a typical time-of-flight experiment: As soon as the trapping potential is suddenly switched off, the atomic cloud ballistically expands for 18 ms, before it is illuminated by a short resonant laser pulse. The shadow printed by the cloud onto the beam is photographed by a CCD camera.

## 24.6.2 Absorption imaging

Let us now detail the experimental process of *absorption imaging* (see Fig. 24.31): The trap confining the atomic cloud is suddenly turned off, thus letting the atoms,

accelerated by the Earth's gravitation, fall for a flight time of a few ms. Then a pulse of a resonant laser light, whose diameter is much larger than the size of the cloud, is irradiated. The local attenuation of the beam intensity  $I \sim |\mathcal{E}|^2$  can be related through the absorption  $b$  (also called *optical density* or *optical depth*) to the atomic density via,

$$-\ln \frac{I(x, y)}{I_0} = b(x, y) = \sigma(\Delta) \int n(\mathbf{r}) dz . \quad (24.141)$$

The shadow printed by the atomic cloud on the transverse profile of the laser beam is recorded by a CCD camera.

We have already noted that the absorption is accompanied by radiative pressure. After some scattering events, due to the photonic recoil, the atoms have accumulated a sufficiently large velocity, and therefore a sufficiently large Doppler shift, to be out of resonance with the laser beam. Subsequent photons are no longer scattered by the atoms and only contribute to increase the illumination of the CCD camera without carrying any information about the presence of atoms. Consequently, it is advantageous to use very short laser pulses. In addition, the intensity of the laser beam should not saturate the transition in order to guarantee an optical cross-section, which is independent of the intensity, and hence to guarantee the validity of the Lambert-Beer law. Finally, the laser frequency must be tuned perfectly to resonance,  $\Delta = 0$ . Otherwise, the interaction between the laser beam and the atomic cloud becomes partially dispersive, which leads to a focusing or defocusing of the laser beam by refraction and a distortion of the image making it impossible to estimate the size of the cloud.

Fig. 24.31 shows examples of absorption images of an atomic cloud taken at different stages of the evaporation process. Fig. 24.31(a,b) was taken at a temperature of 320 nK; the cloud is large and isotropic and therefore purely thermal. At 250 nK [see Fig. 24.31(c,d)] an elliptically shaped part appears in the center of the thermal cloud. And at 180 nK [see Fig. 24.31(e,f)] the thermal cloud almost completely disappeared for the benefit of the condensate. A quantitative evaluation of the condensed fraction is given in Sec. 25.1.4. Solve the Excs. 24.6.6.2 and 24.6.6.1.

### 24.6.3 Dispersive imaging

The absorption imaging technique is destructive, because of the involved ballistic expansion and also because of the radiative pressure exerted by the resonant imaging beam, which accelerates and heats the atomic cloud. That is, the measurement process messes up the distributions of the cloud, such that a second image taken after the first one will give different results. However, there is a non-destructive imaging technique called *dispersive imaging* or *phase contrast imaging*. In this technique, the laser light is tuned sufficiently far from resonance,  $|\Delta| \gg \Gamma$ , for spontaneous emission and heating induced by random photonic recoil to be negligible [18]. This permits to take a series of consecutive images and create a *movie* of the temporal evolution of the cloud. Another advantage of this technique is the low off-resonant optical density, which allows to take pictures of very dense clouds *in situ*, that is, *while they are confined in a trap*.

The physical quantity which is measured by this method is the local phase shift of the wavefront of the probe laser. Wavefront distortions are difficult to measure. To

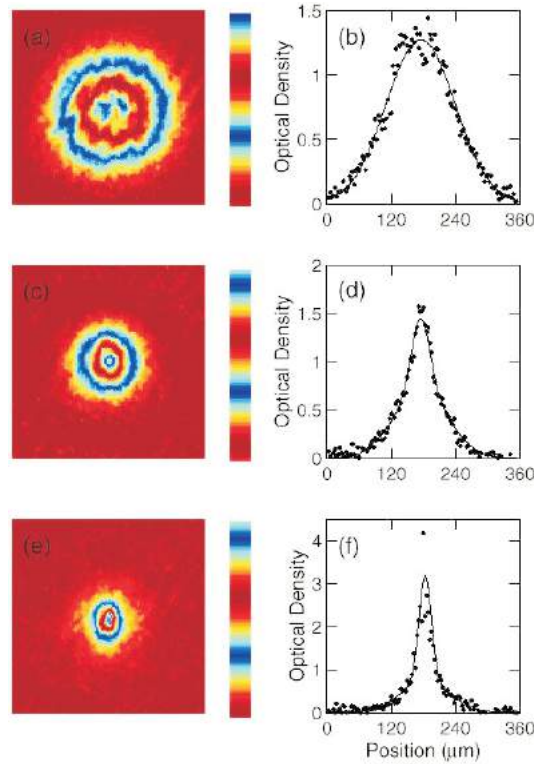


Figure 24.31: Absorption images after a time-of-flight allow to identify the presence of a Bose-condensate through its characteristic momentum distribution. Shown are images (a,b) above, (c,d) slightly below, and (e,f) well below the critical temperature for a Bose-Einstein phase transition (figures [307]).

transform the phase profile into an intensity profile, a method known from classical optics called *Schlieren method* is used. It is based on the interference of the probe beam with its distorted wavefront and a reference plane wave. In practice, there are several possibilities. For *dark-ground imaging*, the part of the incident beam not having interacted with the atoms is blocked behind the interaction zone (see Fig. 24.32)

$$\bar{I}_{dg} = \frac{1}{2} |\mathcal{E} - \mathcal{E}_0|^2 = I_0 \left| e^{-b/2 + i\varphi} - 1 \right|^2 \quad (24.142)$$

$$\xrightarrow{b \rightarrow 0} I_0 \varphi^2 = I_0 b \frac{\Delta^2}{\Gamma^2} .$$

The intensity signal  $\bar{I}_{dg}$  is quadratic in optical density  $b$ .

For *phase contrast imaging*, the part of the beam not having interacted with the atoms receives a phase shift of  $\lambda/4$  with respect to the part of the beam having

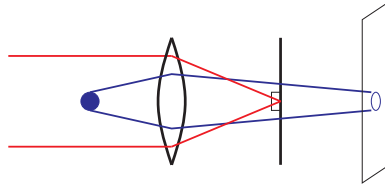


Figure 24.32: Scheme for dispersive images.

interacted with the atoms:

$$\begin{aligned} \bar{I}_{pc} &= \frac{1}{2} |\mathcal{E} - \mathcal{E}_0 + \mathcal{E}_0 e^{\pm i\pi/2}|^2 = I_0 \left| e^{-b/2 + i\varphi} - 1 + e^{\pm i\pi/2} \right|^2 \\ &\xrightarrow{b \rightarrow 0} I_0 (\pm 1 + \varphi)^2 \simeq I_0 \left( 1 \pm b \frac{\Delta}{\Gamma} \right). \end{aligned} \quad (24.143)$$

The intensity  $\bar{I}_{pc}$  is linear in  $b$  and, consequently, more sensitive to weak signals. Finally, a third technique, called *polarization contrast imaging*, detects the local birefringence of the atomic cloud [102, 593].

The imaging techniques shown so far only allow to visualize the instantaneous density distribution of the atomic cloud  $n(\mathbf{r})$ . If we are interested in other quantities, we have to conceive the experiment in such a way, that the desired information leaves its signatures in the density distribution. For example, to measure the excitation frequencies of a condensate, which can perturb its shape and observe the subsequent time evolution of  $n(\mathbf{r}, t)$  via dispersive imaging [372, 478, 19, 390].

#### 24.6.4 Reconstruction of column-integrated absorption images

Assume cylindrical symmetry  $n(\mathbf{r}) = n(r, z)$ , with  $r = \sqrt{x^2 + y^2}$ . Absorption images are *column-integrated*, i.e. they are taken by integration along the  $x$ -axis,

$$\frac{I(y, z)}{I_0(y, z)} = e^{-\sigma \int n(r, z) dx} = e^{-\sigma f(y, z)}. \quad (24.144)$$

The radial density can be recovered by tomography [178, 212, 534],

$$n(r, z) = \frac{1}{(2\pi)^2} \int (\mathcal{F}_y f)(\kappa_y, z) J_0(\kappa_y r) d\kappa_y. \quad (24.145)$$

This is called *image reconstruction* or *Fourier reconstruction* or *inverse Abel transform* and will be studied in Exc. 24.6.6.3.

#### 24.6.5 Condensable atomic species

Early work on BEC has been done by [608, 47, 75, 127, 435]. Proposals for atomic gases were from [315, 671, 667]. An appropriate BEC candidate must fulfill a few conditions: The transition wavelengths must be *accessible by laser light*, the level scheme should exhibit a *closed cycling transition* for laser cooling and have a reasonable pressure in gas phase. Furthermore, it is desirable to have a large HFS,

metastable electronic state, no trapping state, large positive scattering length, Feshbach resonances. For sympathetic cooling it may be nice to have several isotopes of the same element.

The most common elements are alkalis, alkali earths and noble gases. The following gases have already been condensed  $^1\text{H}$ ,  $^1\text{He}^*$ ,  $^7\text{Li}$ ,  $^{23}\text{Na}$ ,  $^{85}\text{Rb}$ , and  $^{87}\text{Rb}$  [16], [173], [103], [102], [594], [156], [307], [311]. Investigations in  $^1\text{Ne}^*$ ,  $^{39}\text{K}$ ,  $^{133}\text{Cs}$ ,  $^x\text{Sr}$ ,  $^x\text{Cr}$  and  $^{40}\text{Ca}$  are underway [646], [292], [403], [561], [634], [55], [248].

## 24.6.6 Exercises

### 24.6.6.1 Ex: Lensing by cold clouds

The interaction of light with two-level atoms generates a susceptibility which gives rise to a refraction index,

$$\eta(\mathbf{r}) = \sqrt{1 - \frac{4\pi n(\mathbf{r})}{k^3(2\Delta/\Gamma + i)}},$$

where  $n(\mathbf{r})$  is the cloud's density distribution and  $\Gamma/2\pi = 30.5$  MHz for strontium.

a. Calculate the phase-shift suffered by a light beam crossing an ultracold atomic cloud ( $N = 10^5$ ,  $T = 1 \mu\text{K}$ ) confined in an isotropic harmonic trap ( $\omega_{trp} = (2\pi) 100$  Hz) as a function of detuning.

b. Estimate the focal distance of the cloud for  $\Delta = -\Gamma$ .

### 24.6.6.2 Ex: Optical density

A cloud of  $N = 10^6$   $^{87}\text{Rb}$  atoms is prepared in a cylindrical harmonic trap characterized by the axial vibration frequencies  $\omega_z = (2\pi) 50$  Hz and the radial one  $\omega_r = (2\pi) 200$  Hz. The experimenter takes the absorption image after 18 ms time-of-flight, as shown in Fig. 24.31(a). A pixel of the CCD camera corresponds to  $5 \mu\text{m}$  in real space.

a. At what temperature is the phase transition to Bose-Einstein condensate to be expected?

b. Determine the temperature of the sample.

c. Evaluate its density distribution.

d. Evaluate the resonant optical density for the  $D_2$ -transition at 780 nm along the symmetry axis of the trapped cloud.

### 24.6.6.3 Ex: Inverse Abel transformation

Calculate the inverse Abel transform using Bessel of an arbitrary function in 2D.

## 24.7 Further reading

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- S.C. Bell et al., *A slow atom source using a collimated effusive oven and a single-layer variable pitch coil Zeeman slower* [DOI]
- R.A. Cline et al., *Spin relaxation of optically trapped atoms by light scattering* [DOI]
- M. Defrise et al., *Three-dimensional image reconstruction from complete projections* [DOI]
- V. Dribinski et al., *Reconstruction of Abel-transformable images: The Gaussian basis-set expansion Abel transform method* [DOI]
- P.A. Vicharelli et al., *Iterative method for computing the inverse Abel transform* [DOI]
- Y. Castin et al., *Limit of Doppler cooling* [DOI]
- D.A. Steck et al., *Rubidium 87 D Line Data* [DOI]
- D.A. Steck et al., *Rubidium 85 D Line Data* [DOI]
- M.G. Raizen et al., *Stochastic cooling of atoms using lasers* [DOI]
- Jiazhong Hu et al., *Creation of a Bose-condensed gas of  $^{87}\text{Rb}$  by laser cooling* [DOI]

### 24.7.1 on gravimetry

- S. Abend et al., *Atom-chip fountain gravimeter* [DOI]
- G. Ferrari et al., *Long-Lived Bloch Oscillations with Bosonic Sr Atoms and Application to Gravity Measurement* [DOI]
- K. Gietka et al., *A supersolid-based gravimeter in a ring cavity* [DOI]

### 24.7.2 on strontium (metrology)

- D.S. Barker et al., *Enhanced magnetic trap loading for atomic strontium* [DOI]
- Y. Bidel et al., *Coherent light transport in a cold strontium cloud* [DOI]
- I. Courtillot et al., *Efficient cooling and trapping of strontium atoms* [DOI]
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- A. Derevianko et al., *Colloquium: Physics of optical lattice clocks* [DOI]
- G. Ferrari et al., *Precision frequency measurement of visible intercombination lines of strontium* [DOI]

- G. Ferrari et al., *Cooling of Sr to high phase-space density by laser and sympathetic cooling in isotopic mixtures* [DOI]
- T. Fukuhara et al., *Degenerate Fermi Gases of Ytterbium* [DOI]
- T. Fukuhara et al., *Mott insulator of ultracold alkaline-earth-metal-like atoms* [DOI]
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- Fachao Hu et al., *Analyzing a single-laser repumping scheme for efficient loading of a strontium magneto-optical trap* [DOI]
- T. Ido et al., *Optical clocks based on ultracold neutral strontium atoms* [DOI]
- C. Javaux et al., *Modulation-free pump-probe spectroscopy of strontium atoms* [DOI]
- H. Katori et al., *Magneto-optical trapping and cooling of strontium atoms down to the photon recoil temperature* [DOI]
- T.H. Loftus et al., *Magnetic trapping of ytterbium and the alkaline-earth metals* [DOI]
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- T. Mukaiyama et al., *Recoil-Limited Laser Cooling of  $^{87}\text{Sr}$  Atoms Near the Fermi Temperature* [DOI]
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- S. Stellmer et al., *Reservoir spectroscopy of  $5s5p\ ^3P_2$ - $5snd\ ^3D_{1,2,3}$  transitions in strontium* [DOI]
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- M. Yasuda et al., *Lifetime Measurement of the  $^3P_2$  Metastable State of Strontium Atoms* [DOI]
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### 24.7.3 on strontium (quantum degeneracy)

- B.J. DeSalvo et al., *Degenerate Fermi gas of  $^{87}\text{Sr}$*  [DOI]
- Y.N. Martinez de Escobar et al., *Bose-Einstein Condensation of  $^{84}\text{Sr}$  resonance at large detuning* [DOI]
- Meng Khoon Tey et al., *Double-degenerate Bose-Fermi mixture of strontium* [DOI]
- P.G. Mickelson et al., *Bose-Einstein Condensation of  $^{88}\text{Sr}$  Through Sympathetic Cooling with  $^{87}\text{Sr}$*  [DOI]
- S. Stellmer et al., *Bose-Einstein condensation of strontium* [DOI]
- S. Stellmer et al., *Bose-Einstein condensation of  $^{86}\text{Sr}$*  [DOI]
- S. Stellmer et al., *Creation of Ultracold  $\text{Sr}_2$  Molecules in the Electronic Ground State* [DOI]
- S. Stellmer et al., *Laser Cooling to Quantum Degeneracy* [DOI]

## Chapter 25

# Thermodynamics of ideal quantum gases

The journey of the quest for Bose-Einstein condensation (BEC) begins with its prediction by Bose and Einstein in 1926. The first hint, that the condensation was more than just a theoretical fantasy came from London [439], who linked the newly discovered phenomenon of superfluidity in  $^4\text{He}$  to BEC. However, the interpretation of the  $\lambda$ -point in terms of BEC was not obvious, because strong interactions between particles concealed the role of quantum statistics, and the thermodynamic potentials exhibited divergences at the critical temperature instead of discontinuities, as expected for an ideal gas BEC. These uncertainties triggered an intense search for other systems. In 1954, Schafroth pointed out that electron pairs can be seen as composite bosons and may form Bose-Einstein condensates at low temperatures [608]. In 1957, Bardeen, Cooper and Schrieffer developed the microscopic theory of superconductivity [47], after other researchers, including Blutt, Schaffrot, Fröhlich and Bogolubov, had suggested a relationship of this phenomenon to Bose condensation of electron pairs (nowadays called Cooper pairs).

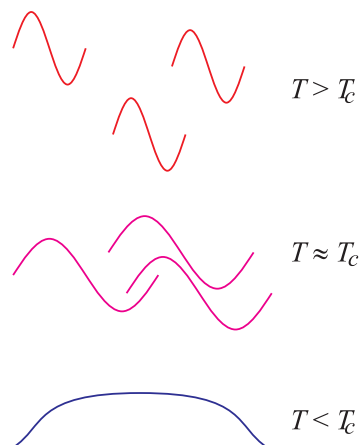


Figure 25.1: Illustration of atomic Broglie waves. From the top to the bottom the temperature of the atoms is decreasing.

Motivated by the need to test the concept of condensation of composite particles

in weakly interacting systems, in 1962 *Blatt et al.* proposed the investigation of the BEC in gases of *excitons* [75]. Excitons are bound electron-hole pairs that can form a weakly interacting gas in certain non-metallic crystals. They are interesting because their small mass allows BEC at high temperatures and gas density can be controlled over a wide range, by only modifying the intensity of the optical excitation. Being *quasi-particles*, excitons can be created and annihilated, that is their number is not conserved. Excitons were discovered in 1968, and the first evidence for Bose-Einstein of biexciton molecules in a CuCl crystal dates back to 1979 [127].

The laser as coherence phenomenon between photons shares many analogies with condensates. However, photons are quasi-particles as well, and again their number is not conserved<sup>1</sup>. Hence, there is no phase transition: When an optical cavity containing photonic modes is cooled, the photons prefer to disappear in the walls of the cavity instead of condensing.

Hecht [315] suggested in 1959, followed by Stwalley and Nosanow [671] in 1976, that an atomic hydrogen gas with polarized spins would be an appropriate candidate for BEC. The advantage of this system is that interactions between atoms are weak and only give rise to a negligible quantum depletion below 1%. In 1978 Greytak and Kleppner started at the MIT intensive efforts to generate BECs in dilute hydrogen gases. In the 1990s, important advances in the cooling of atoms using laser light allowed to reach very low temperatures, and the invention of the magneto-optical trap (MOT) for neutral atoms permitted their spatial confinement and the compression of their density. These successes boosted efforts to try to create BEC in alkaline gases, which have electronic level schemes that lend themselves to optical cooling. Later, it was discovered that the phase space density in MOTs is limited by radiation trapping effects. As a solution to this problem, scientists had to learn how to trap atoms without the use of light in conservative traps, e.g. by their magnetic dipole moment, and to replace optical cooling with *evaporative cooling*. This was the crucial step that finally permitted to reach BEC in alkaline gases in 1995. Later, the hydrogen experiment, which initially stimulated the alkaline experiments, now taking advantage of their success, has been taken to BEC as well [248].

Why did it take so long to reach Bose-Einstein condensation, seven decades after its prediction by Bose and Einstein? How can we *see* when we have a condensate? What are the characteristics of a BEC accessible to observation and how to measure them? These are the answers that we will answer in the following sections. Solve

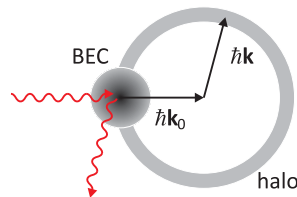


Figure 25.2: Scheme of the Broglie wave of cold atoms. From top to bottom the temperature decreases.

#### Exc. 25.1.5.1.

<sup>1</sup>The chemical potential of photons is  $\mu = 0$ .

## 25.1 Quantum statistics of an ideal Bose gas

The canonical approach to statistical mechanics begins with the probabilistic analysis of Boltzmann's velocity distribution of an ideal gas. For a gas consisting of particles of mass  $m$  at temperature  $T$ , the velocity distribution is given by the well-known *Maxwell-Boltzmann law* (MB) [346]

$$g(\mathbf{v}) = \left( \sqrt{\frac{m}{2\pi k_B T}} \right)^3 e^{-m\mathbf{v}^2/2k_B T}, \quad (25.1)$$

where  $k_B$  is the Boltzmann constant. Maxwell-Boltzmann's law was experimentally proven by Otto Stern in 1920, using a primitive atomic beam and a simple time-of-flight technique based on a rotating drum for selecting atomic velocities. With the advent of laser spectroscopy, the MB law and its limitations can be tested with highly improved accuracy. This law describes well the behavior of weakly interacting hot atoms. Deviations from this law are insignificant until, at low temperatures, quantum effects come into play. For this to happen the temperature must be so low that the atomic Broglie wavelengths become comparable to the average distance between particles. For a gas in thermal equilibrium the characteristic wavelength, called *thermal de Broglie wavelength*, is,

$$\lambda_{therm} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}, \quad (25.2)$$

where  $\hbar = h/2\pi$  is Planck's constant. In a gas of density  $n$ , the mean distance between particles is  $n^{-1/3}$ . So, quantum effects are expected to emerge when  $n^{-1/3} \sim \lambda_{dB}(T)$ , such that the limit for this regime is defined by,

$$k_B T(n) = \frac{2\pi\hbar^2}{m} n^{2/3}. \quad (25.3)$$

For example, an atomic gas with density  $n \sim 10^{16} \text{ cm}^{-3}$  and temperature 900 K is certainly in the classical regime, since  $n^{-1/3} \sim 10^6 \text{ cm} \gg \lambda_{dB} = 10^{-9} \text{ cm}$ . To observe quantum effects, we need relatively dense and cold clouds of atoms. In most gases, lowering the temperature or increasing the density promotes the system to liquidity before the quantum regime is reached. Well-known exceptions are spin-polarized hydrogen ( $\text{H}\uparrow$ ), which does not become liquid and helium, which exhibits quantum degeneracy effects in the liquid phase, although these effects are quite complex due to strong interparticle forces.

We have already seen that all particles in the quantum world are either *bosons* with integer spin or *fermions* with semi-integer spin. Fermions do not share a quantum state, because they must follow the *Pauli's exclusion principle*. They obey a quantum statistical distribution called *Fermi-Dirac distribution* (FD). In contrast, bosons enjoy to share a quantum state and even encourage other bosons to join them in a process called *bosonic stimulation*. Bosons obey a quantum statistical distribution called *Bose-Einstein distribution* (BE). The basic difference between the MB-statistics on one hand and the BE- or FD-quantum statistics on the other is that the former applies to identical particles which, however, are distinguishable from each other, while the

second describes identical indistinguishable particles. For the BE/FD statistics one can derive [?] the occupancy number for a non-degenerate quantum state having the energy  $\varepsilon$  when the system is kept at temperature  $T$ ,

$$w_{T,\mu} = \frac{1}{(2\pi)^3} \frac{1}{e^{\beta(\varepsilon-\mu)} \mp 1}, \quad (25.4)$$

where we used the abbreviation  $\beta \equiv 1/k_B T$ . The upper sign refers to the BE statistics, the lower sign to the FD statistics. The chemical potential  $\mu$  is an important system parameter, which helps to normalize the distribution (25.4) to the total number of particles,

$$N = \sum_{\varepsilon} w_{T,\mu}(\varepsilon). \quad (25.5)$$

Similarly, the total energy of the system is given by,

$$E = \sum_{\varepsilon} \varepsilon w_{T,\mu}(\varepsilon). \quad (25.6)$$

A very remarkable effect occurs in a bosonic gas at a certain characteristic *critical temperature*  $T_c$ : below this temperature a substantial fraction of the total number of particles occupies the lowest energy state, while all other states are occupied by a negligible number of particles. Above the transition temperature the macroscopic observables of the gas, such as pressure, heat capacity, etc., receive contributions of all states with a certain statistical weight, but without favoring the state of lower energy. Below the transition temperature, the observables are altered by a macroscopic occupation of the ground state, which results in dramatic changes of the thermodynamic properties. The phase transition is named after Shandrasekar Bose [97] and Albert Einstein [222] *Bose-Einstein condensation* (BEC).

### 25.1.1 Condensation of a free gas confined in a box potential

One of the keys to understanding BEC is the behavior of the chemical potential  $\mu$  at very low temperatures. The chemical potential is responsible for the concentration of a large number of atoms in the ground state  $N_0$ . A system with a large number of non-interacting bosons condenses to the ground state when the temperature approaches zero,  $N_0 \rightarrow N$ . The Bose-Einstein distribution function (25.4) gives the population of the ground state,  $\varepsilon = 0$ , in the zero temperature limit,  $N = \lim_{T \rightarrow 0} (e^{-\beta\mu} - 1)^{-1} = -1/\beta\mu$ , or in terms of the *fugacity* defined by,

$$Z \equiv e^{\beta\mu}, \quad (25.7)$$

we may write,  $Z \simeq 1 - 1/N$ . It should be noted that the chemical potential in a bosonic system must always be less than the ground state energy in order to guarantee non-negative occupation  $w_{T,\mu}(\varepsilon)$  of any state.  $Z \simeq 1$  denotes macroscopic occupation of the ground state. We define the critical temperature for Bose-Einstein condensation via the occupation of the ground state. Above this temperature the occupancy of ground state is not macroscopic, below it is.

For a Bose gas of  $N$  non-interacting particles with mass  $m$  confined inside a box potential of volume  $V = L^3$  the critical temperature for BEC can be calculated from equation (25.3). The boundary conditions require that the momenta satisfy  $p_j = 2\pi\hbar l_j/L$ , where  $j = x, y$  or  $z$  and  $l_j$  are integers. Each state is labeled by a set of three integers  $(l_x, l_y, l_z)$ . In the *thermodynamic limit*, the sum over all quantum states can be converted into an integral over a continuum of states,

$$\sum_{\mathbf{r}, \mathbf{k}} \xrightarrow{N \rightarrow \infty} \frac{1}{\hbar^3} \int d^3r d^3p = \int d^3r d^3k . \quad (25.8)$$

For a free gas with energy  $\varepsilon = p^2/2m$  we can derive, simplifying the calculation using the *density of states*  $\eta$  defined by (24.19), which basically depends on the geometry of our system<sup>2</sup>. Using the occupation number  $w_{T,\mu}(\varepsilon)$  for the Bose-Einstein distribution (25.4) in the thermodynamic limit and the density-of-states in a box potential (24.22), let us calculate the total number of particles,

$$\begin{aligned} N &= N_0 + \iint w_{T,\mu}(\varepsilon(\mathbf{r}, \mathbf{k})) d^3r d^3k = N_0 + (2\pi)^3 \int_0^\infty w_{T,\mu}(\varepsilon) \eta(\varepsilon) d\varepsilon \\ &= N_0 + \frac{\sqrt{2m}^3}{(2\pi)^2 \hbar^3} V \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{e^{\beta(\varepsilon-\mu)} - 1} , \end{aligned} \quad (25.9)$$

where the ground state population  $N_0$  is maintained explicitly. In the process of converting the sum to an integral (25.8) the density of states disappears when we approach the ground state. This error is corrected by adding a contribution of an explicit term  $N_0$  to the integral.

### 25.1.1.1 Riemann's zeta function

At this point, to help simplifying the notation, we introduce the *Bose function* and its integral representation,

$$g_\xi(Z) = \sum_{t=1}^{\infty} \frac{Z^t}{t^\xi} = \frac{1}{\Gamma(\xi)} \int_0^\infty \frac{x^{\xi-1} dx}{Z^{-1} e^x - 1} . \quad (25.10)$$

where  $\Gamma(\eta)$  denotes the Gamma function. Analogously, we can define the *Fermi function* via,

$$f_\xi(Z) = \sum_{t=1}^{\infty} -\frac{(-Z)^t}{t^\xi} = \frac{1}{\Gamma(\xi)} \int_0^\infty \frac{x^{\xi-1} dx}{Z^{-1} e^x + 1} . \quad (25.11)$$

For classical particles,

$$c_\xi(Z) = \frac{1}{\Gamma(\xi)} \int_0^\infty \frac{x^{\xi-1} dx}{Z^{-1} e^x + 0} = Z . \quad (25.12)$$

A particular value is the *Riemann zeta-function*,

$$g_\xi(1) = \zeta(\xi) . \quad (25.13)$$

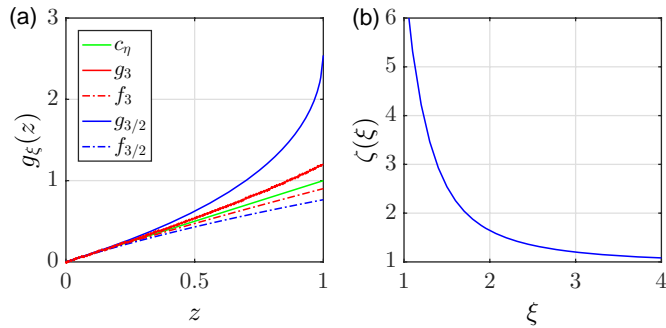


Figure 25.3: (code) (a) Bose and Fermi functions for box potentials ( $g_3$  and  $f_3$ ) and for harmonic potentials ( $g_{3/2}$  and  $f_{3/2}$ ). Also shown is the Boltzmann limit (25.12). (b) Riemann function.

With this definition and the definition of the thermal Broglie wavelength (25.2), Eq. (25.9) becomes,

$$N = N_0 + \frac{V}{\lambda_{th}^3(T)} g_{3/2}(e^{\beta\mu}). \quad (25.14)$$

We can use Eq. (25.14) to calculate the critical temperature<sup>3</sup>  $T_c^{(3/2)}$  defined for  $N_0 \nearrow 0$  and  $\mu \rightarrow 0$ . Above the phase transition,  $T > T_c^{(3/2)}$ , the population is distributed over all states, each individual state being weakly populated. Below  $T_c^{(3/2)}$  the chemical potential is fixed by  $\mu = 0$  and the number of the particles occupying the excited states is,

$$N_{th} = \frac{V}{\lambda_{th}^3(T)} g_{3/2}(1) = N \left( \frac{T}{T_c^{(3/2)}} \right)^{3/2}, \quad (25.15)$$

with  $g_{3/2}(1) = 2.612$ . Since  $N_0 + N_{th} = N$ , the number of particles in the ground state is given by,

$$\boxed{\frac{N_0}{N} = 1 - \left( \frac{\min(T, T_c^{(3/2)})}{T_c^{(3/2)}} \right)^{3/2} \quad \text{with} \quad k_B T_c^{(3/2)} = \frac{2\pi\hbar^2}{m} \left( \frac{N}{V g_{3/2}(1)} \right)^{2/3}}, \quad (25.16)$$

$N_0/N$  is the fraction of the atomic cloud which is condensed in the ground state. The abrupt occurrence of a finite occupation in a single quantum state at temperature below  $T_c^{(3/2)}$  indicates a spontaneous change in the system and a thermodynamic phase transition. Solve Exc. 25.1.5.2.

<sup>2</sup>We must, however, keep in mind that the state density approach is an approximation not valid for experiments with a limited number of atoms.

<sup>3</sup>The superscript (3/2) denotes the box potential shape of the trapping potential. See 25.1.5.3 for an explanation of the notation.

### 25.1.2 Condensation of a harmonically confined gas

The critical temperature  $T_c^0$  can be significantly altered, when the atoms are confined to a spatially inhomogeneous potential. The critical temperature depends on the general shape and the tightness of the potential. Let us consider  $N$  particles of an ideal Bose gas distributed over several quantum states of an arbitrary potential. The occupation number  $w_{T,\mu}(\varepsilon)$  of particles at an energy level  $\varepsilon$  is still given by (25.4), the ground state energy is defined as zero. In the thermodynamic limit, the relation between the chemical potential and the total number of particles is still given by Eq. (25.9), with an adequate density of states  $\eta(\varepsilon)$ . The state density for an arbitrary confinement potential  $U(\mathbf{r})$  can be found by generalizing the calculation to the free gas. The phase space volume between the energy surfaces  $\varepsilon$  and  $\varepsilon + d\varepsilon$  is proportional to the number of states in this energy range. However, the external potential limits the space available for the gas. For a harmonic potential (24.18) with the mean secular frequency  $\bar{\omega}$  the density-of-states  $\eta(\varepsilon)$  has already been calculated in Eq. (24.21). With this, we can analogically to (25.9) calculate,

$$\begin{aligned} N &= N_0 + \iint w_{T,\mu}(\varepsilon(\mathbf{r}, \mathbf{k})) d^3r d^3k = N_0 + (2\pi)^3 \int_0^\infty w_{T,\mu}(\varepsilon) \eta(\varepsilon) d\varepsilon \\ &= N_0 + \frac{1}{2(\hbar\bar{\omega})^3} \int_0^\infty \frac{\varepsilon^2 d\varepsilon}{e^{\beta(\varepsilon-\mu)} - 1} = N_0 + \left( \frac{k_B T}{\hbar\bar{\omega}} \right)^3 g_3(Z). \end{aligned} \quad (25.17)$$

In the same way as for a potential well we find for a harmonic potential,

$$N_{th} = \left( \frac{k_B T}{\hbar\bar{\omega}} \right)^3 g_3(1) = N \left( \frac{T}{T_c^{(3)}} \right)^3, \quad (25.18)$$

with  $g_3(1) = 1.202$ . Since  $N_0 + N_{th} = N$ , the number of particles in the ground state is,

$$\boxed{\frac{N_0}{N} = 1 - \left( \frac{\min(T, T_c^{(3)})}{T_c^{(3)}} \right)^3 \quad \text{with} \quad k_B T_c^{(3)} = \hbar\bar{\omega} \left( \frac{N}{g_3(1)} \right)^{1/3}}. \quad (25.19)$$

The superscript (3) indicates the harmonic shape of the trap.

Fig. 25.4(left) traces the condensed fraction  $N_c/N$  measured as a function of the reduced temperature  $T/T_c^{(3)}$ . Experiments [307, 227] confirm Bose's ideal gas theory in the thermodynamic limit.

We note that smaller trapping volumes (or tighter potentials) increase the critical temperature  $T_c$ , thus allowing for quantum degeneracy at higher temperatures, which can be advantageous in experimentation. Also, at a given temperature, a strongly confining potential reduces the total minimum number of atoms required to reach condensation.

### 25.1.3 Energy and heat capacity

When the number of atoms is limited,  $N < \infty$ , we expect a slightly reduced critical temperature [289]. In addition, the interatomic interaction reduces the critical temperature [37]. The technical resolution of most experiments today is not sufficient to



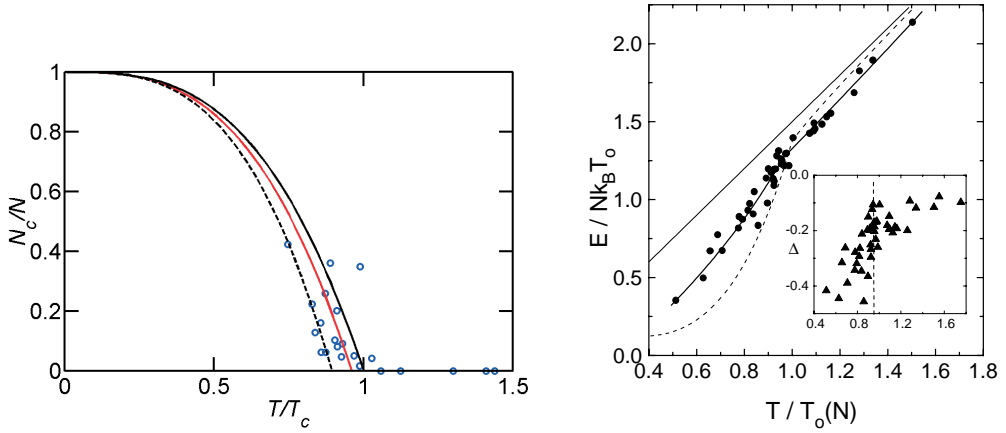


Figure 25.4: Left: Condensed fraction  $N_c/N$  as a function of reduced temperature  $T/T_c^{(3)}$ . The circles represent measured values. The upper solid line shows the theory for an ideal gas, the intermediate solid line shows a curve fitted to the measurements, and the lower part is a theoretical curve taking into account finite size effects and interatomic interactions. Right: Measurement of the release energy [227].

permit the study of these effects. However, measurements of other thermodynamic quantities such as energy and heat capacity [183, 227] showed significant deviations from the ideal gas behavior due to interaction effects. Therefore, although temperature being the most basic variable of the thermodynamic state, the system needs to be characterized by other quantities.

Heat is not a state variable because the amount of heat needed to raise the temperature of the system depends on how the heat is transferred. The *heat capacity* quantifies the system's ability to secure its energy. In conventional systems, the heat capacity is typically given either specified at constant volume or at constant pressure. Together with this specification, heat capacities are extensive state variables. When crossing a phase transition, the temperature-dependent heat capacity measures the degree of change in the system above and below the critical temperature and provides valuable information about the general type of phase transition.

The total energy  $E/N \equiv N^{-1} \int \epsilon w d^3x d^3k$  per particle is given by,

$$\frac{E}{N} = \frac{\int \epsilon w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3x d^3k}{\int w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3x d^3k} = \frac{\int \epsilon \eta(\epsilon) (e^{\beta(\epsilon-\mu)} - 1)^{-1} d\epsilon}{\int \eta(\epsilon) (e^{\beta(\epsilon-\mu)} - 1)^{-1} d\epsilon} = 3k_B T \frac{g_4(Z)}{g_3(Z)}. \quad (25.20)$$

For a confined gas, volume and temperature are interdependent, and the concept of pressure is somewhat vague. In this case, we can not refer to the heat capacity at constant volume or pressure. However, one can define the heat capacity for a fixed number of particles,

$$C(T) = \frac{\partial E(T)}{\partial T}. \quad (25.21)$$

Recalling the implicit dependencies of the thermodynamic variables on temperature,

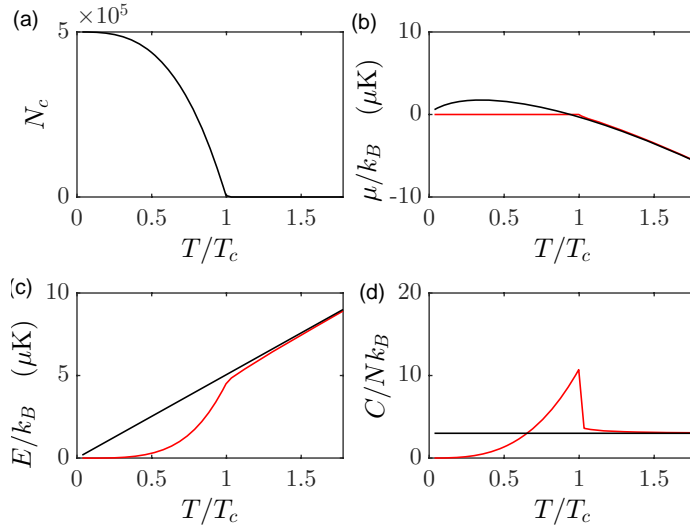


Figure 25.5: (code) Numerical calculation of thermodynamic potentials for a Bose gas as a function of temperature for a given trapping potential. (a) Chemical potential, (b) energy, (c) heat capacity per particle, and (d) total heat capacity.

we can evaluate (25.19):

$$C(T) = \beta \int_0^{\infty} \varepsilon f(\varepsilon)^2 \rho(\varepsilon) \left[ \mu'(T) + \frac{\varepsilon - \mu}{T} \right] e^{\beta(\varepsilon - \mu)} d\varepsilon, \quad (25.22)$$

where the derivative of the chemical potential approaching the phase transition from above,  $T \searrow T_c^0$ , is

$$\mu'(T_c^+) = -\frac{1}{T} \frac{\int_0^{\infty} \varepsilon f(\varepsilon)^2 \rho(\varepsilon) e^{\beta\varepsilon} d\varepsilon}{\int_0^{\infty} f(\varepsilon)^2 \rho(\varepsilon) e^{\beta\varepsilon} d\varepsilon}. \quad (25.23)$$

Calculating the second moments of the distributions obtained for the same density by time-of-flight of absorption images, we obtain the kinetic energy,

$$U = \int \frac{p^2}{2m} n(\mathbf{p}) d^3 \mathbf{p}. \quad (25.24)$$

For confined ideal gases, the virial theorem ensures  $E_{kin} + E_{pot} = 2E_{kin}$ . For real gases, the repulsive energy of the mean field adds to this energy,  $E = E_{kin} + E_{pot} + E_{self}$ . The sudden extinction of the trapping potential before time-of-flight takes away the potential energy  $E_{pot}$  non-adiabatically. The kinetic energy and the self-energy of the condensate are fully converted into kinetic energy during ballistic expansion. It is this energy,  $p^2/2m = E_{kin} + E_{self}$ , which is sometimes called *release energy*, which is measured after ballistic expansion<sup>4</sup>. Fig. 25.4(right) shows a measurement of the release energy. Solve the Exc. 25.1.5.3.

<sup>4</sup>It is interesting to measure the heat capacity of a partially condensed cloud near the critical point and analyze the discontinuity, because it contains important information about interatomic interactions and finite-size effects ([152], Sec. 3.4). In addition, the classification of Bose-Einstein condensation as a phase transition depends very much on the behavior of the thermodynamic potential near the critical point [422, 346].

### 25.1.4 Distribution functions for a Bose gas

Bose-Einstein condensates consist of atoms sharing a single quantum state. In inhomogeneous potentials, the condensate and the thermal fraction form spatially separated clouds, concentrated around the center of the potential and therefore very dense. For this reason, interatomic interaction effects generally dominate the density and momentum distribution of the condensed fraction. However, the non-condensed (or normal, or thermal) fraction is also subject to modifications due to the bosonic nature of the atoms. Since the density of the normal fraction is generally much smaller, these modifications are weak. In this section, we will only discuss these effects briefly, but we note that the calculations are analogous to the calculations for fermionic gases presented in Sec. 25.2.4.

For an ideal Bose gas the density and momentum distributions are expressed by Bose functions  $g_{3/2}(z)$  [152]. For example, as will be derived in Exc. 25.1.5.4(a), the density and momentum distributions are,

$$\boxed{\begin{aligned} n(\mathbf{x}) &= \frac{1}{\lambda_{dB}^3} g_{3/2}(e^{-\beta[U(\mathbf{x})-\mu]}) \\ n(\mathbf{k}) &= \frac{a_{trp}^6}{\lambda_{dB}^3} g_{3/2}(e^{\beta(\mu-\mathbf{p}^2/2m)}) \end{aligned}} \quad \text{bosonic distribution functions} . \quad (25.25)$$

In the classical limit, we can calibrate the chemical potential by Eq. (25.14) for a box potential or by (25.17) for a harmonic potential,

$$g_{3/2}(e^{\beta\mu}) \rightarrow c_{3/2}(e^{\beta\mu}) = e^{\beta\mu} = \begin{cases} \frac{N}{V} \lambda_{th}^3 & \text{for a box potential} \\ c_3(e^{\beta\mu}) = N \left( \frac{\hbar\bar{\omega}}{k_B T} \right)^3 & \text{for a harmonic potential} \end{cases} . \quad (25.26)$$

Hence, we obtain for the classical density distribution,

$$\begin{aligned} n(\mathbf{x}) &= \frac{1}{\lambda_{th}^3} c_{3/2}(e^{-\beta[U(\mathbf{x})-\mu]}) = \frac{e^{\beta\mu}}{\lambda_{th}^3} e^{-\beta U(\mathbf{x})} \\ &= \begin{cases} \frac{N}{V} e^{-\beta U(\mathbf{x})} & \text{for a box potential} \\ N \sqrt{\frac{m\bar{\omega}^2}{2\pi k_B T}}^{-3} e^{-\beta m\bar{\omega}^2 x^2/2} & \text{for a harmonic potential} \end{cases} . \end{aligned} \quad (25.27)$$

Similarly, the momentum density distribution is given by,

$$\begin{aligned} n(\mathbf{k}) &= \frac{a_{trp}^6}{\lambda_{th}^3} c_{3/2}(e^{\beta(\mu-\mathbf{p}^2/2m)}) = \frac{a_{trp}^6 e^{\beta\mu}}{\lambda_{th}^3} e^{-\beta \mathbf{p}^2/2m} \\ &= \begin{cases} \frac{N}{V} a_{trp}^6 e^{-\beta U(\mathbf{x})} & \text{for a box potential} \\ N \hbar^3 \sqrt{\frac{1}{2\pi m k_B T}}^{-3} e^{-\beta \mathbf{p}^2/2m} & \text{for a harmonic potential} \end{cases} . \end{aligned} \quad (25.28)$$

We see that we recover the Maxwell-Boltzmann velocity distribution, as seen in Fig. 25.6,

$$n(\mathbf{v}) = n(\mathbf{k}) \frac{m^3}{\hbar^3} = N \sqrt{\frac{m}{2\pi k_B T}}^3 e^{-\beta m v^2/2} . \quad (25.29)$$

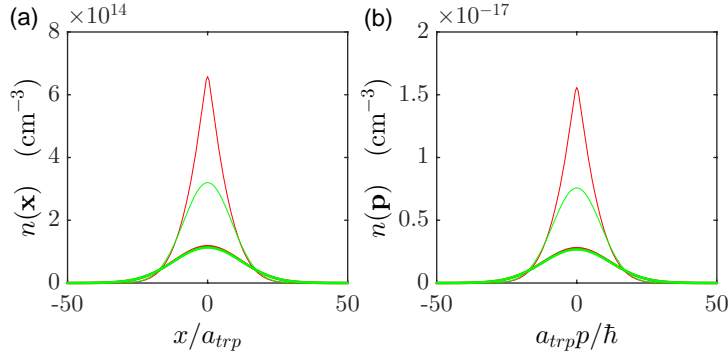


Figure 25.6: (code) (a) Density and (b) momentum distribution of a Bose gas (red) and a Boltzmann gas (green) at  $T = 1.1T_c$  (solid line) and at  $T = 2T_c$  (dotted line).

#### 25.1.4.1 Ballistic expansion

To describe the density distribution of an ultracold Bose-gas after a time-of-flight we replace in the second Eq. (25.25):  $\mathbf{k} = m\mathbf{r}/\hbar t_{tof}$ . We obtain the density distribution,

$$n_{tof}(\mathbf{r}, t_{tof}) = \left(\frac{m}{\hbar t_{tof}}\right)^3 n(\mathbf{k} = m\mathbf{r}/\hbar t_{tof}) = \left(\frac{m}{\hbar t_{tof}}\right)^3 \frac{a_{trp}^6}{\lambda_{th}^3} g_{3/2}(e^{(\mu - mr^2/2t_{tof}^2)/k_B T})$$

$$\xrightarrow{T \rightarrow \infty} \left(\frac{m}{\hbar t_{tof}}\right)^3 N \hbar^3 \sqrt{\frac{1}{2\pi m k_B T}}^3 e^{-mr^2/2t_{tof}^2 k_B T} = \frac{N}{(2\pi)^{3/2} r_{rms}^3} e^{-r^2/2r_{rms}^2}, \quad (25.30)$$

where we defined,

$$r_{rms} \equiv \sqrt{\frac{k_B T}{m}} t_{tof}. \quad (25.31)$$

This distribution does not directly depend on the potential  $U(\mathbf{r})$ , that is, the expansion is isotropic. However, the chemical potential does depend on the potential. For very long flight times (usually several 10 ms) the density resembles a Gaussian distribution [152]. In Exc. 25.1.5.4(b) we determine the time-of-flight density distribution of an ultracold Bose gas.

In a time-of-flight experiment, any deviation observed between the results (25.30) and (25.31) points towards an impact of quantum statistics. However, absorption images only record projections of the time-of-flight distribution on a plane.

#### 25.1.4.2 Temperature and excitations

The *temperature of a Bose condensate* is given by the ratio of the numbers of condensed and thermal atoms. What about collective excitations in pure condensate? Can they be cooled? In fact, an oscillating BEC is not in thermal equilibrium. However, in the presence of some dissipation mechanism the excitations may thermalize evolving towards a steady state. Once the collective excitations have become thermal excitations, they simply increase the thermal fraction.

## 25.1.5 Exercises

### 25.1.5.1 Ex: Boson or fermion?

Whether an atom is a fermion or boson solely depends on its total spin. Half-integer spin particles are fermions, integer spin particles are bosons. For example, Rb atoms have in the ground state  $J = 1/2, I = 7/2$  and  $F$  integer, and therefore are bosons.  $\text{Ca}^+$  ions have  $J = 1/2$  and no hyperfine structure, and thus are fermions.  ${}^6\text{Li}$  has the half-integer  $F$  and is a boson.

Decide on the bosonic or fermionic nature of the following atoms/molecules:

${}^{85}\text{Rb}$  with  $I = 3/2$  in the state  ${}^2S_{1/2}$

${}^{88}\text{Sr}$  with  $I = 0$  in the state  ${}^1S_0$

${}^{88}\text{Sr}$  with  $I = 0$  in the state  ${}^3P_2$

${}^{87}\text{Sr}$  with  $I = 9/2$  in the state  ${}^1S_0$

${}^{172}\text{Yb}^+$  with  $I = 0$  in the state  ${}^2S_{1/2}$

${}^{171}\text{Yb}^+$  with  $I = 1/2$  in the state  ${}^2S_{1/2}$

### 25.1.5.2 Ex: Monoatomic gas

Consider a classical monoatomic gas made up of  $N$  non-interacting atoms of mass  $m$  confined in a container of volume  $V$ , at temperature  $T$ . The Hamiltonian corresponding to an atom is given by  $\hat{H} = (p_x^2 + p_y^2 + p_z^2)/2m$ .

- Show that the atomic canonical partition function is  $\zeta = V/\lambda^3$ , where  $\lambda = h/\sqrt{2\pi mk_B T}$  is the thermal de Broglie wavelength.
- Using  $\zeta$  of the previous item, obtain the system's partition function  $Z$  and the Helmholtz free energy  $F$ . Also obtain the free energy per atom  $f = F/N$  in the thermodynamic limit  $N \rightarrow \infty, V \rightarrow \infty, v = N/V$  fixed.
- Obtain internal energy  $U$  and the gas pressure  $p$ .
- Calculate the chemical potential and entropy per atom in the thermodynamic limit.

### 25.1.5.3 Ex: Generalization for arbitrary potentials in reduced dimensions

The calculation of the thermodynamic potentials can be generalized to arbitrary trapping potentials and dimensions [97, 222, 176, 38, 740, 242, 39, 289, 331, 395, 389, 517, 422, 439, 227]. To do so, we consider a generic power law potential confining an ideal Bose gas in  $\alpha$  dimensions,

$$U(\mathbf{r}) = \sum_{i=1}^{\alpha} \left| \frac{x_i}{a_i} \right|^{t_i},$$

and define a parameter describing the confinement power of the potential,

$$\xi = \frac{\alpha}{2} + \sum_{i=1}^{\alpha} \frac{1}{t_i}.$$

For example, for a three-dimensional potential,  $\alpha = 3$ . Now, for a 3D harmonic potential,  $\xi = 3$ , and for 3D box potential,  $\xi = 3/2$ .

- Calculate the density of states  $\eta$  using the equation (24.19) employing Bose functions (25.10).

b. Prove the following expressions:

bosonic potentials

$$\begin{aligned}
 \frac{N_0}{N} &= 1 - \left( \frac{\min(T, T_c)}{T_c} \right)^\xi \\
 \frac{E}{Nk_B T} &= \xi \frac{g_{\xi+1}(Z)}{g_\xi(Z)} \left( \frac{\min(T, T_c)}{T_c} \right)^\xi \\
 \frac{S}{Nk_B} &= 4 \frac{g_{\xi+1}(Z)}{g_\xi(Z)} - \frac{2\mu}{k_B T} \\
 \frac{C}{Nk_B} &= \xi(\xi+1) \frac{g_{\xi+1}(Z)}{g_\xi(Z)} \left( \frac{\min(T, T_c)}{T_c} \right)^\xi - \xi^2 \frac{g_\xi(Z)}{g_{\eta-1}(Z)} \frac{\max(T - T_c, 0)}{T - T_c} \\
 \frac{C_{T>T_c}}{Nk_B} &= \xi(\xi+1) \frac{g_{\xi+1}(Z)}{g_\xi(Z)} - \xi^2 \frac{g_\xi(Z)}{g_{\xi-1}(Z)}, \quad \frac{C_{T<T_c}}{Nk_B} = \xi(\eta+1) \frac{g_{\xi+1}(1)}{g_\xi(1)} \\
 \frac{\Delta C_{T_c}}{Nk_B} &= \frac{C_{T_c^-} - C_{T_c^+}}{Nk_B} = \xi^2 \frac{g_\xi(1)}{g_{\xi-1}(1)}
 \end{aligned}$$

#### 25.1.5.4 Ex: Time-of-flight distribution of a Bose-gas

- Derive the formulae (25.25) describing the density and momentum distribution of an ultracold Bose-gas.
- Calculate the time-of-flight distribution of a Bose-gas as a function of temperature (i) analytically for a harmonic potential and (ii) numerically for an arbitrary potential.

## 25.2 Quantum statistics of an ideal Fermi gas

Atoms are fermions or bosons, or depending on their spin is integer or semi-integer. For example,  $^{87}\text{Rb}$  atoms with their total integer spin of  $F$  are bosons, while  $^{40}\text{K}$  atoms having a half-integer spin are fermions. At high phase space densities, atoms have to figure out how they will organize their coexistence. Bosons encourage each other to occupy the same phase space cell, in contrast to the reluctant fermions, which prefer to follow Pauli's exclusion principle. The different behavior is described by different quantum statistics that determine how the phase space (i.e., the available energy levels) has to be filled by the atoms. The Bose-Einstein distribution is valid for bosons, the distribution of Fermi-Dirac for fermions and both asymptotically approach the Boltzmann distribution at high temperatures. We have seen that bosons undergo a phase transition and condense in the ground state when the temperature is reduced below a critical threshold. On the other hand, the fermions organize their phase space, so that their energy levels are arranged like a ladder. The impact of fermionic quantum statistics on a cold cloud of atoms were observed experimentally by DeMarco and Jin [183, 525]. They cooled a two-components Fermi gas of  $7 \times 10^5$  potassium atoms down to 300 nK, which corresponded to 60% of the atoms populating energy levels below the Fermi energy. The measured density distribution was found to deviate from the one expected for an ideal Boltzmann gas<sup>5</sup>.

<sup>5</sup>We note that meanwhile ultracold two-components Fermi gas have been demonstrated to form bosonic Cooper-pairs, similarly to the phenomena known as superconductivity in some metals and

### 25.2.1 Chemical potential and Fermi radius for a harmonic trap

The phase space density for a *degenerate Fermi gas* has already been given in (25.4). In the same way as for a Bose gas, the chemical potential must satisfy the normalization condition,

$$\begin{aligned} N &= \iint w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3\mathbf{x} d^3k = (2\pi)^3 \int w_{T,\mu}(\varepsilon) \eta(\varepsilon) d\varepsilon \\ &= \frac{1}{2(\hbar\bar{\omega})^3} \int_0^\infty \frac{\varepsilon^2 d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1} = \left( \frac{k_B T}{\hbar\bar{\omega}} \right)^3 f_3(Z). \end{aligned} \quad (25.32)$$

In the last line, we inserted the density of the states into a harmonic potential (24.21) and used the definition of the Fermi functions (25.11).

For low temperatures,  $x \equiv \mu \gg 1$ , we can use the Sommerfeld expansion which in first order gives  $f_\eta(e^x) \simeq x^\eta / \Gamma(\eta + 1)$ . From this we immediately obtain the energy, the Fermi radius and the momentum of free particles,

$$\begin{aligned} E_F &= \mu(T=0) = \hbar\bar{\omega}(6N)^{1/3} \\ r_F &= \sqrt{\frac{2E_F}{m\omega_r^2}} \quad \text{and} \quad z_F = \sqrt{\frac{2E_F}{m\omega_z^2}} \\ K_F &= \sqrt{\frac{2mE_F}{\hbar^2}}. \end{aligned} \quad (25.33)$$

Using the second order of the Sommerfeld expansion,  $f_\xi(e^x) \simeq \frac{x^\xi}{\Gamma(\xi+1)} \left( 1 + \frac{\pi^2 \xi(\xi-1)}{6x^2} + \dots \right)$ , we obtain for the chemical potential the equation,  $0 = \mu^3 + (\pi k_B T)^2 \mu - E_F^3$ . The approximate solution of this equation, neglecting terms such as  $4\pi^6 k_B^6 T^6 \ll 27E_F^6$ , is

$$\mu = E_F \left[ 1 - \frac{\pi^2}{3} \left( \frac{k_B T}{E_F} \right)^2 \right]. \quad (25.34)$$

In the limit of high temperatures,  $f_\eta(Z) \xrightarrow{Z \rightarrow 1} Z$

$$\begin{aligned} N &= \left( \frac{k_B T}{\hbar\bar{\omega}} \right)^3 e^{\beta\mu} = \left( \frac{k_B T}{\hbar\bar{\omega}} \right)^3 (1 + \beta\mu + \dots), \\ \mu &\approx k_B T \ln N \left( \frac{\hbar\bar{\omega}}{k_B T} \right)^3 = k_B T \ln \frac{1}{6} \left( \frac{E_F}{k_B T} \right)^3. \end{aligned} \quad (25.35)$$

This means that we recover the *Boltzmann gas*, which satisfies an ideal gas equation similar to that of particles in a box potential,

$$N = \left( \frac{k_B T}{\hbar\bar{\omega}} \right)^3 \quad (\text{Boltzmann}). \quad (25.36)$$

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as superfluidity of the fermionic  ${}^3\text{He}$ .

For comparison, for bosons we have,

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^3 \frac{g_3(Z)}{g_3(1)} \quad (\text{Bose}) . \quad (25.37)$$

The chemical potentials are calculated in Fig. 25.7(a).

### 25.2.2 Energy

The total energy  $E_1 \equiv E/N \equiv N^{-1} \int \epsilon w d^3 \mathbf{x} d^3 k$  per particle is given by,

$$\begin{aligned} E_1 &= \frac{\int \epsilon w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3 \mathbf{x} d^3 k}{\int w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3 \mathbf{x} d^3 k} \\ &= \frac{\int \epsilon \eta(\epsilon) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon}{\int \eta(\epsilon) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon} = 3k_B T \frac{f_4(Z)}{f_3(Z)} . \end{aligned} \quad (25.38)$$

Again using the Sommerfeld approximation, we see that for  $T \rightarrow 0$  the energy is limited by

$$\begin{aligned} E_1 &= \frac{3}{N\beta(\beta\hbar\bar{\omega})^3} f_4(e^{\beta\mu}) \\ &= \frac{3\mu^4}{4E_F^3} \left(1 + \frac{2\pi^2}{(\beta\mu)^2} + \dots\right) \xrightarrow{T \rightarrow 0} \frac{3}{4} E_F \quad (\text{Fermi}) . \end{aligned} \quad (25.39)$$

because the atoms are forced to adopt a state of larger dynamics in the outermost regions of the trap. This implies,  $E_1/E_F \xrightarrow{T \rightarrow 0} 3/4$ .

In the limit of high temperatures,  $T \rightarrow \infty$ , a classical gas has the energy per particle,

$$E_1 = \frac{3}{N\beta(\beta\hbar\bar{\omega})^3} f_4 \left( f_3^{-1} \left( \frac{(\beta E_F)^3}{6} \right) \right) \approx 3k_B T \quad (\text{Boltzmann}) , \quad (25.40)$$

which is seen by taking the high temperature limit  $f_\eta(Z) \xrightarrow{Z \rightarrow 0} Z$  and extrapolating to all  $Z$ . This implies,  $E_1/E_F \xrightarrow{T \rightarrow \infty} 3k_B T/E_F$ .

Comparing with bosons,

$$E_1 = 3k_B T \frac{g_4(1)}{g_3(1)} \approx 2.7 \quad (\text{Bose}) . \quad (25.41)$$

### 25.2.3 Entropy and heat capacity

The entropy  $S = -k_B \int g(\epsilon) [w \ln w + (1-w) \ln(1-w)] d\epsilon$  per particle is,

$$S_1 = 4k_B \frac{f_4(Z)}{f_3(Z)} - \frac{\mu}{T} = \frac{4E_1}{3T} - \frac{\mu}{T} . \quad (25.42)$$

The heat capacity per particle  $C_1 = \left. \frac{\partial E_1}{\partial T} \right|_N$  is easily calculated using  $Z f'_\eta(Z) = f_{\eta-1}(Z)$ ,

$$C_1 = 3k_B \frac{f_4(Z)}{f_3(Z)} - \frac{3\mu}{T} \left( 1 - \frac{f_4(Z)f_2(Z)}{f_3(Z)^2} \right) = \frac{E_1}{T} - \frac{3\mu}{T} \left( 1 - \frac{f_4(Z)f_2(Z)}{f_3(Z)^2} \right) . \quad (25.43)$$



For fermions well below the Fermi temperature,  $T \rightarrow 0$ , using the Sommerfeld approximation, we calculate,

$$C_1 \xrightarrow{T \rightarrow 0} \frac{3\pi^2}{2} \frac{k_B T}{T_F} \quad (\text{Fermi}) . \quad (25.44)$$

For high temperature  $T$

$$C_1 \approx 3k_B \quad (\text{Boltzmann}) . \quad (25.45)$$

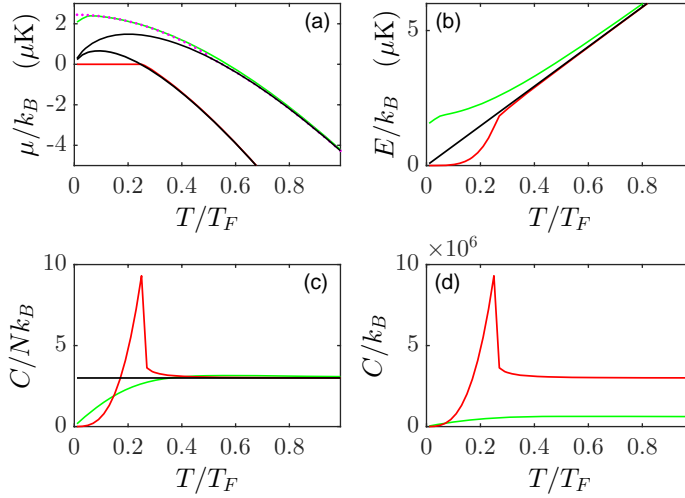


Figure 25.7: (code) Numerical calculation of thermodynamic potentials for Bose (red) and Fermi (green) gases as a function of temperature for a given harmonic trapping potential. (a) Chemical potential, (b) energy, (c) heat capacity per particle, and (d) total heat capacity. The dotted magenta line in (a) shows the chemical potential calculated from the Sommerfeld approximation.

## 25.2.4 Distributions of a Fermi gas

### 25.2.4.1 Spatial distribution

The density distribution is,

$$\begin{aligned} n(\mathbf{x}) &= \int w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3\mathbf{k} = \frac{1}{(2\pi)^2} \int \frac{2k^2 dk}{e^{\beta[\hbar^2 k^2/2m + U(\mathbf{x}) - \mu]} + 1} \\ &= \frac{1}{(2\pi)^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \int \frac{\sqrt{\varepsilon} d\varepsilon}{e^{\beta[\varepsilon + U(\mathbf{x}) - \mu]} + 1} = \frac{1}{(2\pi)^2} \left( \frac{2m}{\beta\hbar^2} \right)^{3/2} \Gamma(3/2) f_{3/2}(e^{-\beta[U(\mathbf{x}) - \mu]}), \end{aligned} \quad (25.46)$$

such that,

$$\boxed{n(\mathbf{x}) = \lambda_{dB}^{-3} f_{3/2}(e^{-\beta[U(\mathbf{x}) - \mu]})} \quad (\text{Fermi}) . \quad (25.47)$$

At low temperatures,  $T \rightarrow 0$ , we can apply the Sommerfeld expansion [115], which to first order gives  $\mu \rightarrow E_F$ ,

$$\begin{aligned} n(\mathbf{x}) &\approx \frac{1}{(2\pi)^2} \frac{\Gamma(3/2)}{\Gamma(5/2)} \left( \frac{2m}{\hbar^2} [\mu - U(\mathbf{x})] \right)^{3/2} \\ &= \frac{1}{(2\pi)^2} \frac{2}{3} \left( \frac{2m}{\hbar^2} \right)^{3/2} \left( E_F - \frac{m}{2} \omega_r^2 \rho^2 \right)^{3/2} = \frac{8\lambda}{\pi^2} \frac{N}{R_F^3} \left( 1 - \frac{\rho^2}{R_F^2} \right)^{3/2}. \end{aligned} \quad (25.48)$$

At high temperatures,  $T \rightarrow \infty$ , we should recover the Boltzmann gas situation,

$$\begin{aligned} n(\mathbf{x}) &= \lambda_{dB}^{-3} f_{3/2}(e^{-\beta[U(\mathbf{x})-\mu]}) \\ &\approx \lambda_{dB}^{-3} N (\beta \hbar \bar{\omega})^3 e^{-\beta U(\mathbf{x})} = \left( \frac{m\beta \bar{\omega}^2}{2\pi} \right)^{3/2} N e^{-\beta m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2}. \end{aligned} \quad (25.49)$$

It's easy to check,  $\int n(\mathbf{x}) d^3\mathbf{x} = N$ . Introducing the peak density  $n_0$ , we obtain,

$$\boxed{n(\mathbf{x}) = n_0 e^{-m\omega^2 \rho^2 / 2k_B T}} \quad (\text{Boltzmann}). \quad (25.50)$$

The *rms*-radius of the distribution is  $\sigma_j = \sqrt{k_B T / m\omega_j^2}$ , which seems contrary to the above results,  $\frac{m}{2} \omega_j^2 \langle x_j^2 \rangle = k_B T$ . In comparison,

$$\boxed{n(\mathbf{x}) = \lambda_{dB}^{-3} g_{3/2} \left[ e^{\beta(\mu - U(\mathbf{x}))} \right]} \quad (\text{Bose gas above } T_c). \quad (25.51)$$

where  $\lambda_{dB} = \sqrt{2\pi\hbar^2 / mk_B T}$  e  $a_{tr} = \sqrt{\hbar / m\bar{\omega}}$ .

#### 25.2.4.2 Momentum distribution

The momentum distribution is,

$$\begin{aligned} \tilde{n}(\mathbf{k}) &= \int w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3\mathbf{x} = \frac{1}{(2\pi)^2} \int \frac{r dr dz}{e^{\beta[\varepsilon(k) + m\omega_r^2 \rho^2 / 2 - \mu]} + 1} \\ &= \frac{1}{(2\pi)^3} \int \frac{4\pi \rho^2 d\rho}{e^{\beta[\varepsilon + m\omega_r^2 \rho^2 / 2 - \mu]} + 1} \\ &= \frac{1}{(2\pi)^2} \left( \frac{2}{\beta m \omega_r^2} \right)^{3/2} \int \frac{\sqrt{t} dt}{e^{\beta[\varepsilon + t - \mu]} + 1} = \frac{1}{(2\pi)^2} \left( \frac{2}{\beta m \omega_r^2} \right)^{3/2} \Gamma(3/2) f_{3/2}(e^{\beta(\mu - \varepsilon)}), \end{aligned} \quad (25.52)$$

such that,

$$\boxed{\tilde{n}(\mathbf{k}) = \lambda_{dB}^{-3} a_{tr}^6 f_{3/2}(e^{\beta(\mu - \varepsilon)})} \quad (\text{Fermi}). \quad (25.53)$$

At low temperatures,  $T \rightarrow 0$ ,

$$\begin{aligned} \tilde{n}(\mathbf{k}) &\approx \frac{1}{(2\pi)^2} \left( \frac{2}{\beta m \omega_r^2} \right)^{3/2} \frac{\Gamma(3/2)}{\Gamma(5/2)} (\beta [\mu - \varepsilon])^{3/2} \\ &\approx \frac{1}{(2\pi)^2} \left( \frac{2}{m\omega_r^2} \right)^{3/2} \frac{2}{3} \left( E_F - \frac{\hbar^2 k^2}{2m} \right)^{3/2} = \frac{8}{\pi^2} \frac{N}{K_F^3} \left( 1 - \frac{k^2}{K_F^2} \right)^{3/2}. \end{aligned} \quad (25.54)$$

This can easily be integrated by dimensions,

$$\begin{aligned} \tilde{n}_{T \rightarrow 0}(k_z) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{n}_{cl}(\mathbf{k}) dk_x dk_y = \frac{8}{\pi^2} \frac{N}{K_F^3} \int \int_{|k| \leq K_F} \left(1 - \frac{k^2}{K_F^2}\right)^{3/2} dk_x dk_y \\ &= \frac{8}{\pi^2} \frac{N}{K_F^3} \int_0^{2\pi} \int_0^{\sqrt{K_F^2 - k_z^2}} \left(1 - \frac{k_z^2}{K_F^2} - \frac{k_\rho^2}{K_F^2}\right)^{3/2} k_\rho dk_\rho d\phi = \frac{16}{5\pi} \frac{N}{K_F} \left(1 - \frac{k_z^2}{K_F^2}\right)^{5/2}. \end{aligned} \tag{25.55}$$

It is easy to check  $\int_{-\infty}^{\infty} \tilde{n}_{T \rightarrow 0} dk_z = N$ , with Maple.

At high temperatures,  $T \rightarrow \infty$ , we should recover the Boltzmann gas situation,

$$\tilde{n}(\mathbf{k}) \approx \left(\frac{\hbar^2 \bar{\omega}^2}{2\pi m \omega_r^2}\right)^{3/2} N e^{-\beta \varepsilon} \quad (\text{Boltzmann}). \tag{25.56}$$

Since  $\varepsilon$  is the kinetic energy, the *rms*-radius  $\sqrt{\langle k^2 \rangle}$  of this distribution is  $\beta \hbar^2 \langle k^2 \rangle = m$ . In comparison,

$$\tilde{n}_B(\mathbf{k}) = \lambda_{dB}^{-3} a_{tr}^6 g_{3/2} \left[ e^{\beta(\mu - \mathbf{p}^2/2m)} \right] \quad (\text{Bose gas above } T_c). \tag{25.57}$$

**Example 114 (Integrated momentum distribution of a Fermi gas):** To integrate the momentum distribution of finite temperature Fermi gas by dimensions,

$$\begin{aligned} \tilde{n}(k_z) &= \frac{1}{(2\pi)^3} \left(\frac{2}{\beta m \tilde{\omega}_{tr}^2}\right)^{3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} \frac{4\pi \tilde{r}^2 d\tilde{r}}{e^{\beta \varepsilon - \beta \mu + \tilde{r}^2} + 1} dk_y dk_x \\ &= \frac{1}{(2\pi)^3} \left(\frac{2}{\beta m \tilde{\omega}_{tr}^2}\right)^{3/2} 2\pi \int_0^{\infty} \int_0^{\infty} \frac{4\pi \tilde{r}^2 d\tilde{r}}{e^{\beta \hbar^2 k_z^2/2m + \beta \hbar^2 k_\rho^2/2m - \beta \mu + \tilde{r}^2} + 1} k_\rho dk_\rho \\ &= \frac{1}{\pi} \left(\frac{2}{\beta m \tilde{\omega}_{tr}^2}\right)^{3/2} \frac{2m}{\beta \hbar^2} \int_0^{\infty} \int_0^{\infty} \frac{\tilde{k}_\rho d\tilde{k}_\rho}{e^{\beta \hbar^2 k_z^2/2m - \beta \mu + \tilde{r}^2 + \tilde{k}_\rho^2} + 1} \tilde{r}^2 d\tilde{r} \\ &= \frac{1}{\pi} \left(\frac{2}{\beta m \tilde{\omega}_{tr}^2}\right)^{3/2} \frac{2m}{\beta \hbar^2} \frac{1}{2} \int_0^{\infty} \tilde{r}^2 \ln \frac{1}{1 + e^{-\beta \hbar^2 k_z^2/2m + \beta \mu - \tilde{r}^2 - k_\rho^2}} \Big|_0^{\infty} d\tilde{r} \\ &= \frac{2}{\pi (\beta \hbar \tilde{\omega}_{tr})^2} \left(\frac{2}{\beta m \tilde{\omega}_{tr}^2}\right)^{1/2} \int_0^{\infty} \tilde{r}^2 \ln \left(1 + e^{\beta \mu - \beta \hbar^2 k_z^2/2m - \tilde{r}^2}\right) d\tilde{r}. \end{aligned} \tag{25.58}$$

### 25.2.4.3 Time-of-flight distribution

To describe time-of-flight images we substitute  $\mathbf{k} = m\mathbf{r}/\hbar t$ . We obtain the density distribution from a convolution,

$$\begin{aligned} n_{ToF}(\mathbf{x}, t) &= \frac{1}{(2\pi)^3} \int d^3 \mathbf{x}_0 d^3 \mathbf{k} \frac{\delta^3(\mathbf{x} - \mathbf{x}_0 - \mathbf{p}t/m)}{e^{\beta(H(\mathbf{x}_0, \mathbf{p}) - \mu)} + 1} \\ &= \frac{1}{(2\pi)^3} \int \frac{d^3 \mathbf{k}}{e^{\beta(H(\mathbf{x} + \mathbf{p}t/m, \mathbf{p}) - \mu)} + 1} \\ &= \frac{1}{(2\pi)^3} \int \frac{dk_x dk_y dk_z}{e^{\beta \Sigma_j [\hbar^2 k_j^2/2m + \frac{1}{2} m \omega_j^2 (x_j + \hbar k_j t/m)^2]} / Z + 1}. \end{aligned} \tag{25.59}$$

We rewrite the exponent,

$$\begin{aligned}
 \hbar^2 k_j^2 / 2m + \frac{1}{2} m \omega_j^2 (x_j + \hbar k_j t / m)^2 &= \hbar^2 k_j^2 / 2m (1 + \omega_j^2 t^2) + \omega_j^2 t x_j \hbar k_j + \frac{1}{2} m \omega_j^2 x_j^2 \\
 &= \left( \sqrt{\frac{\hbar^2 k_j^2}{2m} (1 + \omega_j^2 t^2)} + \frac{\omega_j^2 t x_j \sqrt{2m}}{2\sqrt{1 + \omega_j^2 t^2}} \right)^2 + \frac{m \omega_j^2 x_j^2}{2(1 + \omega_j^2 t^2)} \\
 &= \xi_j + \frac{m}{2} \tilde{\omega}_j^2 x_j^2 .
 \end{aligned} \tag{25.60}$$

where we define  $\tilde{\omega}_i \equiv \omega_i (1 + \omega_i^2 t^2)^{-1/2}$ . With the substitution  $d\xi_j = dk_j \sqrt{\frac{2\hbar^2}{m} \xi_j (1 + \omega_j^2 t^2)}$  we obtain

$$\begin{aligned}
 n_{T_oF}(\mathbf{x}, t) &= \frac{1}{(2\pi)^3} \left( \frac{mk_B T}{2\hbar^2} \right)^{3/2} \frac{1}{\prod_i (1 + \omega_i^2 t^2)} \int \frac{\beta^{3/2} (\xi_x \xi_y \xi_z)^{-1/2} d\xi_x d\xi_y d\xi_z}{e^{\beta \Sigma_j [\xi_j + \frac{m}{2} \tilde{\omega}_j^2 x_j^2]} / Z + 1} \\
 &= \frac{1}{2^3 \pi^{3/2}} \frac{1}{\lambda_{dB}^3} \frac{\tilde{\omega}^3}{\bar{\omega}^3} \int \frac{\beta^{3/2} \xi^{-3/2} 4\pi \xi^2 d\xi}{e^{\beta \Sigma_j [\xi + \frac{m}{2} \tilde{\omega}_j^2 x_j^2]} / Z + 1} ,
 \end{aligned} \tag{25.61}$$

where  $\bar{\omega} \equiv (\omega_x \omega_y \omega_z)^{1/3}$  and  $\tilde{\omega} \equiv (\tilde{\omega}_x \tilde{\omega}_y \tilde{\omega}_z)^{1/3}$ .

$$\boxed{n_{T_oF}(\mathbf{x}, t) = \frac{1}{\lambda_{dB}^3} \frac{\tilde{\omega}^3}{\bar{\omega}^3} f_{3/2} \left( e^{\beta \mu - \frac{1}{2} \beta m \Sigma_j \tilde{\omega}_j^2 x_j^2} \right)} . \tag{25.62}$$

For long times-of-flight  $t \gg \omega^{-1}$ ,

$$n_{T_oF}(\mathbf{x}, t) = \frac{1}{\lambda_{dB}^3} \frac{1}{\bar{\omega}^2 t^2} f_{3/2} \left( e^{\beta(\mu - m\mathbf{x}^2/2t^2)} \right) = \left( \frac{m}{\hbar t} \right)^3 \tilde{n}(m\mathbf{x}/t) . \tag{25.63}$$

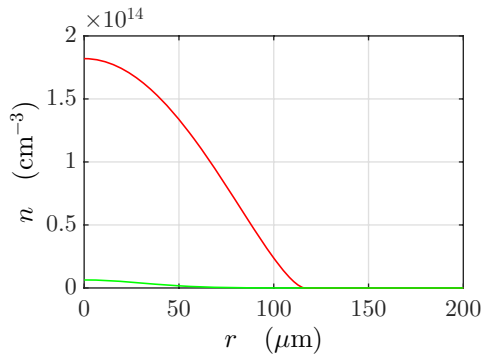


Figure 25.8: (code) Time-of-flight velocity distribution of (red) a Li Fermi gas at  $T = 0$  with vanishing initial spatial distribution [115] and (green) a thermal gas at  $T = T_F$ .

At low temperatures,

$$\begin{aligned} n_{T_oF}(\mathbf{x}, t) &= \left(\frac{m}{\hbar t}\right)^3 \frac{N}{K_F^3} \frac{8}{\pi^2} \left(1 - \frac{(m\mathbf{x}/\hbar t)^2}{K_F^2}\right)^{3/2} \\ &= \left(\frac{m}{\hbar t}\right)^3 \frac{R_F^3}{6\pi^2\lambda} \left[1 - \left(\frac{R_F m\mathbf{x}/\hbar t}{(48N\lambda)^{1/3}}\right)^2\right]^{3/2} \end{aligned} \quad (25.64)$$

At high temperatures,

$$\begin{aligned} n_{T_oF}(\mathbf{x}, t) &= \frac{1}{\lambda_{dB}^3} \frac{1}{\bar{\omega}^2 t^2} f_{3/2}(e^{\beta(\mu - m\mathbf{x}^2/2t^2)}) \\ &\approx \frac{1}{\lambda_{dB}^3} \frac{1}{\bar{\omega}^2 t^2} e^{\beta(\mu - m\mathbf{x}^2/2t^2)} \\ &\approx \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3/2} \frac{1}{\bar{\omega}^2 t^2} N \left(\frac{\hbar\bar{\omega}}{k_B T}\right)^3 e^{-\beta m\mathbf{x}^2/2t^2} \approx N \frac{\bar{\omega}}{t^2} \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\beta m\mathbf{x}^2/2t^2} . \end{aligned} \quad (25.65)$$

A *rms*-width is,

$$\begin{aligned} \langle r_{T_oF}^2 \rangle &= \int r^2 n_{T_oF}(\mathbf{x}, t) d^3\mathbf{x} \\ &= \frac{1}{\lambda_{dB}^3} \frac{\bar{\omega}^3}{\bar{\omega}^3} \int r^2 f_{3/2}\left(e^{\beta\mu - \frac{1}{2}\beta m \Sigma_j \bar{\omega}_j^2 x_j^2}\right) d^3\mathbf{x} \\ &= \frac{2}{m\bar{\omega}_r^2 N} \int \frac{\varepsilon g(\varepsilon) d\varepsilon}{e^{\beta(\varepsilon - \mu)} + 1} = \frac{k_B T}{m\bar{\omega}_r^2} \frac{g_4(Z)}{g_3(Z)} . \end{aligned} \quad (25.66)$$

This shows that the width of the flight-of-time distribution can simply be obtained from the spatial distribution by substituting  $\omega \rightarrow \omega/\sqrt{1 + \omega^2 t^2}$ . Of course this does not hold for condensed gases Bose.

### 25.2.5 Equipartition theorem

We find for harmonic traps,

$$\begin{aligned} E_{pot,1} &= \frac{\int U(\mathbf{x}) w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3\mathbf{x} d^3\mathbf{k}}{\int w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3\mathbf{x} d^3\mathbf{k}} = \frac{1}{(2\pi)^3 N 2} \int \frac{m\omega^2 r^2 d^3\mathbf{x} d^3\mathbf{k}}{e^{\beta[\hbar^2 k^2/2m + m\omega^2 r^2/2 - \mu]} + 1} \\ &= \frac{16}{\pi N \beta^4 (\hbar\omega)^3} \int \frac{u^4 v^2 du dv}{e^{u^2+v^2}/Z + 1} \\ &= \frac{1}{(2\pi)^3 N 2m} \int \frac{\hbar^2 k^2 d^3\mathbf{x} d^3\mathbf{k}}{e^{\beta[\hbar^2 k^2/2m + m\omega^2 r^2/2 - \mu]} + 1} = \frac{\int \hbar^2 k^2 w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3\mathbf{x} d^3\mathbf{k}}{2m \int w_{T,\mu}(\mathbf{x}, \mathbf{k}) d^3\mathbf{x} d^3\mathbf{k}} = E_{kin,1} . \end{aligned} \quad (25.67)$$

This confirms the *equipartition theorem* for confined particles, which postulates,

$$E = E_{kin} + E_{pot} = 2E_{kin} . \quad (25.68)$$

In flight time, however,  $E_{pot}$  suddenly vanishes.

### 25.2.5.1 Calibrating the number of atoms

Experimentally, to calibrate  $N$ , we can use either the measured value of  $\langle k^2 \rangle$  at  $T = 0$ , which gives  $\mu = E_F = 4E/3$  and consequently,

$$N = \frac{32}{3} \left( \frac{\hbar^2 \langle k^2 \rangle}{6m\hbar\bar{\omega}} \right)^3. \quad (25.69)$$

Or we determine the temperature  $T_g$  where the Boltzmann gas turns into a Fermi gas  $3\mu/4 = 3k_B T_g$ ,

$$N = \frac{32}{3} \left( \frac{k_B T_g}{\hbar\bar{\omega}} \right)^3. \quad (25.70)$$

## 25.2.6 Density and momentum distribution for anharmonic potentials

### 25.2.6.1 Width of momentum distribution for anharmonic potentials

If the potential is non-harmonic, the widths of Fermi distributions must in general be calculated numerically. I.e. first  $g(\epsilon)$  is determined by integrating for every value of  $\epsilon$  the root  $\sqrt{\epsilon - U(\mathbf{x})}$  over the entire volume, where  $U(\mathbf{x}) < \epsilon$ , i.e. in the case of cylindrical symmetry,

$$g(\epsilon) = \frac{(2m)^{3/2}}{2\pi\hbar^3} \int \sqrt{\epsilon - U(r, z)} r dr dz. \quad (25.71)$$

Second the chemical potential must also be calculated numerically from  $N = \int g(\epsilon) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon$  by minimizing the function,

$$o(Z) = \left| \beta N - \int \frac{g(x/\beta) dx}{e^{x/Z} + 1} \right|. \quad (25.72)$$

Finally, the *rms*-momentum width of a degenerate Fermi-gas is calculated from,

$$\frac{\langle k^2 \rangle}{k_F^2} = \frac{E_1}{E_F} = \frac{1}{NE_F} \int \frac{\epsilon g(\epsilon) d\epsilon}{e^{\beta(\epsilon-\mu)} + 1}. \quad (25.73)$$

It is important to note that the temperature cannot be obtained from  $\hbar^2 \langle k^2 \rangle / 2m = 3Nk_B T$  any more. Rather for a given  $\langle k^2 \rangle$  the parameter  $\beta$  in the integral (25.71) must be fitted to satisfy the equation.

Alternatively, we may assume a polynomial potential for which the density of states can be described by  $g(\epsilon) \propto \epsilon^n$ . Then,

$$\frac{\langle k^2 \rangle}{k_F^2} = \frac{1}{E_F} \frac{\int \epsilon g(\epsilon) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon}{\int g(\epsilon) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon} = \frac{T}{T_F} \frac{(n+1)f_{n+2}(Z)}{f_{n+1}(Z)}, \quad (25.74)$$

For a harmonic potential we recover the energy formula,

$$\frac{\langle k^2 \rangle}{k_F^2} = \frac{3T}{T_F} \frac{f_4(Z)}{f_3(Z)}, \quad (25.75)$$

and for hot clouds the classical limit holds,

$$\frac{\langle k^2 \rangle}{k_F^2} = \frac{n+1}{\beta E_F} . \quad (25.76)$$

Must for a single dimension the value be divided by three?  $\hbar^2 \langle k_j^2 \rangle = 2mk_B T f_4(Z)/f_3(Z)$  setting  $\epsilon = \hbar^2 k^2/m$ .

For a harmonic potential  $g(\epsilon) \propto \epsilon^2$  and for a linear potential  $g(\epsilon) \propto \epsilon^{7/2}$ . Intermediate values are possible for non isotropic traps, which are linear in some directions and harmonic in others, e.g. for a radially quadrupolar and axially harmonic trap, we expect  $g(\epsilon) \propto \epsilon^3$  and thus  $E = 4Nk_B T$ . In general, we may have more complicated situations, where the trap becomes non-harmonic beyond a certain distance from the origin. In those cases, the density of states may be approximated by series,

$$g(\epsilon) \propto \epsilon^2 + \eta \epsilon^3 , \quad (25.77)$$

where  $\eta$  is a small parameter, so that,

$$\frac{\langle k^2 \rangle}{k_F^2} = \frac{1}{E_F} \frac{\int (\epsilon^3 + \eta \epsilon^4) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon}{\int (\epsilon^2 + \eta \epsilon^3) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon} = \frac{T}{T_F} \frac{3f_4(Z) + 12\eta f_5(Z)}{f_3(Z) + 3\eta f_4(Z)} , \quad (25.78)$$

which in the classical limit gives rise to energies  $E = 3.4Nk_B T$  depending on the value of  $\eta$ .

Such effects must be considered when the time-of-flight method is used for temperatures measurements. For example, if we underestimate  $g(\epsilon)$  by assuming a harmonic potential at all  $\epsilon$ , although the potential is quadrupolar at large  $\epsilon \gg k_B T$ , we get a wrong estimate for the temperature  $T_{wrong} = E/3Nk_B$  instead of  $T_{corr} = E/4Nk_B$ .

### 25.2.6.2 Width of the density distribution for anharmonic potentials

The result also permits to calculate the *rms* spatial width,

$$\sum_{j=1}^3 \frac{m}{2} \omega_j^2 \langle x_j^2 \rangle = 3k_B T \frac{f_4(Z)}{f_3(Z)} . \quad (25.79)$$

Let us for simplicity assume  $\omega_i = \omega_j$ . So in the classical limit,

$$\frac{\langle x_j^2 \rangle}{R_F^2} = \frac{\langle \mathbf{x}^2 \rangle}{3R_F^2} = \frac{E_1}{3E_F} = \frac{1.13T}{T_F} . \quad (25.80)$$

If the potential is non-harmonic, the widths of Fermi distributions must in general be calculated numerically. We may use the same results for the density of states and the chemical potential as for the momentum width calculations. Then,

$$\frac{\langle x_j^2 \rangle}{R_F^2} = \frac{E_1}{3E_F} = \frac{1}{3E_F} \frac{\int \epsilon g(\epsilon) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon}{\int g(\epsilon) (e^{\beta(\epsilon-\mu)} + 1)^{-1} d\epsilon} . \quad (25.81)$$

### 25.2.7 Classical gas

For a harmonic potential [174] the fraction of particles with energy smaller than  $\eta k_B T$  is,

$$\begin{aligned} N(\eta) &= \frac{1}{2N(\hbar\bar{\omega})^3} \int_0^{\eta k_B T} \frac{d\epsilon}{e^{\beta\epsilon}/Z - 0} \approx 1 - \frac{2 + 2\eta + \eta^2}{2e^\eta} \\ E(\eta) &= \frac{1}{2N(\hbar\bar{\omega})^3} \int_0^{\eta k_B T} \frac{\epsilon^2 d\epsilon}{e^{\beta\epsilon}/Z - 0} \approx 3 - \frac{6 + 6\eta + 3\eta^2 + \eta^3}{6e^\eta}, \end{aligned} \quad (25.82)$$

while for a quadrupole potential,

$$\begin{aligned} N(\eta) &\approx -2\sqrt{z} \frac{105 + 70\eta + 28\eta^2 + 8\eta^3}{\sqrt{\pi}105e^\eta} + \text{erf}(\sqrt{\eta}) \\ E(\eta) &\approx -\frac{2}{9}\sqrt{z} \frac{945 + 630\eta + 252\eta^2 + 72\eta^3 + 16\eta^4}{\sqrt{\pi}105e^\eta} + \frac{9}{2}\text{erf}(\sqrt{\eta}). \end{aligned} \quad (25.83)$$

#### 25.2.7.1 Momentum distribution for a classical gas

For high temperatures,  $T \rightarrow \infty$ , we should recover the ideal Boltzmann gas situation,  $f_{3/2} \rightarrow id$ ,

$$\begin{aligned} \tilde{n}_{T \rightarrow \infty}(\mathbf{k}) &= \frac{1}{(2\pi)^3} \int \frac{4\pi\rho^2 d\rho}{e^{\beta[\epsilon + m\omega_{tr}^2 \rho^2/2 - \mu]}} = \frac{1}{2\pi^2} e^{-\beta(\epsilon - \mu)} \int e^{-\beta m\omega_{tr}^2 \rho^2/2} \rho^2 d\rho \\ &= \left( \frac{1}{2\pi\beta m\omega_{tr}^2} \right)^{3/2} e^{-\beta(\epsilon - \mu)} = \lambda_{dB}^{-3} a_{tr}^6 e^{\beta(\mu - \epsilon)}. \end{aligned} \quad (25.84)$$

Since the chemical potential satisfies the normalization,  $\int \tilde{n}_{T \rightarrow \infty}(\mathbf{k}) d^3\mathbf{k} = 1$ ,

$$\tilde{n}_{T \rightarrow \infty}(\mathbf{k}) = \left( \frac{1}{2\pi\beta m\omega_{tr}^2} \right)^{3/2} N \left( \frac{\hbar\omega_{tr}}{k_B T} \right)^3 e^{-\beta\epsilon} = N \sqrt{\frac{\hbar^2}{2\pi m k_B T}} e^{-\hbar^2 k^2 / 2m k_B T}. \quad (25.85)$$

This is easy to integrate by dimensions, so that,

$$\tilde{n}_{T \rightarrow \infty}(k_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{n}_{T \rightarrow \infty}(\mathbf{k}) dk_x dk_y = N \sqrt{\frac{\hbar^2}{2\pi m k_B T}} e^{-\hbar^2 k_z^2 / 2m k_B T}. \quad (25.86)$$

The rms-width of this distribution is,

$$\Delta k_z = \frac{\sqrt{m k_B T}}{\hbar}. \quad (25.87)$$

#### 25.2.7.2 Correlating fluctuations in the number of atoms

Experimentally the atom number will fluctuate. To minimize this problem we can renormalize it to a norm number  $N_{norm}$  by multiplying the measured time-of-flight



variance  $\langle x_{tof}^2 \rangle$  with,

$$\begin{aligned} C_T(N) &= \frac{\langle \tilde{x}_{tof}^2 \rangle}{\langle x_{tof}^2 \rangle} = \frac{N}{N_{norm}} \frac{f_4(\tilde{Z})}{f_4(Z)} \\ &= \frac{N}{N_{norm}} \frac{f_4[f_3^{-1}(N_{norm}(\beta\hbar\bar{\omega})^3)]}{f_4[f_3^{-1}(N(\beta\hbar\bar{\omega})^3)]}. \end{aligned} \quad (25.88)$$

### 25.2.8 Intensive and extensive parameters

The distinction between an *intensive parameter* and an *extensive parameter* is based on the concept that the system under investigation can be subdivided into smaller, identical and non-interconnected entities within which the parameter in question has the same properties, such that this parameter does not change, when the system is divided or subentities are combined.<sup>6</sup> An intensive property is a global property, meaning that it is a physical property of a system that does not depend on the system size or the amount of material in the system. Examples of intensive properties are the temperature and the hardness of an object. No matter how small a diamond is cut, it maintains its intrinsic hardness.

By contrast, an extensive property is one that is additive for independent, non-interacting subsystems. The property is proportional to the amount of material in the system. For example, both the mass and the volume of a diamond are directly proportional to the amount that is left after cutting it from the raw mineral. Mass and volume are extensive properties, but hardness is intensive.

The ratio of two extensive properties, such as mass and volume, is scale-invariant, and this ratio, the density, is hence an intensive property.

Intensive parameter are: chemical potential, concentration, density (or specific gravity), ductility, elasticity, electrical resistivity, hardness, magnetic field, magnetization, malleability, melting point and boiling point, molar absorptivity, pressure, specific energy.

Extensive parameter are: energy, entropy, Gibbs energy, length, mass, particle number, momentum, number of moles, volume, magnetic moment, electrical charge, weight.

### 25.2.9 Signatures for quantum degeneracy of a Fermi gas

Whether an atom is a *fermion* or a *boson* uniquely depends on its total spin. Halfinteger spin particles are fermions, integer spin particles are bosons. E.g. Rb atoms have in the ground state  $J = 1/2, I = 7/2$ , integer  $F$ , and are therefore bosons.  $\text{Ca}^+$  ions have  $J = 1/2$  and no hyperfine structure so that  $F$  is halfinteger, and are therefore fermions.  ${}^6\text{Li}$  has half-integer  $F$  and is a boson.

For a *composite particle* the quantum statistical nature may depend on the interaction strength of the partners. For weak interaction, e.g. Feshbach the total spins of the partners will couple to a total total spin, which determines the nature of the composite particle. A fermion pairing with a fermion or a boson pairing with a boson will

<sup>6</sup>How to derive the thermodynamic potentials from the macrocanonical partition function? How to calculate pressure and volume? [check thermodynamic derivations from Romero-Rochin [see Freddy's thesis].

be bosons. A fermion pairing with a boson will be a fermion. Composite trimers may be either bosonic or fermionic depending on the coupling scheme. Can the quantum nature change with the tightness of the binding? What is the total spin of a deeply bound molecule? [573, 98, 269], [?, 336, 545, ?]

### 25.2.9.1 Optical density of a Fermi gas

With the local density of a Fermi gas,

$$n_{loc} = \frac{k_F^3}{3\pi^2} \quad (25.89)$$

the *optical density* is at  $T = 0$ ,

$$\begin{aligned} \int \sigma ndy &= \frac{8\sigma}{\pi^2} \frac{N}{R_F^3} \int_{-R_F}^{R_F} \left(1 - \frac{x^2 + y^2}{R_F^2} - \frac{z^2}{Z_F^2}\right)^{3/2} dy \\ &= \frac{8\sigma}{\pi^2} \frac{N}{R_F^3} \left(1 - \frac{x^2}{R_F^2} - \frac{z^2}{Z_F^2}\right)^{3/2} \int_{-R_F}^{R_F} \left(1 - \frac{y^2}{R_F^2 - x^2 - R_F^2 z^2 / Z_F^2}\right)^{3/2} dy. \end{aligned} \quad (25.90)$$

Writing  $a = R_F / \sqrt{R_F^2 - x^2 - R_F^2 z^2 / Z_F^2}$ ,

$$\begin{aligned} \int \sigma ndy &= \frac{8\sigma}{\pi^2} \frac{N}{R_F^2 a^4} \int_{-a}^a (1 - \tilde{y}^2)^{3/2} d\tilde{y} \\ &= \frac{2\sigma}{\pi^2} \frac{N}{R_F^2 a^4} \left(9a\sqrt{1 - a^2} - 2a^3\sqrt{1 - a^2} + 3\arcsin a\right). \end{aligned} \quad (25.91)$$

In the center,  $a = 1$ ,

$$\int \sigma ndy = \frac{3N\sigma}{\pi R_F^2} = \frac{9m\omega_r^2 N}{k_L^2 E_F}, \quad (25.92)$$

such that for  $E_F \simeq 1\mu\text{K}$  we expect  $n_{loc} \simeq 4 \times 10^{12} \text{ cm}^{-3}$ .

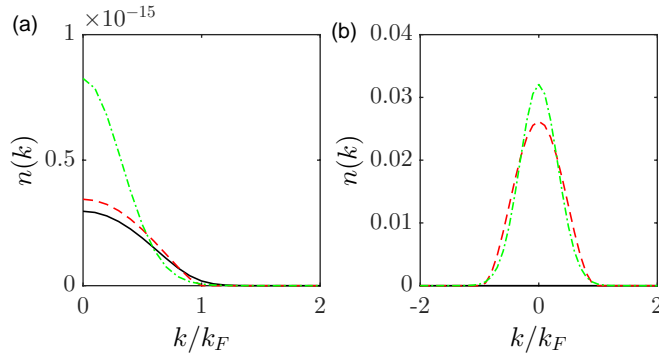


Figure 25.9: (code) (a) Radial momentum distribution and (b) distribution of momentum classes in the direction of  $k_z$  for a Fermi gas at  $T/T_F = 0.2 \mu\text{K}$  (solid), a classical gas (dash-dotted), and a Fermi gas at  $T = 0$  (dashed).

### 25.2.9.2 Superfluid suppression of sympathetic cooling

The fermions inside the bosonic cloud can be regarded as impurities. If they travel too slow,  $v < c$ , and if the condensed fraction is too large, the motion will be frictionless and thermalization stops. If they travel fast, quasiparticles are excited, which can be removed by evaporation. With the typical velocity of sound in the BEC  $c = \hbar\sqrt{16\pi na}/2m_B \approx 2 \text{ mm/s}$ , or  $\frac{m}{2}c^2 \approx k_B \times 20 \text{ nK}$ , we see that this is no real danger.

### 25.2.9.3 Component separation

If the interspecies interaction  $h$  is stronger than the inter-bosonic interaction, the components may separate [524]. Otherwise a small fermionic cloud stays inside the BEC.

### 25.2.9.4 Excess energy modifies 2<sup>nd</sup> moment

Independent on any model, just look deviation from Gaussian (interaction energy plays no role for the fermions). Also calculate the 2<sup>nd</sup> moment  $U = \int E_{kin}(k)n(k)dk$ , where  $n(k)$  is measured in time-of-flight and  $E_{kin} = \hbar^2 k^2/2m$ .

### 25.2.9.5 Modification of light scattering

The unavailability of final momentum states inhibits scattering in a similar way as the Lamb-Dicke effect. Forward scattering is suppressed, because all small momentum states are occupied. Furthermore, spontaneous emission is suppressed like in photonic band gaps. However, here it is rather an atomic momentum band gap. Could it be that because scattering is suppressed, in-situ images of fermions are hampered?

A condition for this effect to play a role is  $k_{rec} \ll k_F$ . For Li the temperature must be  $k_B T_F = \hbar^2 k_F^2/2m = \hbar\bar{\omega}(6N)^{1/3} \gg \hbar^2 k_L^2/2m \approx k_B \times 3 \mu\text{K}$ . I.e. we need quite large Fermi gases.

### 25.2.9.6 Hole heating

Loss processes that remove particles from an atom trap leave holes behind in the single particle distribution if the trapped gas is a degenerate fermion system. The appearance of holes increases the temperature, because of an increase in the energy share per particle if cold particles are removed. Heating is significant if the initial temperature is well below the Fermi temperature. Heating increases the temperature to  $T > T_F/4$  after half of the systems lifetime, regardless of the initial temperature. The *hole heating* has important consequences for the prospect of observing Cooper pairing in atom traps.

## 25.2.10 Fermi gas in reduced dimensions

In  $n$  dimensions with the energy  $\varepsilon = ap^s + br^t$  [?] we have to generalize the results of the last chapter,

$$N = g \frac{\Gamma\left(\frac{n}{s} + 1\right) \Gamma\left(\frac{n}{t} + 1\right)}{(2\hbar)^n a^{n/s} b^{n/t} \Gamma\left(\frac{n}{2} + 1\right)^2} (k_B T)^{n/s+n/t} f_{n/s+n/t}(z). \quad (25.93)$$

This gives for a harmonic trap where  $\varepsilon = \frac{1}{2m}p^2 + \frac{m}{2}\omega^2 r^2$  and with the spin degeneracy factor  $g = 1$ ,

$$N = \left( \frac{k_B T}{\hbar\omega} \right)^n f_n(z) . \quad (25.94)$$

The Fermi energy again follows from Sommerfeld's expansion,

$$E_F = (n!N)^{1/n} \hbar\omega . \quad (25.95)$$

We now assume a 1D potential  $V = \frac{m}{2}\omega_z^2 r^2$  embedded in a 3D trap. A true 1D situation arises when the atoms occupy all low-lying axial levels with the lowest radial vibrational quantum number, i.e.  $E_F \ll \hbar\omega_r$  which gives,

$$N \ll \frac{\omega_r}{\omega_z} . \quad (25.96)$$

Such quantum degenerate 1D fermion gases realize the so-called *Luttinger liquid*. One of the hallmarks of Luttinger liquids is *spin-charge separation*.

**Example 115 (Estimations for 1D):** Let us consider a Fermi gas in a very elongated microtrap:  $\omega_r = \sqrt{\frac{87}{7}} 2\pi \times 1.4$  kHz and  $\omega_z = \sqrt{\frac{87}{7}} 2\pi \times 15$  Hz for Rb. With  $N_{Li} = 10^5$  the Fermi temperature is as high as  $T_F \simeq 5$   $\mu$ K. However we need  $N \ll 100$  to see 1D features. Assume  $\varepsilon = \frac{1}{2m}p^2 + \frac{m}{4}b^4 r^4$ ,

$$N = \frac{1}{(\hbar b)^n} \frac{\Gamma(\frac{n}{4} + 1)}{\Gamma(\frac{n}{2} + 1)} (k_B T)^{3n/4} f_{3n/4}(z)$$

$$E_F \approx (\hbar b)^{4/3} \left( N \frac{\Gamma(\frac{n}{2} + 1) \Gamma(\frac{3n}{4} + 1)}{\Gamma(\frac{n}{4} + 1)} \right)^{4/3n} .$$

In 1D,

$$N = \frac{1.02}{\hbar b} (k_B T)^{3/4} f_{3/4}(z)$$

$$E_F \approx 0.87 (N \hbar b)^{4/3} .$$

## 25.2.11 Exercises

### 25.2.11.1 Ex: Li Fermi gas

Programs on Li Fermi gases.

## 25.3 Further reading

V.S. Bagnato et al., *Bose-Einstein Condensation in an External Potential* [DOI]

D.A. Butts et al., *Trapped Fermi gases* [DOI]



## Chapter 26

# Bose-Einstein condensation

The experimental verification of Bose and Einstein's prediction was for a long time a cherished dream of many physicists. On the one hand, several phenomena have been related to BEC in the past, for example, the phenomenon of superfluidity in liquid helium and superconductivity. On the other hand, these strongly interacting systems are not pure enough to clearly identify the role of BEC. In 1995, however, Bose-Einstein condensation of weakly interacting confined atomic gases was achieved in several laboratories [16, 175, 103, 307]. This success gave rise to a revolution in atom optics documented in an enormous amount of theoretical and experimental work. While initial work focused on the equilibrium thermodynamics of condensates near the phase transition, very soon the dynamic response of condensates to perturbations was the subject of in-depth investigations, followed by the study of superfluid characteristics, quantum transport phenomena, the interaction of condensates with light, of condensed gas mixtures [514, 662], and the behavior of condensates in periodic potentials. To name only a few landmarks, we mention the creation of vortices [463, 448] and quantum turbulence [326], the realization of various types of atom lasers [476, 15, 80, 300] and atom interferometers with condensates [303, 409], the coherent amplification of matter waves [352, 412, 354, 189], the creation of the Mott insulating states in optical lattices [280], the study of condensates in reduced dimensions [504], the Anderson localization of atomic matter waves [126, 580], the observation of Feshbach type collision resonances [155, 351, 703] and Efimov states [413, 50], the creation of homonuclear molecular [281, 374, 160, 753, 738, 328] and heteronuclear condensates [531] and degenerate Fermi gases [183], the observation of BCS type pairing [337, 282], the observation of matter wave superradiance [352] and the interaction of condensates with optical cavities [640, 117] and with surfaces [59].

It is clearly unthinkable to discuss all matters in this course. Let us, however, give a basic and practical introduction to atomic optics with condensates.

### 26.1 Bose-Einstein condensation of dilute gases

The challenge of the experimental realization of Bose-Einstein condensation is the preparation of a very dense sample of very cold atoms. In practice, the first step consists in providing an atomic gas, for example, of an alkali metal. This is done by heating the metal in an oven (or sometimes in a dispenser). The atoms being ejected from the metal and forming a hot gas are then forced through a nozzle out of the oven, where they form a hot atomic beam. Some experiments employ a *Zeeman*

*slower*, which is a device that decelerates the fast atoms of the beam by means of a counterpropagating laser exerting a radiative pressure force. A position-dependent magnetic field applied along the trajectory of the atoms is calculated in order to compensate for the Doppler decreasing shift of the decelerated atoms and to ensure that the laser always stays in resonance with an atomic transition (see Exc. 14.4.6.3). Velocities around 30 m/s are realistic and low enough to allow the capture of the atoms by a magneto-optical (MOT) trap. Usually, some  $10^9$  atoms are captured in a few seconds.

MOTs do not only trap atoms, but simultaneously cool them down to the Doppler limit of typically some  $10\ \mu\text{K}$ . Quasi-resonant optical traps, such as MOT, are afflicted by the problem of radiation trapping (see Sec. 24.3.1), which limits the densities of atomic clouds to typically  $10^{11}\ \text{cm}^3$ . This corresponds (at temperatures close to the Doppler limit) to phase space densities several orders of magnitude away from the threshold to Bose-Einstein condensation. For this reason, the atoms are transferred from the MOT to a potential exempt of radiative pressure force, for example, an optical dipole potential or a magnetic trap.

Once the atoms are confined in such a conservative potential, all the light beams are turned off, and the technique of evaporative cooling is activated (see Sec. 24.4.3). That is, the effective potential is deformed (for example, by an irradiated radiofrequency) in a way to skim out hot atoms and leave behind a cooler sample. This however supposes that the atomic cloud finds back to thermal equilibrium afterwards. As the rethermalization happens by elastic collisions, a high atomic density is necessary, which is often achieved via a compression of the trapping potential. In general, 99.9% of the atoms must be sacrificed to condense the rest. Finally, the momentum distribution is imaged after a time of free expansion. This is done by irradiation of a probe laser pulse (see Fig. 24.31). The entire process of producing a condensed cloud usually takes between 10 s and 60 s.

### 26.1.1 Condensate of alkaline gases

The first experimental observation of Bose-Einstein condensation was done with a dilute rubidium gas by Cornell and Wieman at the Joint Institute for Laboratory Astrophysics (JILA) [16]. A group from the University of Texas [307, 156] used rubidium as well. A group led by Ketterle from the Massachusetts Institute of Technology (MIT) created the first sodium condensate. And a group led by Hulet from Rice University opted for lithium [103, 101], which has a slightly negative scattering length,  $a = -27.3a_B$ . In this situation, only small condensates are expected to be stable [591, 668], which explains the observation of a limited number of about 1400 condensed lithium atoms. Meanwhile, Bose-Einstein condensation has been achieved with many other species, such as  $^1\text{H}$  [248],  $^{85}\text{Rb}$  [150],  $^4\text{He}^*$  [584],  $^{133}\text{Cs}$  [646],  $^{39}\text{K}$  [561],  $^4\text{Ne}$  [55],  $^{88}\text{Sr}$  [659], or even molecules [737].

### 26.1.2 Condensation of hydrogen

Hydrogen is a very interesting element to study condensation, because its short scattering length,  $a \approx 1.23a_B$ , makes it an almost ideal gas. Consequently, the three-body collision rate causing losses is weak, even at very high densities. Since the mass of

hydrogen is small, the critical temperature is high. The simplicity of its electronic structure allows precise calculations of the interaction potentials based on fundamental principles, which can thus be tested experimentally.

Twenty years after having started the project of condensing dilute hydrogen gases, Greytak and Kleppner [248] crossed the phase transition at a temperature of  $50 \mu\text{K}$  with an atomic density of  $5 \times 10^{15} \text{ cm}^{-3}$ . The number of condensed atoms was  $10^9$ , which corresponds to a condensed fraction below 10%<sup>1</sup>. The condensed cloud had a needle-like shape of  $15 \mu\text{m}$  diameter and 5 mm length. It was detected by an *in situ* measurement technique of the atomic velocity distribution.

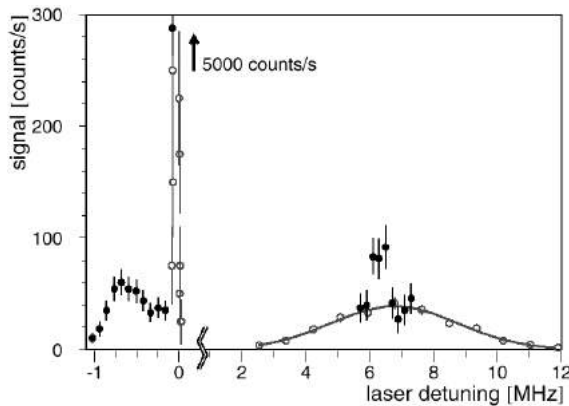


Figure 26.1: Spectrum of condensed hydrogen.

### 26.1.3 Recognizing Bose-Einstein condensates

'How to recognize the presence of a condensate, what are its signatures?' We have already seen in Sec. 25.1.4 that, trapped inside a confinement potential, an ultracold ideal Bose-gas has a modified density distribution when Bose-Einstein statistics come into play. Below the critical temperature the density distribution is well described by a superposition of a condensed cloud concentrated in the trap's ground state and a thermal cloud distributed over several vibrationally excited states. We thus expect distinct distribution functions for both clouds, and the same is true for the momentum distribution. The splitting of the distribution functions in two fractions occurs abruptly during the phase transition to quantum degeneracy. In a real gas, however, the interatomic collisions have a drastic influence on the distribution functions and the behavior of the gas at the phase transition, and we are obliged to develop a more general theory in order to quantitatively understand the thermodynamic properties (temperature, critical point, heat capacity, ...) through the measured static quantities (density, number of atoms, condensed fraction, ...).

'What observables can be measured in the laboratory?' In fact, with few exceptions, the only accessible quantity is the *spatial density distribution* of the atomic cloud

<sup>1</sup>When the condensed fraction and the density are too high, losses induced by dipolar spin-flip processes predominate over the gain due to evaporative cooling of the thermal cloud [334].



$n(\mathbf{r})$  measured after a time of ballistic expansion. Information on non-trivial properties of the condensate, for example, its dynamic behavior (excitations, superfluidity, turbulence, ...) or its coherent features (phase, correlations, ...), can only be gathered through an observation of the condensate's response to applied perturbations. Solve the Excs. 26.1.5.1 and 26.1.5.2.

### 26.1.4 Photon condensation

An interesting question is that of the possibility of *photon condensation* and its relationship to the laser. The relationship is not that obvious because, on one hand atomic condensates are produced by evaporating an ensemble in constant thermal equilibrium, while on the other hand the photonic laser requires inversion, which is a highly non-equilibrium situation. And under the constraint of having to reduce its energy, a photon gas trapped in an optical cavity has the simpler alternative to let photons escape into the void by annihilating them on the cavity walls, as it happens for black-body radiation. Since the number of photons in a cavity is not conserved, the chemical potential disappears,  $\mu = 0$ . The density of states can be written,

$$u(\nu) = \frac{8\pi V}{c^3} \frac{E^2 dE}{h^2} . \quad (26.1)$$

It is the same as in the Debye model. Planck's formula now follows from,

$$u(\epsilon)d\epsilon = \frac{1}{V} \epsilon f_{BE}(\epsilon) \rho(\epsilon) d\epsilon , \quad (26.2)$$

where  $f_{BE}$  is the Bose-Einstein distribution. Hence, the treatment of the photons as indistinguishable particles following the Bose-Einstein distribution is equivalent to assuming a Boltzmann distribution for waves with quantized energies.

Nevertheless, one can imagine a photonic gas in thermal equilibrium with an atomic gas through Compton scattering [390]. In fact, photon condensation was observed experimentally [399]. Also, there are theories about superfluid photon gases [130]<sup>2</sup>.

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<sup>2</sup>*Bose-Einstein condensation occurs in thermal equilibrium when entropy is maximized by putting a macroscopic population of atoms into the ground state of the system. It might appear counter-intuitive that an apparently highly ordered state as the Bose condensate maximizes entropy. However, only the particles in excited states contribute to the entropy. Their contribution is maximized at a given total energy by forming a Bose condensate in the ground state and distributing the remaining atoms among higher energy states. A macroscopic population of atoms in the ground state of the system is achieved simply by lowering the temperature of the sample. This is in contrast to the optical laser where a non-equilibrium process is necessary to place a macroscopic population of photons in a single mode of the electromagnetic field. This is due to the fact that, unlike photons, the number of atoms is conserved. For bosonic atoms, the lowest entropy state below a certain temperature includes a macroscopic population of the ground state. In contrast, when one cools down a blackbody cavity, the cavity empties. Photons do not Bose condense into the ground state of the cavity, but are absorbed by the walls. The absorbed energy leads to a larger entropy than forming a Bose condensate. The laser phenomenon requires inversion of the active medium characterized by a 'negative' temperature. In that sense, 'lasing' of atoms is a simpler phenomenon than lasing of light –all you need to do is cool a gas! However, if a photon gas would thermalize while the number of photons is conserved, it would be described by a Bose-Einstein distribution with non-zero chemical potential and could form a Bose condensate. Thermalization with number conservation is possible, for example, by Compton scattering with a thermal electron gas [390].*

### 26.1.5 Exercises

#### 26.1.5.1 Ex: Condensation of ions

Discuss the possibility of creating Bose-Einstein condensates from ionic clouds.

#### 26.1.5.2 Ex: Isobaric impurities

Discuss the possibility of creating Bose-Einstein condensates with isobaric species.

## 26.2 Quantum theory

As detailed above, interatomic interactions strongly influence the properties of Bose-Einstein condensates, even their density and momentum distributions. For a correct interpretation of the experimental measurements a theoretical many-body treatment taking care of these interactions is compulsory. This is done through a description of the atomic distribution as a *scalar field of matter* called *second quantization*, where the atoms are treated as delocalized Broglie waves. However, we will leave a thorough introduction of this formalism to to [708].

### 26.2.1 Description of the atom as a scalar field

In position space a state with  $n$  particles can be described in a canonically quantized way by a *field operator*,

$$\hat{\Psi}(\mathbf{r}_1, \dots, \mathbf{r}_n, t) = \hat{\psi}^\dagger(\mathbf{r}_1, t) \cdot \dots \cdot \hat{\psi}^\dagger(\mathbf{r}_n, t) \hat{\Psi}_0 \quad , \quad \hat{\psi}(\mathbf{r}) \hat{\Psi}_0 = 0 \quad , \quad (26.3)$$

where  $\Psi_0$  is the vacuum state. The field operators  $\hat{\psi}(\mathbf{r}, t)$  and  $\hat{\psi}^\dagger(\mathbf{r}, t)$  annihilate, respectively create, an atom at position  $\mathbf{r}$  and time  $t$ . This state represents a bosonic Fock state and can be generated from the empty state by a sequence of individual particle creation operators. Applying the notions and rules developed for the harmonic oscillator in Sec. 3.6.1, we can define a coherent state of bosonic matter as,

$$|\hat{\Phi}(t)\rangle = \sum_{n=0}^{\infty} \frac{N^{n/2}}{\sqrt{n!}} |\hat{\Psi}(\mathbf{r}_1, \dots, \mathbf{r}_n, t)\rangle \quad . \quad (26.4)$$

The field operators for particle creation and annihilation are normalized to the number of atoms and satisfy the following commutation rules,

(i)	$[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}') ]_- = 0$
(ii)	$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}') ]_- = \delta^3(\mathbf{r} - \mathbf{r}') \quad , \quad \hat{\psi}^\dagger(\mathbf{r}) = \int d^3r' \hat{\psi}^\dagger(\mathbf{r}') \delta^3(\mathbf{r} - \mathbf{r}')$
(iii)	$[\hat{\psi}(\mathbf{r}), \hat{N} ]_- = \hat{\psi}(\mathbf{r}) \quad , \quad \hat{N} = \int d^3r' \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}')$
(iv)	$[\hat{\psi}(\mathbf{r}), \hat{\mathbf{p}} ]_- = \frac{\hbar}{i} \nabla \hat{\psi}(\mathbf{r}) \quad , \quad \hat{\mathbf{p}} = \int d^3r' \hat{\psi}^\dagger(\mathbf{r}') (\frac{\hbar}{i} \nabla') \hat{\psi}(\mathbf{r}')$
(v)	$[\hat{\psi}(\mathbf{r}), \mathcal{H} ]_- = i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r})$

(26.5)

The last equation is the Heisenberg equation of motion and describes the dynamics of a system whose *many-body Hamiltonian*  $\mathcal{H} \equiv \mathcal{H}_{cm} + \mathcal{H}_{self}$  for  $N$  bosons interacting within an external potential  $V_{trap}$  in second quantization is defined by <sup>3</sup>,

$$\begin{aligned} \mathcal{H}_{cm} &\equiv \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}, t) \right) \hat{\psi}(\mathbf{r}) \\ \mathcal{H}_{self} &\equiv \int d^3r \int d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V_{coll}(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \end{aligned} \quad (26.6)$$

The equations (26.5) and (26.6) represent the foundation of the theory of ultracold bosonic gases. However, to solve the equations, we will need to apply some simplifications, which will be discussed in the following sections. For example, we will generally assume that the temperature of the sample is  $T = 0$ , and that all atoms are condensed. Also, in a first time, we will neglect quantum fluctuations, replacing field operators with complex numbers. And finally, we will need to handle the nonlinear term appearing in  $\mathcal{H}_{self}$  and which signs responsible for collisions between atoms.

## 26.2.2 Quantum scattering at low temperatures

To simplify the term  $\mathcal{H}_{self}$ , we have to go back to Secs. 12.2.5 (and following) and study the phenomenon of the elastic collisions in the ultracold regime. For simplicity, we consider two particles without internal degrees of freedom with masses  $m_1$  and  $m_2$  approaching each other along the  $z$ -axis [141, 714]. Neglecting spin-spin and spin-orbit interactions, the Schrödinger equation in the inertial center-of-mass system is given by (12.115),

$$\left( -\frac{\hbar^2}{2m^*} \nabla^2 + V_{coll}(r) \right) \hat{\psi}(\mathbf{r}) = E \hat{\psi}(\mathbf{r}) , \quad (26.7)$$

where  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  is the momentary interatomic separation,  $r = |\mathbf{r}|$ , and  $m_r \equiv m_1 m_2 / (m_1 + m_2)$  is the reduced mass of atomic collision partners. We assume that the interatomic potential,  $V_{coll}(r)$ , is spherically symmetrical. In the asymptotic limit of large separations <sup>4</sup>, and in the Born-approximation (12.135), the solution of Eq. (26.7) can be seen as the sum of an incident plane wave and a scattered spherical wave modulated with a certain amplitude  $f(\theta)$ ,

$$\psi(\mathbf{r}) = e^{ikz} + f(\theta) \frac{e^{ikr}}{r} , \quad (26.8)$$

where  $k = \sqrt{2m_r E / \hbar^2}$  is the amplitude of the wavevector of the incident and scattered waves and  $\theta$  the angle between  $r$  and  $z$ . The function  $f(\theta)$  is called *scattering amplitude* and determines the scattering cross-section for  $s$ -wave collision through the expression [see (12.123)],

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 . \quad (26.9)$$

<sup>3</sup>Sometimes the *Kamiltonian* is used for canonical and macrocanonic ensembles. It defined by,  $\mathcal{K} = \mathcal{H}_{cm} + \mathcal{H}_{self} - \int d^3\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \mu \hat{\psi}(\mathbf{r})$ , where  $\mu$  is the chemical potential.

<sup>4</sup>This means,  $r \gg r_0$ , where  $r_0$  is the range of potential  $V(r)$ .

where  $d\Omega = \sin\theta d\theta d\phi$  is an element of the solid angle. To calculate the scattering amplitude, we expand the wavefunction (26.8) into spherical partial waves of orders  $\ell$  of the angular momentum, as done in (12.136),

$$f_k(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\cos\theta) e^{i\delta_{\ell}} \sin\delta_{\ell} . \quad (26.10)$$

The collision cross section has been shown in (12.148) to be given by,

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_{\ell} . \quad (26.11)$$

For a potential with finite range, that is, a potential falling faster than  $r^{-3}$  with the distance (interatomic potentials usually fall as  $r^{-6}$  or  $r^{-7}$ ), the phase shift satisfies,

$$\delta_{\ell} \propto k^{2\ell+1} \quad (26.12)$$

for small  $k$ . In ultra-cold gases, the collision energy is very low and  $k \rightarrow 0$ . Thus the scattering will be dominated by terms with  $\ell = 0$ . This is the so-called limit of *s-wave scattering*. In this limit the Eqs. (26.10) can be approximated as,

$$f_k(\theta) = \frac{1}{k} e^{i\delta_0} \sin\delta_0 . \quad (26.13)$$

### 26.2.3 Scattering length

For  $\ell = 0$ , taking the limit  $k \rightarrow 0$ , we define the *scattering length*  $a_s$  via,

$$\frac{\text{Im } f_k(\theta)}{\text{Re } f_k(\theta)} = \tan\delta_0 \equiv -\tan ka_s . \quad (26.14)$$

Therefore, the scattering length and cross section are given at very low temperatures at the asymptotic boundary by,

$$\boxed{a_s = -\frac{\delta_0}{k} \quad \text{and} \quad \sigma = 4\pi a_s^2} . \quad (26.15)$$

The scattering process can be interpreted as follows: During a collision, the system's wavefunction undergoes a phase shift,  $\delta_0$ , which may be positive or negative, depending on the sign of  $a_s$ . If  $a_s < 0$ , the phase is 'delayed' by the collision. This corresponds to an attractive interaction. In contrast, if  $a_s > 0$ , the phase is 'advanced' and the interaction is repulsive. Of course, the intensity of the interaction is proportional to the value of  $|a_s|$ . The expression for  $\sigma$  in Eq. (26.15) indicates, that the atoms behave like *hard spheres* with radius  $|a_s|$ . The specific value of  $a_s$  will depend on the interaction potential, however, the details of the potential are unimportant, as all information about the collision is already contained in  $a_s$ . Consequently, in the low-energy limit, we can assume that the collision is mediated by an effective potential  $V_{coll}(\mathbf{r})$ , which has the particularity,

$$\int V_{coll}(\mathbf{r}) d^3r = \frac{4\pi\hbar^2}{m} a_s \equiv g . \quad (26.16)$$

This has been shown in Sec. 12.1.2. Consequently, the effective interaction between two particles at positions  $\mathbf{r}$  and  $\mathbf{r}'$  can be considered as contact interaction given by <sup>5</sup>,

$$V_{coll}(\mathbf{r}, \mathbf{r}') = \frac{g}{2} \delta(\mathbf{r} - \mathbf{r}') . \quad (26.17)$$

The interatomic interaction potential decides on the value of the scattering length  $a_s$ : A repulsive potential corresponds to a positive  $a_s$ . For a purely attractive potential that does not support bound states  $a_s$  is negative, and for an attractive potential that supports bound states  $a_s$  may be positive or negative depending on the proximity of the last bound vibrational state of the interaction potential below the dissociation limit.

### 26.2.4 The mean field approximation

The *mean-field theory* (MFT) or *local density approximation* (LDA) is based on the assumption of *hard sphere collisions* between atoms (as described by the potential (26.17)) propagating through a locally homogeneous mean-field potential,  $\frac{g}{2} |\hat{\psi}(\mathbf{r})|^2$ . The procedure is also called *regularization of the interaction*.

Thus, the mean-field energy of a condensate is proportional to the density of the gas  $n$  and to a single atomic constant, which is the scattering length  $a_s$ . Its presence in the Gross-Pitaevskii equation emphasizes its impact on shape, dynamic stability and many other properties of the condensate. For example, the mean-field interaction contributes to the broadening of a condensed wavepacket, and consequently contracts its momentum distribution in comparison with an ideal gas. Homogeneous condensates with a negative scattering length are unstable, because the attempt of such a condensate to lower its self-energy by increasing its density also increases the rate of inelastic three-body collisions until the condensate collapses.

### 26.2.5 Gross-Pitaevskii equation

The Heisenberg equation [last line of (26.5)] is equivalent to the *variational principle*, as stated by the Ehrenfest theorem,

$$i\hbar \frac{d\hat{\psi}}{dt} = \frac{\delta \mathcal{H}}{\delta \hat{\psi}^\dagger} . \quad (26.18)$$

This facilitates the derivation of the equation of motion for the atomic field. With the Hamiltonian (26.6) in the mean-field approximation,

$$\mathcal{H}_{atom} \equiv \mathcal{H}_{cm} + \mathcal{H}_{mf} \quad \text{with} \quad \mathcal{H}_{mf} \equiv \int d^3r \hat{\psi}^\dagger(\mathbf{r}, t) \frac{g}{2} |\hat{\psi}(\mathbf{r}, t)|^2 \hat{\psi}(\mathbf{r}, t) , \quad (26.19)$$

we find the *non-linear Schrödinger equation*,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}, t) + g |\hat{\psi}(\mathbf{r}, t)|^2 \right] \hat{\psi}(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t) . \quad (26.20)$$

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<sup>5</sup>The *Hartree-Fock-Bogolubov method* (HFB) for the mean-field theory disregards corrections of higher orders, for example, due to the renormalization of the scattering length. It also neglects quantum depletion due to the correlation effects of the order of  $N_{out}/N = \frac{5}{8} \sqrt{\pi} \sqrt{a^3 n_0}$ . The theory mean-field supposes the validity of the *Born approximation*, that is, two-body correlations are neglected,  $\hat{\psi}(\mathbf{r}') \approx \hat{\psi}(\mathbf{r})$  and  $\int d^3R V_{coll}(\mathbf{R}) = \frac{g}{2}$ .

Remember that, despite their symbol  $\hat{\psi}$ , which usually is associated to wavefunctions, and the fact that they satisfy a non-linear Schrödinger equation the field operators are represented by matrices acting of many-body states. That is, Eq. (26.20) also represents a Heisenberg equation for the field operators.

A common approximation is the *Bogolubov prescription*, where the field operators describing the condensate and its fluctuations are decomposed into a complex function,  $\psi_0(\mathbf{r}) \equiv \langle \hat{\psi}(\mathbf{r}) \rangle$  called *condensed wavefunction*, which can be chosen as the *order parameter* of the system, and a small perturbation,  $\delta\hat{\psi}(\mathbf{r}) \equiv \hat{\psi}(\mathbf{r}) - \psi_0(\mathbf{r})$  describing *thermal excitations*. At zero temperature, we can neglect the excitations [53], and our system is completely described by a single wavefunction,  $\psi_0(\mathbf{r}, t)$ , obeying the famous *Gross-Pitaevskii equation (GPE)*,

$$\left[ \frac{-\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(\mathbf{r}, t) + g|\psi_0(\mathbf{r}, t)|^2 \right] \psi_0(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \psi_0(\mathbf{r}, t). \quad (26.21)$$

### 26.2.5.1 Spontaneous breaking of gauge symmetry

The description of a condensate by a single macroscopic wavefunction means that we attribute a well-defined phase to it. However, the GPE does not allow us to predict, which phase between 0 and  $2\pi$  this will be, and we have to assume, that the BEC chooses its phase spontaneously when it undergoes the phase transition to quantum degeneracy. This principle is called *spontaneous breaking of gauge symmetry*<sup>6</sup>. In Exc. 26.2.6.2 we study the relation between the fact of having exactly  $N$  atoms in a condensate and a well-defined phase  $\varphi$ , knowing that these two quantities are conjugate variables having to satisfy a Heisenberg uncertainty relation.

## 26.2.6 Exercises

### 26.2.6.1 Ex: Derivation of the non-linear Schrödinger equation

Derive the non-linear Schrödinger equation using (a) the commutator relation (26.5)(v) and (b) the variational expression (26.18).

### 26.2.6.2 Ex: Spontaneous breaking of gauge symmetry

One of the primary characteristics of a condensate is its phase coherence. Now, consider a condensate with exactly  $N$  atoms. The exact knowledge of the atom number implies a totally uncertain phase of the condensate, according to Heisenberg's uncertainty relation. Explain this contradiction!

## 26.3 Approximate solutions of the Gross-Pitaevskii equation

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<sup>6</sup>An alternative way of modeling the development of a BEC phase is based on measurement theory. See also (??) for an analogy to the correct state of a laser.

### 26.3.1 Stationary GPE

In cases where the external potential is stationary,  $V_{trap}(\mathbf{r}, t) = V_{trap}(\mathbf{r})$ , the temporal dependency of the GPE can be removed by the ansatz,

$$\psi_0(\mathbf{r}, t) = \psi_0(\mathbf{r})e^{-i\mu t/\hbar} . \quad (26.22)$$

This gives the stationary Gross-Pitaevskii equation,

$$\left[ \frac{-\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + g|\psi_0(\mathbf{r})|^2 \right] \psi_0(\mathbf{r}) = \mu\psi_0(\mathbf{r}) , \quad (26.23)$$

where  $\mu$  is called the *chemical potential*. Solve Exc. 26.3.4.1.

### 26.3.2 Trapped condensates and the Thomas-Fermi limit

#### 26.3.2.1 Free particles

The wavefunction of free particles,  $V(\mathbf{r}) = 0$ , can be described by a plane wave,

$$\psi(\mathbf{r}) = \sqrt{n}e^{i\mathbf{k}\cdot\mathbf{r}} , \quad (26.24)$$

also called the Hartree solution. Inserted it into the equation of Gross-Pitaevskii equation,

$$E(k) = \frac{\hbar^2 k^2}{2m} + gn , \quad (26.25)$$

we observe a *gap* in the energy spectrum due to the interaction.

#### 26.3.2.2 Ideal gas in a harmonic potential

Most experiments apply non-isotropic (often cylindrical) potentials, which are additionally distorted by the mean-field. Hence, the non-linear term of the GPE is important, and the spatial coordinates can not be separated. However, assuming an ideal gas and a harmonic potential, the dimensions could be separated, as demonstrated in Sec. 3.5.5, even when the potential is not isotropic. It is then sufficient to consider one-dimensional problems with  $g = 0$ ,

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m}{2} \omega_x^2 \hat{x}^2 \right] \psi_n = \mu_n \psi_n . \quad (26.26)$$

In this limit, the GPE is nothing more than the usual Schrödinger equation, which has the well-known spectrum (3.107) and the solutions (3.106).

#### 26.3.2.3 Ideal gas in an isotropic potential

In the case of an ideal gas trapped in a spherically symmetric potential, as shown in (4.34), the Schrödinger equation can be reduced to its radial component,

$$\left[ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} + V_{trap}(r) \right] f_{nlm}(r) = \mu_{nl} f_{nlm}(r) , \quad (26.27)$$

with the solution (4.18),

$$\psi_n(r, \vartheta, \varphi) = \sum_{l,m} f_{nlm}(r) Y_{lm}(\vartheta, \varphi) \quad (26.28)$$

The differential equation (26.27) can be solved numerically by Runge-Kutta type methods,

$$\begin{pmatrix} f'' \\ f' \end{pmatrix} = \begin{pmatrix} \frac{2}{r} & \mu + \frac{l(l+1)}{r^2} - V_{trap}(r) \\ 1 & 0 \end{pmatrix} \begin{pmatrix} f' \\ f \end{pmatrix}. \quad (26.29)$$

#### 26.3.2.4 Thomas-Fermi limit for strong interactions

In the case of strong interactions, the kinetic energy term can be neglected, at least in the center of the cloud, where the mean-field energy is stronger. For this case, called *Thomas-Fermi limit*, the GPE solution is easy,

$$|\psi_0(\mathbf{r})|^2 = \frac{\mu - V_{trap}}{g}. \quad (26.30)$$

The chemical potential follows from the normalization condition,

$$N = \int_{n(\mathbf{r})>0} n(\mathbf{r}) d^3\mathbf{r}. \quad (26.31)$$

In the case of an cylindrical harmonic oscillator potential,  $V_{trap}(r, z) = \frac{m}{2}(\omega_r^2 r^2 + \omega_z^2 z^2)$ , the chemical potential is,

$$\mu = \left( \frac{15Ng}{8\pi} \right)^{2/5} \left( \frac{m}{2}(\omega_r^2 \omega_z^2)^{2/3} \right)^{3/5}. \quad (26.32)$$

The radial size  $\sigma$  of the condensate follows from  $n(r_{hw}, 0) = \frac{n(0,0)}{2}$ ,

$$r_{hw} = \sqrt{\frac{\mu}{m\omega_r^2}}. \quad (26.33)$$

Solve the Excs. 26.3.4.2 and 26.3.4.3.

### 26.3.3 Variational treatment of the GPE

The many-body Hamiltonian (26.19) can be used as an *energy functional*,

$$E[\psi_0] \equiv \langle \mathcal{H}[\psi_0] \rangle = \int d^3r \left[ \frac{\hbar^2}{2m} |\nabla \psi_0|^2 + V_{trap}(\mathbf{r}) |\psi_0|^2 + \frac{g}{2} |\psi_0|^4 \right], \quad (26.34)$$

from which, using the variational condition (26.18), we have derived the Gross-Pitaevskii equation (26.21). Hence, the wavefunction  $\psi_0$  minimizes the functional [204]. By inserting an ansatz for the wavefunction with adjustable parameters, the functional provides conditions to optimize these parameters.

The *variational method* is useful e.g. for finding the ground state wavefunction of a condensate in an arbitrarily shaped trap or to perform a stability analysis of a condensate with attractive interatomic forces.



### 26.3.3.1 Finding the fundamental state of the GPE

This problem of finding the ground state wavefunction of a condensate consists in finding the  $\psi$  for which the energy  $\mathcal{H}[\psi]$  goes to a minimum. In general, the functional has the form  $\mathcal{H}[\psi] = \int f[\psi, \nabla\psi] d^3r$ . The fastest way to the minimum is to reduce the energy by varying  $\psi$  in that direction, where the gradient  $\delta\mathcal{H}/\delta\psi^*$  is largest, that is,

$$\begin{aligned}\mathcal{H} &\rightarrow \mathcal{H}[\psi + \tau \frac{\delta\mathcal{H}}{\delta\psi^*}] \\ \psi &\rightarrow \psi + \tau \frac{\delta\mathcal{H}}{\delta\psi^*},\end{aligned}\tag{26.35}$$

with the boundary condition, that the normalization must be preserved. Formally, this problem is similar to a time-dependent Gross-Pitaevskii equation, but with *imaginary time*. Physically, the procedure, called the *steepest descent method*, can be interpreted as applying a heavily 'overdamped' friction force,

$$\frac{\partial\psi}{\partial\tau} = \frac{\delta\mathcal{H}}{\delta\psi^*}.\tag{26.36}$$

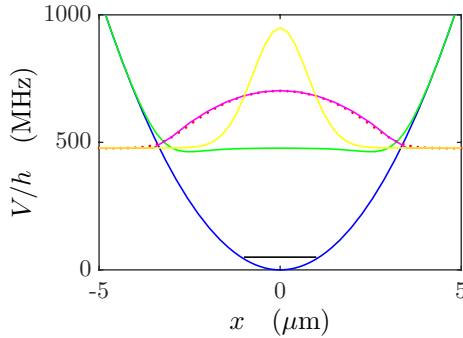


Figure 26.2: (code) Calculation of the BEC wavefunction by the steepest descent method (red dots). Also shown are the ideal gas approximation (yellow line) and the Thomas-Fermi approximation (magenta line), as well as the ground state energy (black line) and the chemical potential (green line).

In practice, the procedure is as follows: we start with a trial wavefunction, for example, the exact solution of the interaction-free case. This function is now propagated in imaginary time, using the complete Hamiltonian including the non-linear term, and then renormalized:

$$\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \mathcal{H}(\mathbf{r}) \psi(\mathbf{r}, t).\tag{26.37}$$

Substituting the imaginary unit  $i$  in the time-dependent Gross-Pitaevskii equation (26.21) by  $-1$ , we obtain,

$$\begin{aligned}\psi(\mathbf{r}, t + dt) &= [1 - \hbar^{-1} \mathcal{H}(\mathbf{r}) dt] \psi(\mathbf{r}, t) \\ \psi'(\mathbf{r}, t) &\equiv \frac{\psi(\mathbf{r}, t + dt)}{|\psi(\mathbf{r}, t + dt)|} \rightarrow \psi(\mathbf{r}, t).\end{aligned}\tag{26.38}$$

This procedure is repeated until the function converges. Since this method is derived from a variational principle, it only serves to find the ground state of the trapping potential. It can not be used for excited states (with the exception of vortex states, where in cylindrical coordinates the Hamiltonian differs by an additional centrifugal term).

### 26.3.3.2 Collapse and stabilization of condensates with attractive interactions

Attractive interactions destabilize a Bose-Einstein condensate. Since the interaction energy,  $4\pi\hbar^2 a_s n/m$ , of a condensate with negative scattering length decreased with increasing density  $n$ , the condensate attempts to lower its interaction energy by increasing its density until it succumbs to inelastic two-body spin-changing collisions of to three-body collisions leading to the formation of molecules [668]. Strictly speaking, this only holds true for homogeneous condensates. In the presence of a trapping potential, however, the zero-point energy exerts a kinetic pressure, which counteracts the *condensate collapse* to a certain extent, such that small condensates are stabilized. This can be verified by inserting a Gaussian wavefunction  $\psi_0 \propto e^{-r^2/2\bar{r}^2}$  into the energy functional (26.34). Varying the radius  $\bar{r}$  of the condensate, we find a local minimum where the condensate is stable. Calculations for spherical traps predict [591, 166],

$$N_{min} \simeq 0.575 \frac{a_{trp}}{|a_s|}, \quad (26.39)$$

where  $a_{trp} = \sqrt{\hbar/m\omega_{trp}}$ .

The atomic species  ${}^7\text{Li}$  has a slightly negative scattering length  $a_s = -27.3a_B$ . As can be seen in Fig. 26.3, small condensates can survive in a confining trap, since the energy functional has a local minimum [103, 101, 592]. Solve Exc. 26.3.4.4.

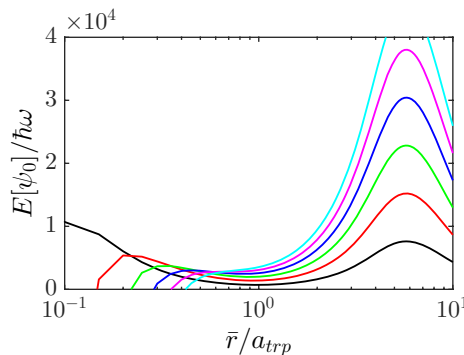


Figure 26.3: (code) Energy of a  ${}^7\text{Li}$  condensate in a harmonic isotropic potential with  $\omega_{trp} = (2\pi) 50$  Hz with  $N = 500$  atoms (linha inferior) up to  $N = 3000$  (linha superior) when the radius  $\bar{r}$  of the condensate is varied.

## 26.3.4 Exercises

**26.3.4.1 Ex: GPE in dimensionless units**

Use the following abbreviations to rewrite the Gross-Pitaevskii equation and its solution for a harmonic isotropic potential in dimensionless units,

$$\begin{array}{ll}
 V_1 \equiv V_{\text{trap}}/\hbar\omega_{\text{trap}} & V_{\text{trap}} = \frac{m}{2}\omega_{\text{trap}}^2 r^2 \\
 \mathbf{r}_1 \equiv \mathbf{r}/a_{\text{trap}} & a_{\text{trap}} = \sqrt{\hbar/m\omega_{\text{trap}}} \\
 \mu_1 \equiv \mu/\hbar\omega_{\text{trap}} & T_1 \equiv k_B T/\hbar\omega_{\text{trap}} \\
 \psi_1 \equiv \psi/a_{\text{trap}}^{3/2} & p_1 \equiv a_{\text{trap}}p/\hbar \\
 g \equiv 4\pi\hbar^2 a/m & g_1 \equiv 8\pi N_0 a/a_{\text{trap}}
 \end{array}$$

**26.3.4.2 Ex: Interacting gas in an isotropic potential**

Consider the potential  $V(\mathbf{r}) = V(r)$ , such that the wavefunction will have radial symmetry,  $\psi(\mathbf{r}) = \frac{\phi(r)}{r}$ . Rewrite the Gross-Pitaevskii equation for the function  $\phi$  [339].

**26.3.4.3 Ex: Interacting gas in a cylindrical potential**

Consider the potential  $V(\mathbf{r}) = V(\rho, z)$ , such that the wavefunction will have rotational symmetry,  $\psi(\rho, z, \varphi) = \frac{\phi(\rho, z)}{\rho}$ . Rewrite the Gross-Pitaevskii equation for the function  $\phi$  [339].

**26.3.4.4 Ex: Collapse of condensate with attractive interactions**

A Bose-Einstein condensate of  ${}^7\text{Li}$  may become unstable due to attractive interatomic forces, the scattering length being  $a_s = -27.3a_B$ . Consider the radial Gross-Pitaevskii Hamiltonian with an external harmonic potential with the oscillation frequency  $\omega_{\text{trap}}/(2\pi) = 50$  Hz. Using the variational method, determine the maximum number of atoms allowing for a stable condensate. (Note that the derived minimization condition must be evaluated numerically.)

**26.4 Elementary excitations**

The dynamics of Bose-Einstein condensates is usually studied by observing the change of their shape in response to temporal variations in the trapping potential. The simplest variation surely consists in suddenly removing the trapping potential altogether. Consequently, the first experiment performed with a BEC was the study of its ballistic expansion [16, 228, 124] (see Sec. 26.7.1).

On the other hand, the temporal variation of the potential can also be a small oscillatory or pulsed perturbation, for example, a small modification of the amplitude of the trapping field, a displacement or a local anisotropy induced by the dipole force of a laser beam tuned far away from resonance. It is even conceivable to manipulate the self-energy of the condensate or to irradiate electromagnetic waves, which couples internal atomic excitation levels or states of the atomic motion [53, 17, 655, 372, 478, 637, 219, 669, 373, 527, 654, 262]. The response of the condensate to such

small perturbations can be understood by a linearized model of the Gross-Pitaevskii equation, which we will present in the following sections.

### 26.4.1 Bogolubov spectrum of excitations

To analyze the spectrum of a condensate's response to small perturbations, let us follow Bogolubov's treatment of the time-dependent Gross-Pitaevskii equation [652]. We start by substituting Eq. (26.20) [218],

$$\hat{\psi}(\mathbf{r}, t) \longrightarrow \hat{\psi}(\mathbf{r}, t)e^{-i\mu t/\hbar}, \quad (26.40)$$

which gives us,

$$\left[ -\frac{\hbar^2}{2m}\nabla^2 + V_{trap}(\mathbf{r}) + g|\hat{\psi}(\mathbf{r}, t)|^2 \right] \hat{\psi}(\mathbf{r}, t) = \left[ \mu + i\hbar\frac{\partial}{\partial t} \right] \hat{\psi}(\mathbf{r}, t). \quad (26.41)$$

The *Bogolubov prescription* now consists in approximating the field operators of the condensate by a sum of the equilibrium wavefunction, which is interpreted as a complex number, and a small perturbation, which conserves its operator character,

$$\hat{\psi}(\mathbf{r}, t) \simeq \psi_0(\mathbf{r}) + \delta\hat{\psi}(\mathbf{r}, t). \quad (26.42)$$

This treatment assumes that most atoms are condensed,  $N - N_0 \ll N_0$ , and only a few thermal atoms are left out.

Applying the *Bogolubov transform*,

$$\boxed{\delta\hat{\psi}(\mathbf{r}, t) \equiv \sum_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r})\hat{a}_{\mathbf{k}}(t) + v_{\mathbf{k}}^*(\mathbf{r})\hat{a}_{\mathbf{k}}(t)^\dagger}, \quad (26.43)$$

the perturbation is expressed as a superposition of amplitudes for annihilation and creation of non-interacting *quasi-particles*. By inserting this ansatz into the Gross-Pitaevskii equation, we obtain a linear system of equations called *Bogolubov-de Gennes equations*.

#### 26.4.1.1 Semi-classical approximation

To simplify the equations, let us neglect the operator character of the quasi-particle by doing the substitutions,

$$\hat{a}_{\mathbf{k}} \rightarrow e^{-i\omega_{\mathbf{k}}t} \quad \text{and} \quad \hat{a}_{\mathbf{k}}^\dagger \rightarrow e^{i\omega_{\mathbf{k}}t}. \quad (26.44)$$

That is, we insert the ansatz (26.42) with,

$$\delta\hat{\psi}(\mathbf{r}, t) \equiv u_{\mathbf{k}}(\mathbf{r})e^{-i\omega_{\mathbf{k}}t} + v_{\mathbf{k}}^*(\mathbf{r})e^{i\omega_{\mathbf{k}}t}, \quad (26.45)$$

into the Gross-Pitaevskii equation (26.41), we look for the lowest order,

$$\left( -\frac{\hbar^2}{2m}\nabla^2 + V_{trap} + g|\psi_0|^2 \right) \psi_0 = \mu\psi_0, \quad (26.46)$$

and we collect the terms of first order in  $e^{\pm i\omega_{\mathbf{k}}t}$ , neglecting terms of order  $u_{\mathbf{k}}^2, v_{\mathbf{k}}^{*2}$  or higher,

$$\begin{aligned} -\frac{\hbar^2}{2m}\nabla^2 u_{\mathbf{k}} + V_{\text{trap}}u_{\mathbf{k}} + 2g\psi_0^2 u_{\mathbf{k}} - g\psi_0^2 v_{\mathbf{k}}^* &= \mu u_{\mathbf{k}} + \hbar\omega_{\mathbf{k}}u_{\mathbf{k}} \\ \frac{\hbar^2}{2m}\nabla^2 v_{\mathbf{k}} - V_{\text{trap}}v_{\mathbf{k}} - 2g\psi_0^2 v_{\mathbf{k}} + g\psi_0^2 u_{\mathbf{k}}^* &= -\mu v_{\mathbf{k}} + \hbar\omega_{\mathbf{k}}v_{\mathbf{k}} . \end{aligned} \quad (26.47)$$

Introducing the abbreviations  $n = \psi_0^2$  and,

$$\mathcal{L} \equiv \frac{-\hbar^2\nabla^2}{2m} + V_{\text{trap}} + 2gn - \mu , \quad (26.48)$$

we can write

$$\begin{pmatrix} \mathcal{L} - \hbar\omega_{\mathbf{k}} & gn \\ gn & \mathcal{L} + \hbar\omega_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \left[ \begin{pmatrix} \mathcal{L} & gn \\ gn & \mathcal{L} \end{pmatrix} - \hbar\omega_{\mathbf{k}}\hat{\sigma}_z \right] \phi_{\mathbf{k}} = 0 , \quad (26.49)$$

with  $\hat{\sigma}_z$  being the third Pauli matrix. The solution of Eq. (26.49) is given by the requirement, that the determinant of the matrix be 0,

$$\hbar\omega_{\mathbf{k}} = \sqrt{\mathcal{L}^2 - (gn)^2} . \quad (26.50)$$

The object

$$\phi_{\mathbf{k}} \equiv \begin{pmatrix} u_{\mathbf{k}}(\mathbf{r}) \\ v_{\mathbf{k}}(\mathbf{r}) \end{pmatrix} \quad (26.51)$$

is called a *normal mode* of the condensate. The normal modes (26.50) are orthonormal,

$$\langle \phi_{\mathbf{k}} | \phi_{\mathbf{k}'} \rangle = \int d\mathbf{r} \phi_{\mathbf{k}}^\dagger(\mathbf{r}) \hat{\sigma}_z \phi_{\mathbf{k}'}(\mathbf{r}) = \delta_{\mathbf{k},\mathbf{k}'} , \quad (26.52)$$

which means that *the modes do not interact*, that is, the quasi-particles *do not collide*.

For homogeneous systems or at the interior of a large condensate with strong interactions, we can assume that the potential is approximately constant,  $V_{\text{trap}} \rightarrow 0$ , and kinetic energy negligible compared to the self-energy, and Eq. (26.41) shows us,  $\mu \rightarrow gn$ . Assuming plane waves,

$$u_{\mathbf{k}}(\mathbf{r}) \equiv ue^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{and} \quad v_{\mathbf{k}}(\mathbf{r}) \equiv ve^{i\mathbf{k}\cdot\mathbf{r}} , \quad (26.53)$$

we obtain the *Bogolubov spectrum* of elementary excitations,

$$\boxed{\hbar\omega_{\mathbf{k}} = \sqrt{\frac{\hbar^2\mathbf{k}^2}{2m} \left( \frac{\hbar^2\mathbf{k}^2}{2m} + 2\mu \right)}} . \quad (26.54)$$

which corresponds to a *dispersion relation* for Bose-Einstein condensates. For an interacting gas, the collective modes are distortions of the condensate, caused by restoring forces originating in the finite compressibility of the gas.

### 26.4.1.2 Phonon- and particle-like excitations

The coefficients  $u$  and  $v$  describe the annihilation and  $u^*$  and  $v^*$  the creation of *quasi-particles* called *fonons* or *elementary excitations*. Two limits are interesting. In the low energy limit,  $\frac{\hbar^2 \mathbf{k}^2}{2m} \ll gn(\mathbf{r})$ , we create *phonon-like excitations*. The Bogolubov spectrum becomes,

$$\hbar\omega_{\mathbf{k}}^{ph} \simeq c_s \hbar k \quad \text{with} \quad c_s \equiv \sqrt{\frac{ng}{m}}. \quad (26.55)$$

Here is  $c_s$  the *sound velocity* inside the condensate. The fact that, comparing (26.54) and (26.55), we find,

$$\hbar\omega_{\mathbf{k}} > \hbar\omega_{\mathbf{k}}^{ph} \quad (26.56)$$

for all  $\mathbf{k}$  is the *Landau criterion* for the superfluidity of the condensate. It means that, for an object being dragged through the condensate with a velocity less than  $c_s$ , it does not become energetically favorable to produce excitations, see Fig. 26.4. Therefore, the object will move without dissipation, which is an important characteristic of superfluids. Experiments demonstrated this manifestation of superfluidity by slowly stirring a strongly focused blue-detuned laser through a condensate. We will come back to this in Sec. 27.1.1.

In the high energy limit,  $\frac{\hbar^2 \mathbf{k}^2}{2m} \gg gn(\mathbf{r})$ , we create *particle-like excitations*. The Bogolubov spectrum becomes,

$$\hbar\omega_{\mathbf{k}}^{pa} = \frac{\hbar^2 \mathbf{k}^2}{2m}. \quad (26.57)$$

In this limit, we recover the quadratic dispersion relation of free particles, as seen in Fig. 26.4.

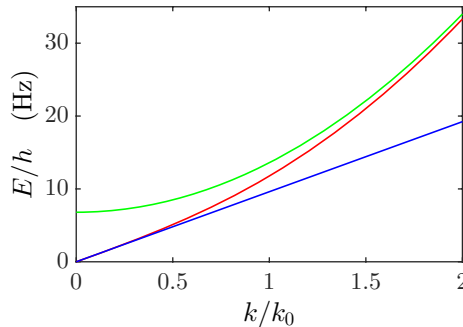


Figure 26.4: (code) Bogolubov spectrum (red), phonon limit (blue line) and particle limit (green line).

Experimentally, the complete Bogolubov spectrum (26.54) can be measured by Bragg spectroscopy [661, 653] (see Sec. 28.2). Solve Exc. 26.4.3.1.

### 26.4.2 Excitation of normal modes

In the simplest case, we generate a perturbation as a weak additional potential in the Gross-Pitaevskii equation (26.41),

$$[\mathcal{L} - gn + f_+(\mathbf{r})e^{-i\omega_p t} + f_-(\mathbf{r})e^{i\omega_p t}] \hat{\psi} = i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t). \quad (26.58)$$

After the Bogolubov transform (26.45) we now have,

$$\left[ \begin{pmatrix} \mathcal{L} & gn \\ gn & \mathcal{L} \end{pmatrix} - \hbar\omega_{\mathbf{k}}\sigma_3 \right] \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = - \begin{pmatrix} f_+(\mathbf{r})\psi_0(\mathbf{r}) \\ f_-^*(\mathbf{r})\psi_0^*(\mathbf{r}) \end{pmatrix}. \quad (26.59)$$

The solution of this equation is found by expanding the amplitudes  $u(\mathbf{r})$  and  $v(\mathbf{r})$  into normal modes,

$$\begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = \sum_{\mathbf{k}} c_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}) \quad \text{and} \quad \begin{pmatrix} f_+(\mathbf{r})\psi_0(\mathbf{r}) \\ f_-^*(\mathbf{r})\psi_0^*(\mathbf{r}) \end{pmatrix} = \sum_{\mathbf{k}} g_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}), \quad (26.60)$$

where  $g_{\mathbf{k}}$  is given by the overlap integral,

$$g_{\mathbf{k}} = \int d\mathbf{r} \phi_{\mathbf{k}}^\dagger(\mathbf{r}) \sigma_3 \begin{pmatrix} f_+(\mathbf{r})\psi_0(\mathbf{r}) \\ f_-^*(\mathbf{r})\psi_0^*(\mathbf{r}) \end{pmatrix}. \quad (26.61)$$

To calculate the response of the condensate to a given perturbation  $f_{\pm}(\mathbf{r})$ , we must first calculate the normal mode spectrum  $\phi_{\mathbf{k}}(\mathbf{r})$  from the Bogolubov equation (26.49). After that, we can calculate the coefficients (26.61). Inserting the expansions into the Eq. (26.59), we obtain the response of the condensate,

$$\begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = - \sum_{\mathbf{k}} \frac{g_{\mathbf{k}}/\hbar}{\omega_{\mathbf{k}} - \omega} \phi_{\mathbf{k}}. \quad (26.62)$$

The deviation, which is observed for resonant excitation, is due to the neglected losses and non-linear effects.

#### 26.4.2.1 Classification of normal modes

BECs often have cylindrical symmetry,  $\psi(\mathbf{r}) = \psi_0(r, z)$ . In this case, similar calculations to those shown above, result in analytical expressions for the frequencies of the elementary excitations. These frequencies were derived by [165]<sup>7</sup>. The modes can be classified by their main quantum numbers  $n_r$ , and by their multipolar moment  $\ell$ . Examples are the *surface excitation* or *shape oscillation* ( $n_r = 0$ ) and the *compression oscillation* ( $n_r \neq 0$ ). Special cases are called *shaking mode*, *breathing mode* ( $n_r = 1, \ell = 0$ ), and *swirling mode*. In the case of cylindrical symmetry, the projection of the angular momentum onto the symmetry axis  $m$  is the relevant quantum

<sup>7</sup>It is worth mentioning that the linearized theory applies to *small perturbations*. Strong disturbances render the dynamics chaotic, since the energy is coupled to many modes of excitation.

number. The dispersion relations are,

$$\begin{aligned} \omega(\ell, \mp m = \ell) &= |m|\omega_r^2 & (26.63) \\ \omega(\ell, \mp m = \ell - 1) &= |m|\omega_r^2 + \omega_z^2 \\ \omega(\ell, \mp m = \ell - 2) &= \omega_r^2 \left[ 2|m| + 2 + \frac{3}{2}\lambda^2 \mp \sqrt{(|m| + 2 - \frac{3}{2}\lambda^2)^2 + 2\lambda^2(|m| + 1)} \right] \\ \omega(\ell, \mp m = \ell - 3) &= \omega_r^2 \left[ 2|m| + 2 + \frac{7}{2}\lambda^2 \mp \sqrt{(|m| + 2 - \frac{5}{2}\lambda^2)^2 + 6\lambda^2(|m| + 1)} \right], \end{aligned}$$

where  $\lambda$  is the aspect ratio  $\lambda = \omega_z/\omega_r$ . Obviously, higher excitation orders depend on the trap geometry. Moreover, we can easily see, that occasional degeneracies must arise for specific aspect ratios. For example, when  $\omega_+(2, 0) = 2\omega(2, 2)$ , we derive from (26.63) the condition  $\lambda = \sqrt{16/7}$ , and when  $\omega_+(2, 0) = 2\omega_-(2, 0)$ , we derive  $\lambda = \frac{1}{6}\sqrt{77 + 5\sqrt{145}}$ .

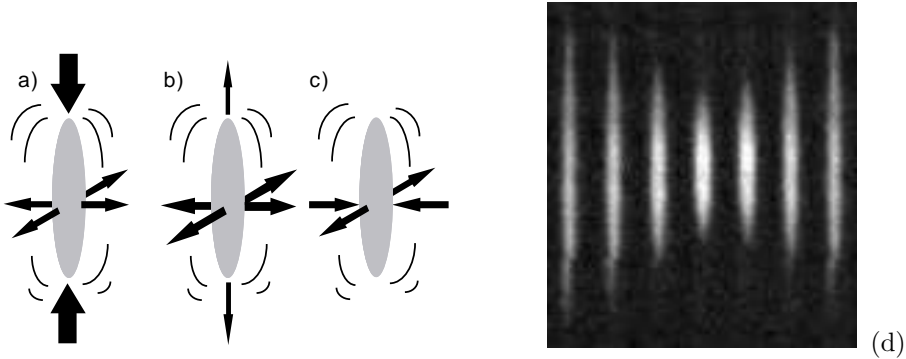


Figure 26.5: Normal modes of a BEC. (a) Shape oscillation, (b) breathing oscillation, and (c) quadrupole oscillation. (d) Non-destructive measurements of quadrupolar vibrations of a BEC [654].

### 26.4.2.2 Quantum depletion

Following Bogolubov’s theory the *quantum depletion* is given by,

$$\frac{\delta N}{N} = \frac{1}{N} \sum_{\mathbf{k}} \int d^3r |v_{\mathbf{k}}(\mathbf{r})|^2. \quad (26.64)$$

### 26.4.2.3 Fluctuations in BECs

Fluctuations in condensates are reduced as compared to thermal ensembles. Non-linearities are always very sensitive to fluctuations (see the laser). Therefore, we have to look at closer at collisions. For 3-body decay in a thermal source,  $\langle \rho(\mathbf{r})^3 \rangle \sim 6\langle \rho(\mathbf{r}) \rangle^3$ , and in a coherent source:  $\langle \rho(\mathbf{r})^3 \rangle \sim \langle \rho(\mathbf{r}) \rangle^3$  [113, 646].



### 26.4.3 Exercises

#### 26.4.3.1 Ex: Sound velocity in the Thomas-Fermi regime

Consider a condensate of  $N = 10^5$   $^{87}\text{Rb}$  atoms confined to an isotropic harmonic potential with secular frequency  $\omega_{trp} = (2\pi) 50$  Hz. Remember  $a_s = 110a_B$  and use the Thomas-Fermi approximation.

- Evaluate the chemical potential.
- Calculate the sound velocity at the center of the condensate.

## 26.5 Hydrodynamics and the propagation of sound

The question arises how the elementary excitations relate to the phenomenon of *sound*, well known from the hydrodynamic theory of superfluid  $^4\text{He}$  proposed by Landau [422]. The *hydrodynamic regime* is characterized by the dominance of collisions <sup>8</sup>. On the other hand, Bogolubov's theory describes elementary excitations in the *collisionless regime*, where *quasi-particles* do not interact <sup>9</sup>. There is, therefore, a great motivation to study excitations with condensates in a very dense regime, where one can expect to recover predictions of hydrodynamic theory.

The hydrodynamic regime is reached, when the *free path* of the particles is smaller than the wavelength of the sound, that is <sup>10</sup>,

$$l_{mfp} < \lambda/2\pi . \quad (26.65)$$

### 26.5.1 Zero, first and second sound

The occurrence of several types of sound was related by Tisza and London to the existence of superfluid and normal components in  $^4\text{He}$  [520]. The *second sound* is a quantum phenomenon, where the heat transfer occurs as an *wave-like motion* instead of being diffusive. Heat takes the place of pressure in normal sound waves called *first sound*. This induces a very high thermal conductivity. At temperatures below the  $\lambda$ -point,  $^4\text{He}$  has the highest known conductivity of all materials (a few hundred times higher than copper).

The *zero sound* was introduced by Landau to name quantum vibrations in Fermi quantum liquids. This sound can not be seen as a simple wave of compression and rarefaction. In gaseous condensates, the zero sound corresponds to the elementary excitation called *phonon-like*.

Finally, the excitation called *particle-like* or *ballistic*, observed in gaseous condensates has no correspondence in dense superfluids, since the mean free path there is too short. The various regimes accessible in condensed gasses are listed in the following table [17, 19, 285, 387, 631, 655, 654, 241]:

<sup>8</sup>Collisions prevent condensation, because they localize the particles. This is the reason for the large quantum depletion, which in  $^4\text{He}$  is of the order of 10% and hides effects of quantum statistics. Quantum depletion prevents any form of long-range order, as this requires delocalization.

<sup>9</sup>Bogolubov's theory assumes that the only impact of collisions is to deform the dispersion relationship, keeping the collective modes orthogonal.

<sup>10</sup>Note the similarity to the Ioffe-Regel criterion.

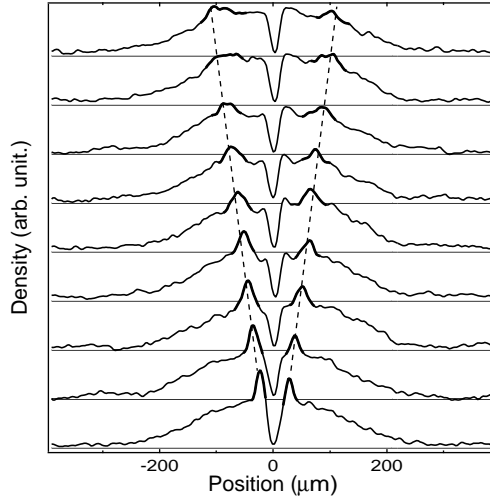


Figure 26.6: (code) Consecutive measurements of the BEC density profile showing the propagation of zero sound. The sound was excited by a blue-detuned laser tuned focused into the middle of the BEC (lower curve). The other curves show how the perturbation propagates towards the edges of the BEC.

regime	range scale	energy range	condensate	thermal cloud
collision-less	$k^{-1} < \xi < l_{mfp}$	$\frac{\hbar^2}{2ml_{mfp}^2} < gn_0 < \frac{\hbar^2 k^2}{2m}$	ballistic	ballistic
collision-less	$\xi < k^{-1} < l_{mfp}$	$\frac{\hbar^2}{2ml_{mfp}^2} < \frac{\hbar^2 k^2}{2m} < gn_0$	zero sound	ballistic
hydrodynamic	$\xi < l_{mfp} < k^{-1}$	$\frac{\hbar^2 k^2}{2m} < \frac{\hbar^2}{2ml_{mfp}^2} < gn_0$	second sound	first sound

(26.66)

normal modes			$qR \ll 1$
macroscopic beyond Bogolubov			$qa \ll 1$ $qa > 1$
superfluid (TF limit, LDA) ???	$E_{self} \gg E_{kin}$ $E_{self} \ll E_{kin}$	$8\pi Na \gg a_{ho}$ $8\pi Na \ll a_{ho}$	$a_{ho} \gg \xi$ $a_{ho} \ll \xi$
collision-less	$\gamma_{coll} \ll \frac{\hbar q^2}{2m}$		$ql_{mfp} \ll 1$
hydrodynamic	$\gamma_{coll} > \frac{\hbar q^2}{2m}$		$ql_{mfp} > 1$

(26.67)

With  $l_{mfp} \simeq 1/n_{th}\sigma$ . Typical values are,

$$\begin{aligned}
 a &= 0..1000a_B & = 0..50 \text{ nm} \\
 n^{-1/3} & & = 20..200 \mu\text{m} \\
 2\pi/q & & = 0.2..\infty \mu\text{m} \\
 \xi &= \sqrt{8\pi na}^{-1} & = 0.03..30 \mu\text{m} \\
 a_{ho} &= \sqrt{\hbar/m\omega_{tr}} & = 0.1..3 \mu\text{m} \\
 2\pi/k_F &= 2\pi a_{ho}(48N)^{-1/6} & = 30..70 \mu\text{m}
 \end{aligned} \tag{26.68}$$

The various regimes of sound are distinguished by frequency shifts and damping rates of the collective modes, which depend on the density (determining the mean-field energy and the mean free path) and the temperature (controlling the ratio between condensed and normal fraction). The quantity

$$\xi \equiv \frac{1}{\sqrt{8\pi a_s n}} \tag{26.69}$$

is called *healing length*.

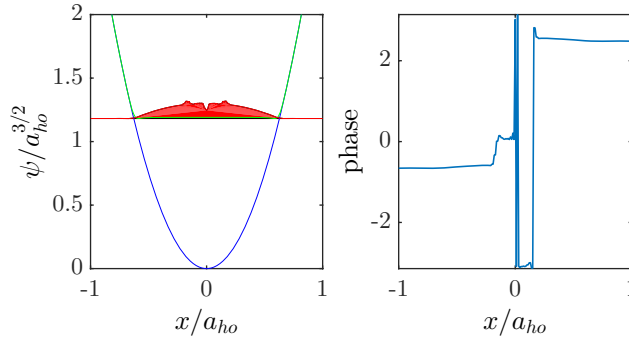


Figure 26.7: Simulation of the propagation of sound toward the edges of the condensate.

## 26.6 Momentum representation

We showed in Sec. 2.3.7, that the wavefunctions can be represented in the spatial or the momentum domain. These notions can be extended to the second quantization procedure by generalizing the equations (2.101),

$$\hat{a}_{\mathbf{k}} \equiv \frac{1}{\sqrt{(2\pi)^3 V}} \int \hat{\psi}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3 r \quad , \quad \hat{\psi}(\mathbf{r}) \equiv \sqrt{\frac{V}{(2\pi)^3}} \int \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} d^3 k \tag{26.70}$$

Differently from (2.101) we chose here a normalization, which leaves the field operators  $a_{\mathbf{k}}$  without unit.

### 26.6.1 Confined particles

In the case of confined atoms,  $\mathcal{H} = \mathcal{H}_{cm} + V_{trap}(\mathbf{r}) + \mathcal{H}_{self}$ , we get sharp eigenvalues,

$$\hat{a}_{\mathbf{k}} = \frac{1}{V} \sum_{\mathbf{k}'} \hat{a}_{\mathbf{k}'} \delta^{(3)}(\mathbf{k} - \mathbf{k}') . \quad (26.71)$$

We insert this in equation (26.70),

$$\begin{aligned} \hat{\psi}(\mathbf{r}) &= \sqrt{\frac{1}{(2\pi)^3V}} \sum_{\mathbf{k}'} \hat{a}_{\mathbf{k}'} \int \delta^{(3)}(\mathbf{k} - \mathbf{k}') e^{i\mathbf{k}\cdot\mathbf{r}} d^3k \\ &= \sqrt{\frac{1}{(2\pi)^3V}} \sum_{\mathbf{k}'} \hat{a}_{\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r}) \hat{a}_{\mathbf{k}} , \end{aligned} \quad (26.72)$$

thus making an expansion of the condensate into plane waves,

$$u_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{(2\pi)^3V}} e^{i\mathbf{k}\cdot\mathbf{r}} , \quad (26.73)$$

which is particularly adapted to the 3D box potential,  $V_{trap}(\mathbf{r}) \equiv \infty$  se  $r > R$ . Also, we calculate,

$$\hat{a}_{\mathbf{k}} = \sqrt{\frac{1}{(2\pi)^3V}} \int \hat{\psi}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3r = \int \hat{\psi}(\mathbf{r}) u_{\mathbf{k}}^*(\mathbf{r}) d^3\mathbf{r} . \quad (26.74)$$

We obtain the observable commutation rules from (26.5),

$$[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \quad , \quad [\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}] = 0 \quad , \quad \hat{N} = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} . \quad (26.75)$$

Using the following mathematical relationships,

$$\frac{1}{(2\pi)^3V} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \delta^3(\mathbf{r} - \mathbf{r}') \quad \text{and} \quad \frac{1}{(2\pi)^3V} \int d^3\mathbf{r} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} = \delta_{\mathbf{k},\mathbf{k}'} , \quad (26.76)$$

and easy to show for plane waves,

$$\sum_{\mathbf{k}} u_{\mathbf{k}}^*(\mathbf{r}) u_{\mathbf{k}}(\mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}') \quad \text{and} \quad \int u_{\mathbf{k}}^*(\mathbf{r}) u_{\mathbf{k}'}(\mathbf{r}) d^3\mathbf{r} = \delta_{\mathbf{k}\mathbf{k}'} . \quad (26.77)$$

In Exc. 26.6.4.1 we will check the validity of the commutation rules (26.75), and in Exc. 26.6.4.2 we derive the following representation of the Hamiltonian:

$$\begin{aligned} \mathcal{H} &= \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) \right) \hat{\psi}(\mathbf{r}) \\ &\quad + \frac{g}{2} \int d^3r \int d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \\ &= \sum_{\mathbf{k}} \frac{\hbar^2 \mathbf{k}^2}{2m} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} \hat{a}_{\mathbf{k}}^\dagger V_{\mathbf{k},\mathbf{k}'} \hat{a}_{\mathbf{k}'} + \frac{g}{2} \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}'}^\dagger \hat{a}_{\mathbf{k}''} \hat{a}_{\mathbf{k}+\mathbf{k}'-\mathbf{k}''} \end{aligned} , \quad (26.78)$$

with the abbreviation,

$$V_{\mathbf{k},\mathbf{k}'} = \int u_{\mathbf{k}}^*(\mathbf{r}) V_{\text{trap}}(\mathbf{r}) u_{\mathbf{k}'}(\mathbf{r}) d^3\mathbf{r} = \frac{1}{(2\pi)^3} \int V_{\text{trap}}(\mathbf{r}) e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} d^3\mathbf{r}. \quad (26.79)$$

The equation of motion for the momentum wavefunction now becomes,

$$i\hbar \frac{\partial}{\partial t} \hat{a}_{\mathbf{k}} = [\hat{a}_{\mathbf{k}}, \mathcal{H}] = \frac{\hbar^2 \mathbf{k}^2}{2m} \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \hat{a}_{\mathbf{k}'} + g \sum_{\mathbf{k}',\mathbf{k}''} \hat{a}_{\mathbf{k}'}^\dagger \hat{a}_{\mathbf{k}''} \hat{a}_{\mathbf{k}+\mathbf{k}'-\mathbf{k}''}. \quad (26.80)$$

### 26.6.1.1 Harmonically confined particles

In harmonic traps,  $V_{\text{trap}}(r) = \frac{m}{2} \omega_{\text{trap}}^2 r^2$ , the motion can be canonically quantized,

$$\hat{a} = \frac{1}{\sqrt{2}} \left( \frac{\hat{r}}{a_{\text{trap}}} \mp i a_{\text{trap}} \hat{p} \right), \quad \mathcal{H}_{cm} = \sum_{\mathbf{k}} \hbar \omega_{\text{trap}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}, \quad (26.81)$$

with the size of the ground state,

$$a_{\text{trap}} \equiv \sqrt{\frac{\hbar}{m\omega_{\text{trap}}}}. \quad (26.82)$$

As an alternative notation we could introduce,

$$|\mathbf{r}\rangle \equiv \hat{\psi}^\dagger(\mathbf{r}) \quad \text{and} \quad |\mathbf{k}\rangle \equiv \hat{a}_{\mathbf{k}}^\dagger. \quad (26.83)$$

Hence, just considering the ground state of the trap, that is, assuming that the atomic motion be frozen, our Hamiltonian becomes:

$$\mathcal{H}_{cm} + \mathcal{H}_{\text{self}} = \hbar \omega_{\text{trap}} \hat{a}^\dagger \hat{a} + \frac{g}{2} \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a}. \quad (26.84)$$

### 26.6.2 Thomas-Fermi limit

In the limit of negligible kinetic energy (that is, in the middle of a large condensate) with the analytical form of the condensate wavefunction,

$$\hat{\psi}(\mathbf{r}) \propto \sqrt{n_0} \left( 1 - \frac{\mathbf{r}^2}{\mathbf{r}_0^2} \right), \quad (26.85)$$

the transformation (26.70) allows us to derive an expression for the momentum distribution,

$$|a(\mathbf{k})| \propto \frac{J_1(\mathbf{k} \cdot \mathbf{r}_0)}{(\mathbf{k} \cdot \mathbf{r}_0)^2}. \quad (26.86)$$

#### 26.6.2.1 Width of the momentum distribution

It is interesting to compare the size of an ideal gas condensate with the size of an interacting condensate. We can express the Thomas-Fermi radius as,

$$\Delta r_{TF} = a_{\text{trap}} \sqrt{\frac{\mu}{\hbar \omega_{\text{trap}}}}. \quad (26.87)$$

The Heisenberg limit requires,

$$\Delta p_{TF} = \frac{\hbar}{\Delta r_{TF}} . \quad (26.88)$$

Since  $\sqrt{\mu/\hbar\omega_{trap}} > 1$ , the interaction increases the volume of the condensate, but restricts the distribution of its velocities. For a hypothetical thermal Boltzmann gas having the same temperature,

$$\Delta r_{th} = a_{trap} \sqrt{\frac{k_B T}{\hbar\omega_{trap}}} \quad \text{and} \quad \Delta p_{th} = \frac{\hbar}{a_{trap}} \sqrt{\frac{k_B T}{\hbar\omega_{trap}}} . \quad (26.89)$$

The thermal cloud *is not at the Heisenberg limit*, because  $\sqrt{k_B T/\hbar\omega_{trap}} > 1$ .

These relationships were experimentally confirmed [661] by measurements of the velocity distributions of condensates using a Bragg spectroscopy technique (see Sec. 28.2). It is interesting to note that the measured widths of velocity distributions were *lower than the photonic recoil limit*,  $\hbar k/m \simeq 30$  mm/s for  $^{87}\text{Rb}$ .

### 26.6.3 Master equation approach

The Hamiltonian that describes a BEC in second quantization in an orthonormal set of energy eigenfunctions reads:

$$\begin{aligned} \mathcal{H} &= \sum_{i,j} \mathcal{H}_{atom}^{(ij)} \hat{a}_i^\dagger \hat{a}_j + \sum_{i,j,k,l} \frac{1}{2} W^{(ijkl)} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \quad (26.90) \\ \mathcal{H}_{atom}^{(ij)} &= \langle \phi_i | \frac{1}{2m} \mathbf{P}^2 + V_{trap}(\mathbf{r}) | \phi_j \rangle \\ W^{(ijkl)} &= g \int \phi_i(\mathbf{r}) \phi_j(\mathbf{r}) \phi_k(\mathbf{r}) \phi_l(\mathbf{r}) d^3 r . \end{aligned}$$

The inclusion of spontaneous processes (one-body-loss, dephasing) requires a master equation including a *Lindblad term* within a density matrix formalism. The von Neumann equation for the density operator reads:

$$\begin{aligned} \frac{d}{dt} \hat{\rho} &= -i[V, \hat{\rho}] + \mathcal{L} \hat{\rho} \quad (26.91) \\ \mathcal{L}_{one-body\ loss} &\equiv \kappa(2\hat{a}\hat{\rho}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}) \\ \mathcal{L}_{one-body\ feeding} &\equiv \kappa(2 + 2\hat{a}^\dagger\hat{\rho}\hat{a} - \hat{a}\hat{a}^\dagger\hat{\rho} - \hat{\rho}\hat{a}\hat{a}^\dagger) \\ \mathcal{L}_{two-body\ loss} &\equiv \kappa(2\hat{a}^2\hat{\rho}\hat{a}^{\dagger 2} - \hat{a}^{\dagger 2}\hat{a}^2\hat{\rho} - \hat{\rho}\hat{a}^{\dagger 2}\hat{a}^2) . \end{aligned}$$

### 26.6.4 Exercises

#### 26.6.4.1 Ex: Commutators in momentum space

Demonstrate the validity of the commutation rules (26.75).

#### 26.6.4.2 Ex: Commutators in momentum space

Derive the representation (26.78) of the Hamiltonian.

## 26.7 Condensates at finite temperature

### 26.7.1 Ballistic expansion of a bosonic gas

As discussed in Sec. 24.6, the atomic density distributions are revealed through their interaction with a laser beam. The problem with imaging a confined condensate is, on the one hand, its very high optical density, which inhibits the penetration of resonant light and, on the other hand, its very small size, which is often below the diffraction limit and prevents its optical resolution. As discussed in Sec. 24.6, both problems can be avoided by the time-of-flight imaging technique, which consists in quickly switching off the trap and dropping the atomic cloud (see Fig. 24.30). If the switching-off process is fast enough, the potential energy is lost, but in the course of ballistic expansion, the self-energy is transformed into kinetic energy. Both the self-energy transformed to kinetic energy and the inherent initial kinetic energy contribute to blow up the size of the atomic cloud, so that the density rapidly decreases. After a few 10 ms, when the optical density is sufficiently low (on the order of 1), the cloud can be imaged via its absorption of a resonant laser beam. The condensate, which is about 10 times denser than the thermal cloud, has a much larger repulsive self-energy. When the condensate is suddenly released from its trap, its explosion is accelerated by this self-energy, and the acceleration is faster in those directions, where the confining potential was stronger [339, 124]. Therefore, the aspect ratio of the condensate's shape is inverted during the flight time [390, 124]. In contrast, the self-energy of the thermal cloud is relatively insignificant. Therefore, its spatial density after a time of free expansion reflects the pure velocity distribution of the atomic cloud while it was trapped. This allows the interpretation of the spatial distribution of the expanded cloud in terms of a *temperature* of the trapped cloud.

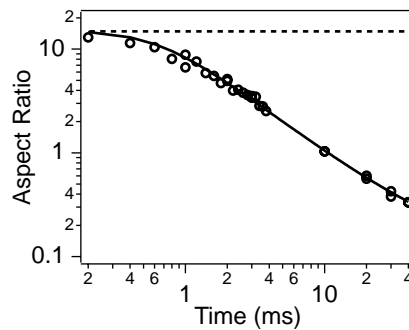


Figure 26.8: Inversion of aspect ratio during time-of-flight. The frequencies of the harmonic trap were  $\omega_r = (2\pi) \cdot 248$  Hz and  $\omega_z = (2\pi) \cdot 16$  Hz [390].

#### 26.7.1.1 Popov approximation

The Popov decomposition separates the condensed part, described by a  $c$ -number  $\phi \equiv \langle \hat{\psi} \rangle$  and normalized to the number of condensed atoms  $N_0$  from the thermal part

$\tilde{\psi} \equiv \hat{\psi} - \phi$ , which keeps track of the quantum nature of the Bose-gas [206],

$$\begin{aligned} \mathcal{K} &= \mathcal{K}_0 + \mathcal{K}_1 + \mathcal{K}_1^\dagger + \mathcal{K}_2 & (26.92) \\ \mathcal{K}_0 &= \int d^3r \phi^*(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + \frac{g}{2} |\phi|^2 - \mu \right) \phi(\mathbf{r}) \\ \mathcal{K}_1 &= 0 \quad \text{if} \quad [\mathcal{L} - gn_0(\mathbf{r})] \phi(\mathbf{r}) = 0 \\ \mathcal{K}_2 &= \int d^3r \left[ \tilde{\psi}^+(\mathbf{r}) \mathcal{L} \tilde{\psi}(\mathbf{r}) + \frac{g}{2} \left( \phi(\mathbf{r})^2 \tilde{\psi}^+(\mathbf{r}) \tilde{\psi}^+(\mathbf{r}) + \phi^*(\mathbf{r})^2 \tilde{\psi} + (\mathbf{r}) \tilde{\psi}(\mathbf{r}) \right) \right] \\ \mathcal{L} &\equiv -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) - \mu + 2gn(\mathbf{r}) \\ n(\mathbf{r}) &= n_0(\mathbf{r}) + n_T(\mathbf{r}) = |\phi(\mathbf{r})|^2 + \langle \tilde{\psi}^\dagger(\mathbf{r}) \tilde{\psi}(\mathbf{r}) \rangle . \end{aligned}$$

We perform the Bogolubov transform to the diagonalized Hamiltonian,

$$\begin{aligned} \mathcal{K}_{Popov} &= \mathcal{K}_0 + \sum_j \varepsilon_j \hat{b}_j^\dagger \hat{b}_j & (26.93) \\ \tilde{\psi}(\mathbf{r}) &= \sum_j u_j(\mathbf{r}) \hat{b}_j - v_j^*(\mathbf{r}) \hat{b}_j^\dagger \\ \delta_{jk} &= \int d^3r (u_j u_k^* - v_j v_k^*) \\ \delta_{jk} &= [\hat{b}_j, \hat{b}_k^\dagger] . \end{aligned}$$

This yields a set of equations for elementary excitations (quasi-particle excitations in a diagonalized energy space),

$$\begin{aligned} N_j &= [\exp(\varepsilon_j/k_B T) - 1]^{-1} & (26.94) \\ n_T(\mathbf{r}) &= \sum_j [ (|u_j|^2 + |v_j|^2) N_j + |v_j|^2 ] \\ \mathcal{L}u_j(\mathbf{r}) - gn_0(\mathbf{r})v_j(\mathbf{r}) &= \varepsilon_j u_j(\mathbf{r}) , \\ \mathcal{L}v_j(\mathbf{r}) - gn_0(\mathbf{r})u_j(\mathbf{r}) &= -\varepsilon_j v_j(\mathbf{r}) . \end{aligned}$$

The quantum depletion at  $T = 0$  [last term in the density  $n(\mathbf{r})$ ] may be neglected. In this zero-temperature limit, the equations simplify to yield the Gross-Pitaevskii equation. We may separate these equations using auxiliary functions [349],

$$\begin{aligned} \tilde{\psi}_j^{(\pm)}(\mathbf{r}) &\equiv u_j(\mathbf{r}) \pm v_j(\mathbf{r}) & (26.95) \\ \hat{h}_0 &\equiv \mathcal{L} - gn_0(\mathbf{r}) \\ \hat{h}_0 \tilde{\psi}_j^{(+)}(\mathbf{r}) &= E_j \tilde{\psi}_j^{(-)}(\mathbf{r}) . \end{aligned}$$

The eigenvalue equations that one gets after substituting (III.2.5) into (III.2.4) may be solved by expanding in a set of eigenfunctions of  $\hat{h}_0$ :

$$\begin{aligned} \tilde{\psi}_j^{(\pm)}(\mathbf{r}) &\equiv \sum_\alpha c_\alpha^{(j)} \phi_\alpha(\mathbf{r}) & (26.96) \\ \hat{h}_0 \phi_\alpha(\mathbf{r}) &\equiv \varepsilon_\alpha \phi_\alpha(\mathbf{r}) \\ \sum_\beta (M_{\alpha\beta} + \varepsilon_\alpha \delta_{\alpha\beta}) \varepsilon_\beta c_\alpha^{(j)} &= E_j^2 c_\alpha^{(j)} \\ M_{\alpha\beta} &= 2g \int \phi_\alpha^*(\mathbf{r}) n_0(\mathbf{r}) \phi_\beta(\mathbf{r}) d^3r . \end{aligned}$$



## 26.7.2 Hartree-Fock approach

### 26.7.2.1 Two-gas model for $T > 0$

The two phases of a condensate above  $T = 0$  have a specific interdependence, which makes it possible to treat the problem with an approximation, where only the condensed part influences the non-condensed and not vice versa [205]<sub>DOI</sub>. The HFB equation (III.2.11) is solved for the condensed part alone, assuming  $n_{th} = 0$ . The condensate wavefunction and the chemical potential are derived from that, *f.e.* using numerical methods like the method of steepest descent. The effective potential for the thermal cloud in the presence of a condensate is:

$$V_{1,eff}(\mathbf{r}_1) = V_{1,trap}(\mathbf{r}_1) + g_1 |\psi_1(\mathbf{r}_1)|^2 . \quad (26.97)$$

Next, we diagonalize the Schrödinger equation:

$$[-\nabla_1^2 + V_{1,eff}(\mathbf{r}_1)]\psi_{1,j}(\mathbf{r}_1) = 2E_{1,j}\psi_{1,j}(\mathbf{r}_1) , \quad (26.98)$$

maintaining the normalization,

$$1 = \int |\psi_{1,j}(\mathbf{r}_1)|^2 d^3\mathbf{r}_1 . \quad (26.99)$$

This provides us with the energy eigenvalues of the excited trap states and their eigenfunctions. One can *f.e.* guess an eigenvalue and numerically solve the Schrödinger equation using Runge-Kutta integration routines. The eigenfunction will probably diverge. In this case, we vary the eigenvalue until the solution converges.

Finally, we can calculate the thermal density distribution:

$$N_j \equiv [\exp((E_{1,j} - \mu_1)/k_B T_1) - 1]^{-1} \quad (26.100)$$

$$n_{th}(\mathbf{r}_1) = \sum_j N_j |\psi_{1,j}(\mathbf{r}_1)|^2 ,$$

and all thermodynamic potentials, as shown in Sec. 25.1.2.

A more sophisticated method uses self-consistent recursion [349]. Here, the thermal density is plugged back into the HFB equation, and the whole procedure is repeated until it converges.

### 26.7.2.2 Hartree-Fock approximation

We have already seen that, inside a trap the condensate occupies the lowest vibrational level, whereas the atoms of the thermal gas are distributed among all levels. The trapping potential is often harmonic,  $U_{trap}(\mathbf{r}) = \frac{m}{2}\omega_r^2 r^2$ , with secular frequencies  $\omega_r$  typically on the order of several tens or hundreds of Hz. The spatial (radial) extent of the vibration levels varies a lot with their quantum number,  $r_j = \sqrt{(2j+1)\hbar/m\omega_r}$ . This naturally produces a *separation of the thermal (or normal) and condensate fractions* at  $T > 0$ , which does not exist for a homogeneous gas and which allows (up to a certain degree) an individual treatment of the two fractions. The details of the interaction between the two fractions are very complicated and are still under intense theoretical investigation. However, to understand the shape of a trapped atomic cloud and other characteristics, we can use a simple approximate model [?, 349], assuming

that the condensate is only weakly disturbed by the thermal cloud. In contrast, the presence of the condensate dramatically modifies the potential for the thermal atoms. Therefore, we must *first* calculate the density of the condensate  $n_0(\mathbf{r})$ , *before* calculating that of the thermal cloud. If this procedure is applied iteratively, it is called *Hartree-Fock method*:

i. We start with  $n_{th}(\mathbf{r}) = 0$ ;

ii. we solve the GPE  $\left(-\frac{\hbar^2}{2m}\Delta + V_{trap}(\mathbf{r}) - \mu + g[|\psi(\mathbf{r})|^2 + n_{th}(\mathbf{r})]\right)\psi(\mathbf{r})$  numerically with the steepest descent method, we derive  $\mu$  and  $\psi$ , and also  $n(\mathbf{r}) = |\psi(\mathbf{r})|^2 + n_{th}(\mathbf{r})$ ;

iii. assuming that collisions between atoms of the thermal cloud, the density of which is weak, can be neglected, we can view the cloud as an ideal gas in a potential modified by the strongly anharmonic mean field of the condensate,  $V_{trap}(\mathbf{r}) + 2gn(\mathbf{r})$ , we calculate the thermal density  $n'_{th}(\mathbf{r}) = \lambda_{dB}^{-3} g_{3/2} \left(\exp \frac{V_{trap}(\mathbf{r}) - \mu + 2gn(\mathbf{r})}{k_B T}\right)$ ;

iv. we start over at (ii) using the new thermal density.

We can now calculate the total energy,

$$\begin{aligned} U &= \int d^3r \left( \psi(\mathbf{r}) \frac{-\hbar^2 \nabla^2}{2m} \psi(\mathbf{r}) + V_{trap}(\mathbf{r})n(\mathbf{r}) + \frac{g}{2}[2n(\mathbf{r})^2 - n_0(\mathbf{r})] + \hbar^{-3} \int d^3k \frac{-\hbar^2 k^2}{2m} n(\mathbf{r}, \mathbf{k}) \right) \\ &= \int d^3r \left( \psi(\mathbf{r}) \frac{-\hbar^2 \nabla^2}{2m} \psi(\mathbf{r}) + V_{trap}(\mathbf{r})n(\mathbf{r}) + \frac{g}{2}[2n(\mathbf{r})^2 - n_0(\mathbf{r})] + \frac{3k_B T}{2\lambda_{dB}^3} g_{3/2} \left[ \exp \frac{V_{trap}(\mathbf{r}) - \mu + 2gn(\mathbf{r})}{k_B T} \right] \right) \end{aligned} \quad (26.101)$$

and other thermodynamic quantities.

### 26.7.3 Ideal gas limit

Consider the ideal gas in an isotropic harmonic potential. The excitation spectrum then takes the form:

$$\begin{aligned} f(\mathbf{k}, \mathbf{r}) &= n(\mathbf{k}, \mathbf{r}) \\ \varepsilon_{HF}(\mathbf{k}, \mathbf{r}) &= \mathcal{L}(\mathbf{k}, \mathbf{r}) = \frac{\hbar^2 \mathbf{k}^2}{2m} + V(\mathbf{r}) - \mu . \end{aligned} \quad (26.102)$$

We can immediately calculate:

$$\begin{aligned}
 g &\longrightarrow 0 & (26.103) \\
 \mu &\xrightarrow{g \rightarrow 0} \frac{3}{2} \hbar \omega \\
 \phi(\mathbf{r}) &\xrightarrow{g \rightarrow 0} \frac{\sqrt{N_0}}{\pi^{3/4} a_{\text{trap}}^{3/2}} \exp\left(-\frac{\mathbf{r}^2}{2a_{\text{trap}}^2}\right) \\
 E_{\text{kin}} &= \int \phi(\mathbf{r}) \frac{-\hbar^2 \Delta}{2m} \phi(\mathbf{r}) d^3 r = -\frac{9}{4} N_0 \hbar \omega \\
 n_{\text{th}}(\mathbf{r}) &\xrightarrow{g \rightarrow 0} \int f(\mathbf{r} \cdot \mathbf{k}) d^3 \mathbf{k} = \frac{1}{\lambda_{dB}^3} g_{3/2} \left[ \exp\left(\frac{V_{\text{trap}}(\mathbf{r}) - \mu}{k_B T}\right) \right] \\
 N_{\text{th}} &\xrightarrow{g \rightarrow 0} \int n_{\text{th}}(\mathbf{r}) d^3 \mathbf{r} = \left(\frac{k_B T}{\hbar \omega}\right)^3 g_3 \left[ \exp\left(\frac{\mu}{k_B T}\right) \right] \\
 U &\xrightarrow{g \rightarrow 0} \int \varepsilon_{HF} f(\mathbf{r} \cdot \mathbf{k}) d^3 \mathbf{r} \cdot \mathbf{d}^3 k = 3k_B T \left(\frac{k_B T}{\hbar \omega}\right)^3 g_4 \left[ \exp\left(\frac{\mu}{k_B T}\right) \right] .
 \end{aligned}$$

## 26.7.4 Exercises

### 26.7.4.1 Ex: Ballistic expansion of a condensate

Calculate the ballistic expansion of a  $^{87}\text{Rb}$  BEC initially confined in a cylindrically symmetric trap with secular frequencies  $\omega_z = 20 \text{ Hz}$  and  $\omega_r = 100 \text{ Hz}$ .

## 26.8 Numerical simulations of the Gross-Pitaevskii equation

To simulate the one-dimensional evolution of a wavepacket following the Gross-Pitaevskii equation,

$$i\hbar \frac{\partial}{\partial t} \psi(z, t) = \left[ \frac{-\hbar^2}{2m} \frac{d^2}{dz^2} + V_{\text{trap}}(z) + |\psi(z, t)|^2 \right] \psi(z, t) . \quad (26.104)$$

we solve iteratively [554],

$$\psi(z, t + dt) = \psi(z, t) + dt \dot{\psi}(z, t) . \quad (26.105)$$

As initial state we choose,  $\psi(z, 0) = e^{-z^2/2z^2} e^{ikz}$ , where  $k \equiv \sqrt{2mE}/\hbar$  is the wavevector.

The numerical propagation is conveniently performed using the *time-splitting spectral algorithm* [45, 44, 43, 256], which can be easily extended to two dimensions.

### 26.8.1 Crank-Nicholson-Crout algorithm

### 26.8.1.1 Crank-Nicholson-Crout algorithm for the time-dependent Schrödinger equation

The *Crank-Nicholson algorithm* goes as follows. The time-dependent Schrödinger equation in one dimension,

$$\frac{\partial}{\partial t} \psi(x, t) = \frac{i\hbar}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) - \frac{iV(x)}{\hbar} \psi(x, t) \quad (26.106)$$

is a parabolic partial differential equation. We usually seek a solution on an interval  $x \in [a, b]$  and  $t > 0$ . The solution is uniquely determined from boundary conditions:  $\psi(a, t) = \psi(b, t) = 0$  and  $\psi(x, 0) = g(x)$ . One method for numerical solution solves for the values of the wavefunction on a regular grid of dimension  $h = (b - a)/N_x$  in  $x$  and  $\tau$  in  $t$ ,

$$\psi_j^k = \psi(a + jh, k\tau) . \quad (26.107)$$

The derivatives are replaced by simple finite differences. The r.h.s. of the equation at the grid point  $(i, j)$  is then,

$$\frac{i\hbar}{2m\hbar^2} (\psi_{j+1}^k - 2\psi_j^k + \psi_{j-1}^k) - \frac{iV(a + jh)}{\hbar} \psi_j^k = \sum_{m=0}^N iH_{jm} \psi_j^k , \quad (26.108)$$

where  $H$  is a real symmetric tridiagonal matrix (provided  $V(x)$  is real). The l.h.s. of the equation can be replaced either by a forward or backward difference,

$$\frac{\psi_j^{k+1} - \psi_j^k}{\tau} \quad \text{or} \quad \frac{\psi_j^k - \psi_j^{k-1}}{\tau} , \quad (26.109)$$

which, when combined with the r.h.s. gives the explicit algorithm,

$$\psi^{k+1} = (1 + iH\tau)\psi^k \quad \text{or} \quad \psi^k = (1 - iH\tau)\psi^{k+1} . \quad (26.110)$$

The Crank Nicholson Algorithm averages both,

$$(1 - iH\tau/2)\psi^{k+1} = (1 + iH\tau/2)\psi^k . \quad (26.111)$$

This method is a second order algorithm in  $t$ , i.e. the discretization error decreases as  $\tau^2$ . The finite difference representation of the second derivative  $d^2/dx^2$  is also good to second order in  $h^2$ . The Crank-Nicholson Algorithm also gives a unitary evolution in time. That is especially useful for quantum mechanics where unitarity assures that the normalization of the wavefunction is unchanged over time. The algorithm steps the solution forward in time by one time unit, starting from the initial wavefunction at  $t = 0$ . According to the Crank-Nicholson scheme, the time stepping process is half explicit and half implicit. The implicit part involves solving a tridiagonal system. That solution is accomplished by Crout reduction, a direct method related to Gaussian elimination and LU decomposition.

To simplify the algorithm we have chosen units in which the Planck constant  $\hbar = 1$ , time step  $\tau = 1$  and the spatial separation  $h = 1$ . This can always be arranged by an appropriate redefinition of mass and potential:  $m = m_{SI} \hbar^2/\tau\hbar$  and  $V = V_{SI} \tau/\hbar$ .

### 26.8.1.2 Crank-Nicholson algorithm for the time-dependent Gross-Pitaevskii equation

The Crank-Nicholson algorithm [4],

$$\frac{i(\varphi_j^{n+1} - \varphi_j^n)}{\Delta} = -\frac{\varphi_{j+1}^{n+1} - 2\varphi_j^{n+1} + \varphi_{j-1}^{n+1} + \varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n}{2h^2} \quad (26.112)$$

$$+ \frac{1}{2} \left( \frac{c(x_j)^2}{4} + n \frac{|\varphi_j^n|^2}{(x_j)^2} \right) (\varphi_j^{n+1} + \varphi_j^n).$$

Introducing abbreviations,

$$B(\varphi_j^{n+1} - \varphi_j^n) = -A(\varphi_{j+1}^{n+1} - 2\varphi_j^{n+1} + \varphi_{j-1}^{n+1} + \varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n) + C_j^n (\varphi_j^{n+1} + \varphi_j^n). \quad (26.113)$$

Can be rewritten as,

$$A\varphi_{j+1}^{n+1} + (-2A + B - C_j^n)\varphi_j^{n+1} + A\varphi_{j-1}^{n+1} = -A\varphi_{j+1}^n + (2A + B + C_j^n)\varphi_j^n - A\varphi_{j-1}^n = X_j^n. \quad (26.114)$$

The set of equations,

$$\begin{pmatrix} -2A - B - C_1^n & A & 0 & \cdots & 0 \\ A & -2A - B - C_2^n & A & \cdots & 0 \\ 0 & A & -2A - B - C_3^n & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & A & -2A - B - C_J^n \end{pmatrix} \begin{pmatrix} \varphi_1^{n+1} \\ \varphi_2^{n+1} \\ \varphi_3^{n+1} \\ \vdots \\ \varphi_J^{n+1} \end{pmatrix} = \begin{pmatrix} X_1^n \\ X_2^n \\ X_3^n \\ \vdots \\ X_J^n \end{pmatrix} \quad (26.115)$$

can be solved by inverting tridiagonal matrix. Set  $\varphi_0^{n+1} = \varphi_{J+1}^{n+1} = 0$ . Run a loop  $j = 1, \dots, J$ . Assume given  $\varphi_1^{n+1} = \varphi_j^{n+1}$ ,

$$\varphi_{j+1}^{n+1} = \frac{X_j^n}{A} + \frac{2A - B + C_j^n}{A} \varphi_j^{n+1} - \varphi_{j-1}^{n+1}. \quad (26.116)$$

### 26.8.2 Time-splitting spectral algorithm: Coherent propagation

We write the one-dimensional GPE in the form,

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(x, t) + V(x) \psi(x, t) + \frac{4\pi \hbar^2 a_s}{m(2r_h)^2} |\psi(x, t)|^2 \psi(x, t) \quad (26.117)$$

for  $a < x < b$ . Choose periodic boundary conditions,  $\psi(a, t) = \psi(b, t)$  and  $\psi_x(a, t) = \psi_x(b, t)$ . Various methods are known to solve the GPE numerically, such as the *Crank-Nicholson algorithm*. The *time-splitting spectral algorithm* (TSSA) consists in solving the first and the second of the following equations in two distinct steps [45, 44, 43, 256],

$$\frac{\partial \psi(x, t)}{\partial t} = -i \frac{V(x)}{\hbar} \psi(x, t) - i \frac{g_{1D}}{\hbar} |\psi(x, t)|^2 \psi(x, t) \quad (26.118)$$

$$\frac{\partial \psi(x, t)}{\partial t} = i \frac{\hbar}{2m} \psi_{xx}(x, t),$$

i.e. we discretize in space using  $x = a + j(b - a)/M$  and  $k = 2\pi l/(b - a)$  such that  $k(x - a) = 2\pi lj/M$ . We propagate half the way,  $\Delta t/2$ , in time,

$$\varphi_x \equiv e^{-\frac{i}{\hbar}(V(x)+g_{1D}|\psi(x,t)|^2)\frac{\Delta t}{2}} \psi(x, t) \quad (26.119)$$

for  $j = 0, \dots, M-1$ . Now we propagate the spectral components,  $(\mathcal{F}\varphi)_k \equiv \sum_{j=0}^{M-1} \varphi_x e^{-2\pi ilj/M}$ , in momentum space and transform back,  $(\mathcal{F}^{-1}\varphi)_x \equiv M^{-1} \sum_{l=-M/2}^{M/2-1} \varphi_k e^{2\pi ilj/M}$ ,

$$\phi_x \equiv \mathcal{F}^{-1} \left[ e^{i\frac{\hbar}{2m}k^2\Delta t} (\mathcal{F}\varphi)_k \right]. \quad (26.120)$$

for  $l = -M/2, \dots, M/2 - 1$ . Finally, we propagate the remaining time,  $\Delta t/2$ ,

$$\psi(x, t + dt) = e^{-\frac{i}{\hbar}(V(x)+g_{1D}|\phi_x|^2)\frac{\Delta t}{2}} \phi_x. \quad (26.121)$$

Compared to the Crank-Nicholson algorithm time-splitting spectral algorithm has several advantages:

- TSSA is much much faster, especially, for large arrays;
- No divergence, perfect reversibility;
- Imaginary version yields same density shape as steepest descent.

But there are problems:

- The coherent version changes shape, maybe it's due to  $\text{ifft}(\text{fft}(x)) \neq x$ ;
- The imaginary version mixes up real and imag parts;
- Don't know how to generalize to coupled GPEs.

### 26.8.2.1 Time-splitting spectral algorithm for coupled GPEs

Write the one-dimensional GPE in the form,

$$\begin{aligned} i\hbar \frac{\partial \psi_1(x, t)}{\partial t} &= -\frac{\hbar^2}{2m} \nabla^2 \psi_1(x, t) + V(x)\psi_1(x, t) + \frac{4\pi\hbar^2 a_s}{m(2r_h)^2} |\psi_1(x, t)|^2 \psi_1(x, t) \quad (26.122) \\ &\quad + \frac{\hbar}{2} \Omega_{mw} \psi_2(x, t) + \hbar \Delta_{mw} \psi_1(x, t) \\ i\hbar \frac{\partial \psi_2(x, t)}{\partial t} &= -\frac{\hbar^2}{2m} \nabla^2 \psi_2(x, t) + V(x)\psi_2(x, t) + \frac{4\pi\hbar^2 a_s}{m(2r_h)^2} |\psi_2(x, t)|^2 \psi_2(x, t) \\ &\quad + \frac{\hbar}{2} \Omega_{mw} \psi_1(x, t) \end{aligned}$$

for  $a < x < b$ . Choose periodic boundary conditions,  $\psi(a, t) = \psi(b, t)$  and  $\psi_x(a, t) = \psi_x(b, t)$ . We generalize the *time-splitting spectral algorithm*,

$$\begin{aligned}\frac{\partial\psi_1(x, t)}{\partial t} &= -\frac{\imath}{\hbar}V(x)\psi_1(x, t) - \frac{\imath}{\hbar}g_{1D}|\psi_1(x, t)|^2\psi_1(x, t) - \imath\Delta_{mw}\psi_1(x, t) - \frac{\imath}{2}\Omega_{mw}\psi_2(x, t) \\ \frac{\partial\psi_2(x, t)}{\partial t} &= -\frac{\imath}{\hbar}V(x)\psi_2(x, t) - \frac{\imath}{\hbar}g_{1D}|\psi_2(x, t)|^2\psi_2(x, t) - \frac{\imath}{2}\Omega_{mw}\psi_1(x, t) \\ \frac{\partial\psi_1(x, t)}{\partial t} &= i\frac{\hbar}{2m}\psi_{xx1}(x, t) \\ \frac{\partial\psi_2(x, t)}{\partial t} &= i\frac{\hbar}{2m}\psi_{xx2}(x, t),\end{aligned}\tag{26.123}$$

i.e. we discretize in space and propagate half the way,  $\Delta t/2$ , in time,

$$\begin{aligned}\varphi_{x1} &\equiv \psi_1(x, t) - \left[ \left( \frac{\imath}{\hbar}V(x) + \frac{\imath}{\hbar}g_{1D}|\psi_1(x, t)|^2 + i\Delta_{mw} \right) \psi_1(x, t) - \frac{\imath}{2}\Omega_{mw}\psi_2(x, t) \right] \frac{\Delta t}{2} \\ \varphi_{x2} &\equiv \psi_2(x, t) - \left[ \left( \frac{\imath}{\hbar}V(x) + \frac{\imath}{\hbar}g_{1D}|\psi_2(x, t)|^2 \right) \psi_2(x, t) - \frac{\imath}{2}\Omega_{mw}\psi_1(x, t) \right] \frac{\Delta t}{2}.\end{aligned}\tag{26.124}$$

Since we here use the first order Taylor expansion of the exponential function, we introduce an error that we have to keep low by renormalizing the wavefunction after each step. Now we propagate the spectral components in momentum space and transform back,

$$\begin{aligned}\phi_{x1} &\equiv \mathcal{F}^{-1} \left[ e^{i\frac{\hbar}{2m}k^2\Delta t} (\mathcal{F}\varphi_{x1})_k \right] \\ \phi_{x2} &\equiv \mathcal{F}^{-1} \left[ e^{i\frac{\hbar}{2m}k^2\Delta t} (\mathcal{F}\varphi_{x2})_k \right],\end{aligned}\tag{26.125}$$

for  $l = -M/2, \dots, M/2 - 1$ . Finally, we propagate the remaining time,  $\Delta t/2$ ,

$$\begin{aligned}\psi_1(x, t + dt) &= \phi_{x1} - \left[ \left( \frac{\imath}{\hbar}V(x) + \frac{\imath}{\hbar}g_{1D}|\phi_{x1}|^2 + \frac{\imath}{2}\Delta_{mw} \right) \phi_{x1} - \frac{\imath}{2}\Omega_{mw}\phi_{x2} \right] \frac{\Delta t}{2} \\ \psi_2(x, t + dt) &= \phi_{x2} - \left[ \left( \frac{\imath}{\hbar}V(x) + \frac{\imath}{\hbar}g_{1D}|\phi_{x2}|^2 \right) \phi_{x2} - \frac{\imath}{2}\Omega_{mw}\phi_{x1} \right] \frac{\Delta t}{2}.\end{aligned}\tag{26.126}$$

### 26.8.2.2 Spinor notation

It may be possible to simplify the notation by writing the wavefunction as a spinor,  $\vec{\psi} \equiv \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ . Now the non-kinetic part of the coupled GPE can be written,

$$\frac{\partial\vec{\psi}(x, t)}{\partial t} = M\vec{\psi}(x, t),\tag{26.127}$$

with the matrix,

$$M = \begin{pmatrix} -\frac{\imath}{\hbar}V(x) - \frac{\imath}{\hbar}g_{1D}|\psi_1(x, t)|^2 - \imath\Delta_{mw} & -\frac{\imath}{2}\Omega_{mw} \\ -\frac{\imath}{2}\Omega_{mw} & -\frac{\imath}{\hbar}V(x) - \frac{\imath}{\hbar}g_{1D}|\psi_2(x, t)|^2 \end{pmatrix},\tag{26.128}$$

and the solution,

$$\vec{\psi}(x, t) = e^{Mt} \vec{\psi}(x, 0) . \quad (26.129)$$

Let us now abbreviate the matrix by,

$$M = \begin{pmatrix} A & B \\ B & D \end{pmatrix} . \quad (26.130)$$

The matrix is diagonalized with the unitary transforms,

$$U = \frac{1}{\sqrt{2\Delta}} \begin{pmatrix} \frac{A-D}{2B} + \Delta & \frac{A-D}{2B} - \Delta \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad U^{-1} = \frac{1}{\sqrt{2\Delta}} \begin{pmatrix} 1 & -\frac{A-D}{2B} + \Delta \\ -1 & \frac{A-D}{2B} + \Delta \end{pmatrix} . \quad (26.131)$$

The eigenvalue matrix is,

$$U^{-1}MU = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \quad (26.132)$$

with  $E_{1,2} = \frac{1}{2}A + \frac{1}{2}D \pm B\Delta$ . Here we used the abbreviation  $\Delta = \sqrt{\left(\frac{D-A}{2B}\right)^2 + 1}$ . The formal solution now reads,

$$\vec{\psi}(x, t) = \exp \left[ U \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} U^{-1}t \right] \vec{\psi} = U \begin{pmatrix} e^{E_1 t} & 0 \\ 0 & e^{E_2 t} \end{pmatrix} U^{-1} \vec{\psi}(x, 0) . \quad (26.133)$$

This formula can easily be computed, because the block matrices of transform  $U$  are diagonal in  $x$ .

## 26.8.3 Wavepacket propagation

### 26.8.3.1 1D simulations

We want to describe the one-dimensional evolution of an atomic wavepacket according to the Schrödinger equation. The problem is fully described by [554],

$$i\hbar \frac{\partial}{\partial t} \psi(z, t) = \frac{-\hbar^2}{2m} \frac{d^2}{dz^2} \psi(z, t) + V(z)\psi(z, t) . \quad (26.134)$$

Numerically the Schrödinger equation is integrated via,

$$\psi(z, t + dt) = \psi(z, t) + dt\dot{\psi}(z, t) . \quad (26.135)$$

The initial state of the wavepacket is set to  $\psi(z, 0) = e^{-z^2/2z^2} e^{ikz}$ , where  $k \equiv \sqrt{2mE}/\hbar$  is its wavevector.

The numerical propagation is conveniently done with the time-splitting spectral algorithm [45, 44, 43, 256].

The flux is,

$$\psi \nabla \psi = 0 . \quad (26.136)$$



### 26.8.3.2 2D simulations

We want to describe the two-dimensional evolution of an atomic wavepacket according to the Schrödinger equation. The problem is fully described by,

$$\frac{-\hbar^2}{2m} \left( \frac{d^2}{dx^2} + \frac{d^2}{dz^2} \right) \Psi(x, z, t) + V(x, z) \Psi(x, z, t) = i\hbar \frac{\partial}{\partial t} \Psi(x, z, t). \quad (26.137)$$

Since the potential is conservative, we separate the time-evolution,

$$\Psi(x, z, t) = \psi(x, z) e^{-iEt/\hbar} \quad (26.138)$$

The initial shape of the wavefunction moving along the  $y$  coordinate could be a Gaussian,

$$\psi(x, z) = \psi_x(x, 0) \psi_z(0, z) = (2\pi\sigma_x\sigma_z)^{-1/2} e^{-x^2/4\sigma_x^2 - z^2/4\sigma_z^2}. \quad (26.139)$$

We can assume  $\sigma_z \gg \sigma_x$  and obtain an effectively one-dimensional model,  $E = E_{k_z}$ . Set,

$$\psi(x, z, 0) = \phi(x, z) e^{-ik_z z} \quad (26.140)$$

and,

$$-\frac{d^2}{dz^2} \phi(x, z) + 2ik_z \frac{d}{dz} \phi(x, z) = \frac{d^2}{dx^2} \phi(x, z) + \left[ \frac{2m}{\hbar^2} E_{k_z} - \frac{2m}{\hbar^2} V(x, z) - k_z^2 \right] \phi(x, z), \quad (26.141)$$

and,

$$\frac{d}{dz} \phi(x, z) = \frac{d^2}{dx^2} \phi(x, z) - \frac{2m}{\hbar^2} V(x, z) \phi(x, z) \quad (26.142)$$

$$\frac{d}{dz} \phi(x, z) = \frac{1}{2ik_z} \frac{1}{dx^2} [\phi(x - dx, z) - 2\phi(x, z) + \phi(x + dx, z)] - \frac{m}{ik_z \hbar^2} V(x, z) \phi(x, z).$$

Discretize in steps  $dz$ .

### 26.8.3.3 Reflection from a potential barrier

Now we allow for a change of direction. We assume that a matter wave with wavevector  $\mathbf{k}_0 = k_{0x} \hat{\mathbf{e}}_x + k_{0y} \hat{\mathbf{e}}_y = k_0 \hat{\mathbf{e}}_x \sin \alpha + k_{0y} \hat{\mathbf{e}}_y \cos \alpha$ , runs towards a potential step. If the step is sharp,  $V(x) = V_1 \theta(-x) + V_2 \theta(x)$ , the following ansatz is reasonable,

$$\psi_0(x, y) = e^{ixk_x + iyk_y} \quad (26.143)$$

$$\psi_1(x, y) = r e^{-ixk_x + iyk_y}$$

$$\psi_2(x, y) = t e^{ixk'_x + iyk_y}$$

and we have to solve the equations,

$$\begin{aligned} \frac{-\hbar^2}{2m} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) (\psi_0 + \psi_1) &= (E - V_1) (\psi_0 + \psi_1) \\ \frac{-\hbar^2}{2m} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) \psi_2 &= (E - V_2) \psi_2. \end{aligned} \quad (26.144)$$

In the step is smooth,  $V(x \rightarrow -\infty) = V_1 < V_2 = V(x \rightarrow \infty)$ , the situation is more complicated. Let us set  $V(x) = (V_1 - V_2) \frac{1}{\pi} \arctan x + \frac{1}{2}(V_1 + V_2)$ .

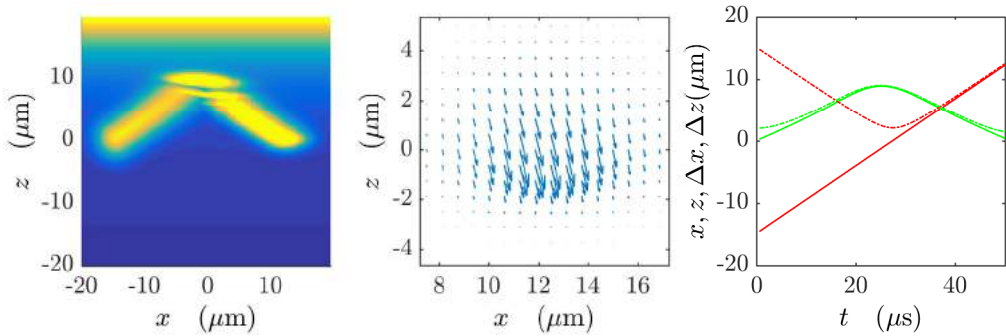


Figure 26.9: (code) Reflection of a wavepacket at a potential barrier. Do evanescent matter waves propagate along the barrier? Is there an atomic analogue to the Goos-Hänchen shift?

## 26.8.4 Exercises

### 26.8.4.1 Ex: Propagation of wavefunctions

Programs on the propagation of wavefunctions.

### 26.8.4.2 Ex: Programs on wavepackets reflected from potential barriers

Programs on wavepackets reflected from potential barriers.

## 26.9 Further reading

F. Dalfovo et al., *Theory of Bose-Condensation in Trapped Gases* [\[DOI\]](#)

Ph.W. Courteille et al., *Bose-Einstein Condensation of Trapped Atomic Gases* [\[DOI\]](#)

A.J. Leggett, *Bose-Einstein condensation in the alkali gases Some fundamental concepts* [\[DOI\]](#)

C.J. Myatt et al., *Production of Two Overlapping Bose-Einstein Condensates by Sympathetic Cooling* [\[DOI\]](#)

W. Ketterle et al., *Making, probing and understanding Bose-Einstein condensates* [\[DOI\]](#)



# Chapter 27

## Superfluid and coherent properties of Bose-Einstein condensates

Superfluid liquids or gases are distinguished by their ability to sustain flow without dissipation, i.e. flow which is free of viscous damping. The phenomenon of superfluidity is a well-known property of liquid  $^4\text{He}$ , but the relationship between superfluidity and Bose-Einstein condensation in this strongly interacting system is not trivial. The situation is much simpler in weakly interacting Bose gases, where the superfluid fraction is almost identical with the condensed fraction and the normal phase of the fluid with the thermal fraction. The availability of dilute gas Bose-Einstein condensates now offers the unique opportunity to study the complicated interdependence between superfluidity and condensation.

### 27.1 Superfluidity in quantum gases

The *superfluidity* of a gaseous condensate, which is one of its most apparent properties, is intrinsically linked to interatomic collisions. To characterize this phenomenon, it is useful to define some parameters. In the local-density approximation, the *homogeneity* of a gas of  $N$  atoms with the thermal de Broglie wavelength (24.9) confined inside a harmonic trap with the ground state size defined by (3.82), is characterized by,

$$\frac{k_B T}{\hbar\omega_{trp}} = \frac{2\pi a_{trp}^2}{\lambda_{therm}^2} . \quad (27.1)$$

For a typical experimental situation,  $k_B T/\hbar\omega_{trp} \approx N^{1/3} \approx 100$ . This shows that the assumption of a locally homogeneous gas is generally a good approximation. With the definition of the *healing length* (26.69), the degree of superfluidity of a condensate with density  $n$  can be cast into the form,

$$\frac{gn}{\hbar\omega_{trp}} = \frac{a_{trp}^2}{\xi^2} . \quad (27.2)$$

For a typical experimental situation,  $a_{trp}^2/\xi^2 \approx 100$ . A parameter that well characterizes the importance of interatomic forces within a condensate is the gas *dilution*,

$$na_s^3 = \frac{a_s^2}{8\pi\xi^2} . \quad (27.3)$$

The typical numerical value  $na_s^3 \approx 10^{-5}$  shows, that atomic gases are usually very dilute, although interatomic forces play an important role in the dynamics of condensates. In contrast, three-body collisions can be totally neglected, because the probability to have three atoms close to each other is even lower than the probability for two atoms.

There are several manifestations of phenomena linked to superfluidity, such as the behavior of collective elementary excitations, superfluid flow of non-circulating topological modes, quantized flux in vortices and matter wave solitons, which will be discussed in the following sections.

### 27.1.1 Landau's criterion for superfluidity

According to Landau, the phenomenon of superfluidity is rooted in the particular character of the Bogolubov spectrum of elementary excitations (26.54). Let us consider a bosonic fluid at a given temperature moving with velocity  $v$ . A macroscopic obstacle in the path of the superfluid can generate elementary excitations. That is, a fraction of the kinetic energy of the fluid is transferred to these excitations, thereby decelerating the fluid and causing *viscosity*. With the excitation energy  $\mathcal{E}(p)$  and the momentum  $\mathbf{p}$ , the total energy of the fluid interacting with the obstacle is,

$$E = \mathcal{E}(p) + \frac{(\mathbf{p} + M\mathbf{v})^2}{2M} = \mathcal{E}(p) + \mathbf{p} \cdot \mathbf{v} + \frac{1}{2}Mv^2 + \frac{p^2}{2M} \simeq \mathcal{E}(p) + \mathbf{p} \cdot \mathbf{v} + \frac{1}{2}Mv^2 , \quad (27.4)$$

where  $M$  is the total mass of the superfluid. Since the term  $Mv^2/2$  is the initial kinetic energy of the fluid,  $\mathcal{E}(p) + \mathbf{p} \cdot \mathbf{v}$  represents the excitation energy. And since the kinetic energy of the superfluid can only be diminished by the excitation, we need  $\mathcal{E}(p) + \mathbf{p} \cdot \mathbf{v} < 0$ . Finally, as  $\mathcal{E}(p)$  must be positive, the condition for generating elementary excitations is,

$$\mathcal{E}(p) \leq pv , \quad (27.5)$$

where  $\mathbf{p}$  and  $\mathbf{v}$  are antiparallel.

Therefore, there is a relative *minimum velocity* between the fluid and the obstacle, called *critical Landau velocity*, for creating excitations,

$$v_c = \min \left( \frac{\mathcal{E}(p)}{p} \right) . \quad (27.6)$$

For velocities below  $v_c$ , it is impossible to generate excitations, and there is no mechanism to decrease the kinetic energy of the fluid. As a result, the system becomes superfluid [422].

The spectrum of elementary excitations for a weakly interacting condensate, is the Bogolubov spectrum (26.54). The graph Fig. 27.1 shows, that for velocities below the sound velocity given by (26.56),  $v < c_s$ , the curve representing the propagation of

the perturbation does not cross the Bogolubov spectrum. That is, the perturbation can not be converted into excitations, which is only possible when  $v > c_s$ .

In an ideal condensate without interactions,  $a_s = 0$ , the Bogolubov spectrum reduces to the quadratic dispersion relation of free particles, which means that there is no critical velocity,  $v_c = c_s$ . Consequently, it is always possible to excite the condensate, that is, an ideal condensate can not be superfluid, and, as first pointed out by Landau: *superfluidity and Bose-Einstein condensation are different phenomena*.

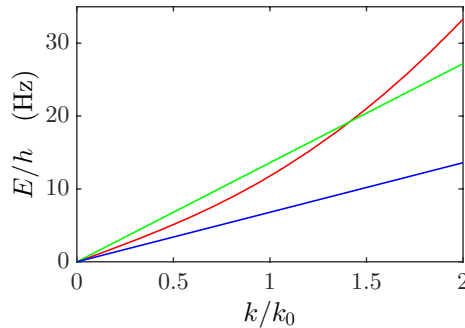


Figure 27.1: (code) Landau's criterion for superfluidity. Slow perturbations (blue line) do not cross the Bogolubov spectrum (red line) and do not generate excitations. Rapid perturbations (green line) cross the spectrum and can be dissipated.

### 27.1.2 Impurity scattering

A first hint for the superfluid nature of Bose-Einstein condensates is the fact that the hydrodynamic theory of superfluidity describes well the collective excitations (see Sec. ??). Moreover, several experiments provided direct evidence for the superfluid nature of condensates. For example, via a calorimetric measurement [569]: A condensate, stirred around by a rotating far blue-detuned laser beam, dissipated atoms to the thermal fraction of the atomic cloud, provided the stirring velocity exceeded a certain *critical velocity*  $v_c$ : At lower velocities, the perturbation did not lead to dissipation. At higher velocities, phonons were excited and the cloud was heated. In a subsequent experiment, perturbation-induced density fluctuations were observed *in vivo* and *in situ* [528]. When the stirring speed was below the critical velocity, the density was almost homogeneous, thus indicating superfluid flow. When, however, the stirring speed exceeded  $v_c$ , atoms piled up in front of the stirring beam, and the resulting pressure gradients led to a turbulent flow around the perturbation and to dissipation.

The critical velocity  $v_c$  found in the stirring experiments was about ten times smaller than the local sound velocity  $c_s$ ,

$$c_s \equiv \sqrt{\frac{gn}{m}} = \frac{\hbar}{\sqrt{2m\xi}}. \quad (27.7)$$

In fact, while the onset of dissipation is accelerated by turbulence around the *macroscopic object* traversing the superfluid, the local sound velocity (27.8) is derived for

a *microscopic object*. Puzzled by this discrepancy, Chikkatur *et al.* [131] studied the motion of microscopic atomic impurities through a condensate. The *impurity* was created by transferring a few atoms out of the original BEC from the trapped state  $|F = 1, m_F = -1\rangle$  to the free state  $|F = 1, m_F = 0\rangle$  via induced Raman transitions. The initial velocity was adjusted by the laser beams exciting the Raman transition (polarization, incident angle and relative detuning) to satisfy the Bragg condition (see Sec. 28.2). After the free impurity passed through the BEC, the trap was switched off, a Stern-Gerlach magnetic field gradient was pulsed to separate atoms in different Zeeman states, and finally the atoms were detected via time-of-flight imaging (see Sec. 24.6.1). When the initial velocity of the impurity was well above a critical value given by the local velocity of sound, ultracold *s*-wave collisions between impurity atoms and the stationary condensate distributed the momenta of the collision partners uniformly. In TOF images this appeared as a *circular halo* centered around the center-of-mass momentum of the collision partners (see Fig. 27.2). When, however, the initial velocity of the impurity was reduced, its collision rate with the stationary condensate was suppressed and the trajectory became superfluid.

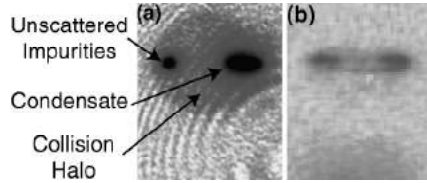


Figure 27.2: (a) Scattering of impurities at velocities above the critical velocity. The presence of a halo indicates the occurrence of collisions between the impurity and the condensate dissipating the relative kinetic energy. (b) For velocities below the critical velocity the halo disappears.

### 27.1.3 Hydrodynamic theory of superfluidity

For the description of superfluidity a hydrodynamic theory is adequate. Therefore, we will rewrite the time-dependent Gross-Pitaevskii equation (26.21). We consider the general case, in which the external potential  $V_{trp}(\mathbf{r}, t)$  depends on time. The wavefunction can be written by defining the density and the velocity fields,

$$\begin{aligned}\phi(\mathbf{r}, t) &= \sqrt{n_0(\mathbf{r}, t)} e^{i\theta(\mathbf{r}, t)} \\ \mathbf{v}_s(\mathbf{r}, t) &= \frac{\mathbf{j}(\mathbf{r}, t)}{n_0(\mathbf{r}, t)} = \frac{1}{2im} \frac{1}{n(\mathbf{r}, t)} [\phi^*(\mathbf{r}, t) \nabla \phi(\mathbf{r}, t) - \nabla \phi^*(\mathbf{r}, t) \phi(\mathbf{r}, t)].\end{aligned}\quad (27.8)$$

This gives,

$$\mathbf{v}_s(\mathbf{r}, t) = \frac{\hbar}{m} \nabla \theta(\mathbf{r}, t). \quad (27.9)$$

From the GPE we derive the continuity and the Navier-Stokes equations:

$$\begin{aligned}\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{v}_s n) &= 0 \\ m \frac{\partial \mathbf{v}_s}{\partial t} + \nabla \cdot \left( V_{trp} + gn - \frac{\hbar^2 a}{2m\sqrt{n}} \nabla^2 \sqrt{n} - \mu + \frac{m}{2} \mathbf{v}_s^2 \right) &= 0.\end{aligned}\quad (27.10)$$

We can see that the hydrodynamic behavior of a BEC depends greatly on the quantum phase  $\theta$ . When the kinetic pressure is small compared to the mean-field energy,

$$m \frac{\partial \mathbf{v}_s}{\partial t} + \nabla \left( V_{trp} + gn + \frac{m}{2} \mathbf{v}_s^2 \right) = 0 . \quad (27.11)$$

This is the *Euler equation* for a fluid with a potential flow. This equation and the *continuity equation* have the typical structure of equations describing superfluids at  $T = 0$ . This is due 1. to the presence of a Bose-Einstein condensate allowing us to formulate an equation for a complex *order parameter*, and 2. to the presence of interactions, included via the pressure term in the Euler equation, which are necessary condition for superfluidity.

At zero temperature, the entire fluid is superfluid. Moreover, in the Gross-Pitaevskii approximation, the whole fluid is condensed. Therefore,  $\mathbf{v}_s(\mathbf{r}, t)$  is the velocity flow of the superfluid <sup>1</sup>.

## 27.2 Topological modes

Significant manifestations of superfluidity are associated with rotational phenomena. An example is the occurrence of *scissor modes* [293], which are excited, when an angular momentum is suddenly applied to a condensate confined in an anisotropic trap. This can be done via a sudden reorientation of the symmetry axis of the trap [454, 453]. The condensate responds to this perturbation by an oscillation of its inclination implemented by an *irrotational superfluid flow*. The excitation spectrum reflects the strong reduction of the inertial momentum for superfluids.

The most rigorous manifestation of superfluidity, however, is the occurrence of a quantized and persistent current, called *quantized vortex*. In contrast to the elementary excitations, which must be created by perturbations, the vortex is a *stationary* (or *topological mode*) solution of the Gross-Pitaevskii equation Eq. (26.21).

Work on vortices has been done by [464, 448, 569, 528, 131, 293, 454, 449, 129, 14, 587, 203, 360, 116, 750].

### 27.2.1 Vortices

From Eq. (27.9) it is easy to see, that the superfluid is non-rotational, that is,

$$\nabla \times \mathbf{v}_s(\mathbf{r}, t) = 0 . \quad (27.12)$$

This raises the question, how vortices are possible. The solution to this apparent contradiction is, that Eq. (27.12) does not apply, when the phase exhibits a singularity. Consider, for example, a closed loop  $C$  around the singularity. In a vortex, the superfluid current is pulled by the phase gradient,  $\mathbf{v} = \frac{\hbar}{m} \nabla \theta$ . For the condensate wavefunction to be well defined, the phase variation  $\Delta \theta$  around the loop must be a multiple of  $2\pi$ , that is,

$$\Delta \theta = \oint_C \nabla \theta \cdot d\mathbf{l} = 2\pi \ell . \quad (27.13)$$

<sup>1</sup>This is not the case for strongly interacting superfluids, such as superfluid helium, where the normal fluid fraction is considerable.



where  $\ell$  is an integer. Therefore, we can calculate the *circulation*  $\Gamma$  around the closed loop, that is,

$$\Gamma = \oint_C \mathbf{v}_s(\mathbf{r}, t) \cdot d\mathbf{l} = \frac{h}{m} \ell. \quad (27.14)$$

Apparently, the superfluid circulation is quantized in units of  $\hbar/m$ . The parameter  $\ell$  is called *charge of the vortex* and measures, in unit of  $h$ , the quantized angular momentum of the vortex.

In addition, the flow must be persistent, because its circulation can only be changed in a discontinuous way, by overcoming a discrete energy barrier, which requires energy coming e.g. from thermal excitations. Clearly, the normal (thermal) fraction of a gas can also have a circular flow. However, the disordered microscopic motion of each individual particle causes a viscous drag that prevents the persistence of the flow in the absence of a torque. This is in contrast to superfluid flow, which persists even without external torque. The issues of vortex stability, formation, and topology were addressed in recent experiments [463, 448, 449, 129, 14]. Solve the Excs. 27.2.6.1 and 27.2.6.2.

The kinetic energy per unit vortex length can be estimated from a semi-classical approach. First, we define as the mass density  $\rho_m$  of the superfluid. If  $n$  is the particle density,  $\rho_m = nm$ . The kinetic energy of a flux line at the radius  $r$  is,

$$\mathcal{E}_{kin} = \frac{1}{2} \rho_m v_s^2 = \frac{\hbar^2 \ell^2}{2m} \frac{n}{r^2}. \quad (27.15)$$

To obtain the kinetic energy per unit length, we integrate the expression (27.21) over a plane perpendicular to the vortex axis. Note, however, that the velocity field is  $v_s \propto r^{-1}$  and, therefore, can not be integrated from zero. Instead, we begin the integration at a radius given by the *healing length*  $\xi$ , which represents a measure of the vortex core size. Now, the kinetic energy per unit length is,

$$E_{semi} = \int_0^{2\pi} \int_{\xi}^R \mathcal{E}_{kin}(\mathbf{r}) r dr d\theta = \pi n \frac{\hbar^2 \ell^2}{m} \ln \frac{R}{\xi}. \quad (27.16)$$

Note, that a multiply charged vortex carrying the entire angular momentum  $\ell = \ell_0$  of the superfluid is energetically less favorable than an ensemble of  $\ell_0$  vortices with unit charge  $\ell = 1$ . Therefore, a multiply charged vortex is unstable and may decay to several single charge vortices.

To calculate exactly the energy of a vortex, we do the following ansatz,

$$\Phi_0(\mathbf{r}) = \phi(r, z) e^{i\ell\theta}, \quad (27.17)$$

we then solve the Gross-Pitaevskii equation (26.21) numerically, and calculate the expectation value of the energy of the vortex through the expression,

$$\langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \int d^3\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla \Phi_0(r, z)|^2 + V_{trp} |\phi(r, z)|^2 + g |\phi(r, z)|^4 \right], \quad (27.18)$$

where  $\hat{H}$  is the Gross-Pitaevskii Hamiltonian.

The calculation yields for energy per unit length of a single charge vortex in a uniform cylindrical condensate [543],

$$E_{unif} = \pi n \frac{\hbar^2}{m} \ln \left( 1.464 \frac{R}{\xi} \right), \quad (27.19)$$

which is very close to our semi-classical prediction. Although the wavefunction  $|\phi(r, z)|$  has no analytic form, it can be shown by a variational approach, that the trial wavefunction,

$$|\phi(r, z)| = \frac{nr}{\sqrt{2\ell^2\xi^2 + r^2}} \quad (27.20)$$

is a good approximation [543]. Note that the healing length  $\xi$  characterizes the size of the vortex. For a superfluid, we can calculate the total energy of the vortex exactly, because the fluid is confined in all directions,

$$E_{tot} = \frac{4\pi n_0}{3} \frac{\hbar}{m} \ln \left( 0.671 \frac{R_r}{\xi_0} \right), \quad (27.21)$$

where  $n_0$  and  $\xi_0$  are, respectively, the density and healing length at the center of the fluid.  $R_z$  and  $R_r$  are, respectively, the extensions of the cloud along the axial and radial directions within the Thomas-Fermi approximation.

### 27.2.1.1 Creation and detection of vortices

The first superfluid vortex was observed 1979 in  $^4\text{He}$  [744]. For gaseous condensates, two approaches have been employed to produce vortices. Either one stirs the atomic cloud in order to impart an angular momentum to it. This can be done by rotating the (anisotropic) trap during the process of forced evaporation with time-orbiting magnetic fields or with an optical spoon. The vortex state is formed when the critical temperature for condensation is crossed. An alternative method is to imprint a  $2\pi$  circular phase gradient into a previously created condensate. Indeed, the local phase of a matter wave can be manipulated via a local modification of the potential depth, which can be achieved by a Stark shift induced by a far-detuned laser beam [203]. Focused into a tiny spot which is moved across the condensate, the laser beam will create a phase gradient, which in turn will cause a velocity flow. It is important to force the local density at the center of the vortex to zero, which can be achieved via a proper design of the trapping potential (e.g., a Mexican hat-shaped potential), and let the BEC then relax to the vortex state.

A variation of this method [723] avoids the need for relaxation processes. In this configuration the phase gradient is created through a *local* Raman coupling between two internal atomic states (for example, in  $^{87}\text{Rb}$  the two trappable Zeeman states  $|F, m_F\rangle = |1, -1\rangle$  to  $|2, 1\rangle$ ). At the spots, where the focused Raman beams hit the condensate, atoms were dynamically converted from the ground state to the excited state. The circular trajectory of the spots and the rotation speed were calculated such as to generate a toroidal topology for the adiabatic population transfer. The process was coherent and allowed to directly construct and shape the vortex wave function. We study this experiment in more detail in the Exc. 27.2.6.3.

In confined single-species condensates the diameter of the vortex core is on the order of the healing length,  $2\xi$ . With typical values of  $2\xi \approx 0.4 \mu\text{m}$  it is thus way too small to be imaged *in situ*, and ballistic expansion times of several 10 ms are necessary. On the other hand, in double condensates formed by two repelling species (e.g. the two states  $|2, 1\rangle$  and  $|1, -1\rangle$  in  $^{87}\text{Rb}$ ), one of the species can form a vortex around the second. In this case, the diameter of the vortex core, is determined by the diameter of the condensate of the second species and, hence, much larger. When

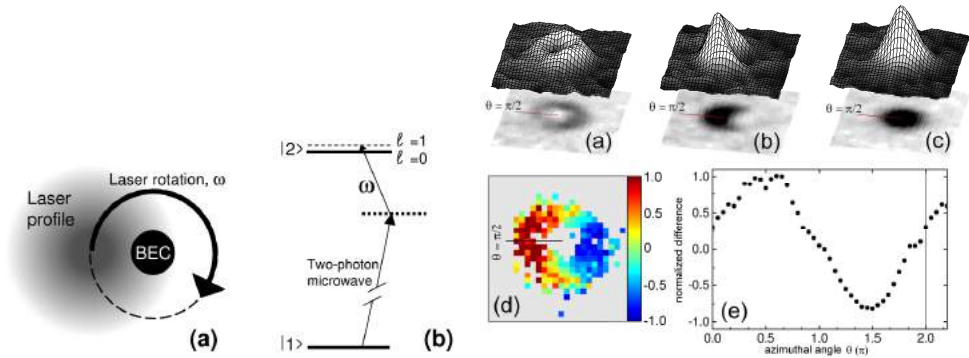


Figure 27.3: (Left) Scheme of the experiment [463]. (Medium) Level system used. (Right) Density distribution of a vortex state: (a) (the visible atoms are in the upper hyperfine state), (b) after a  $\pi/2$ -pulse and (c) after a  $\pi$ -pulse (the visible atoms are in the lower hyperfine state). The images (d) and (e) visualize the phase slip around the vortex.

the second species is selectively removed (e.g. by the radiative pressure exerted by a resonant laser), and the vortex in the first species can be studied by *in situ* imaging of the confined density distribution [464].

A particularly smart detection method for vortices is based on matter wave interferometry (see Sec. 27.3.3). Here, two matter waves, that is, the vortex state in  $|2, 1\rangle$  and a (reference) ground state BEC in  $|1, -1\rangle$  are coherently mixed via a resonant two-photon radiofrequency  $\pi/2$ -pulse. The resulting matter wave interference patterns reveal the phase profile of the vortex (see Fig. 27.3).

### 27.2.1.2 Stability

In a topologically 'singly-connected' trap, for example a potential harmonic, vortices do not represent the lowest energy eigenstate, and they must decay to the ground state. If the mean-field energy of the condensate is weak compared to the kinetic energy,  $gm_0/\hbar\omega_z \ll 1$ , the healing length will exceed the size of the BEC,  $\xi \gg a_{trp}$ , and the vortex rapidly decays by dissipating its excess energy to thermal excitation. Such BECs can not be considered superfluid. If the mean-field interaction is strong, the vortex spontaneously breaks azimuthal symmetry, moves away from the center and exits the condensate on a spiral-shaped trajectory [587]. Nevertheless, the decay time may be quite long.

On the other hand, a vortex can be the ground state of a 'multiply-connected' trap (for example, a toroidal potential). Such a potential can be realized as the temporal average of a harmonic potential with a small rotating anisotropy [448]. In such geometries vortices are extremely stable.

### 27.2.1.3 Vortex precession

A radial force acting on a vortex results in a radial displacement and a precession about the symmetry axis. The effect, known as *Magnus effect* [360], is due to pressure

imbalances on the vortex surface. A radial force naturally arises, when the core is displaced from the center, because local pressure gradients will force the vortex out of the center toward regions with lower densities. Experimentally, a slow precession ( $\sim 1$  Hz) spiraling the vortex toward the rim of the condensate has been observed [14] by taking a succession of nondestructive images.

### 27.2.2 Vortex lattices

Superfluid  $^4\text{He}$  in a rotating bucket spontaneously develops symmetrically organized vortex patterns. Similar phenomena can be observed, when a dilute gas Bose-Einstein condensate is forced to rotate [116] at a given frequency  $\Omega$ . The energy in the rotating system receives an additional contribution from the centrifugal term,  $U_{rot}(\mathbf{r}) = U_{trap}(\mathbf{r}) - \Omega L_z$ , where  $L_z = \hbar N l_z$ , and  $l_z = i(y\partial_x - x\partial_y)$  is the angular momentum of the individual atoms. If the rotation is slow, the energy  $\Omega L_z$  is too small to force the condensed wavefunction to rotate. If the rotation frequency is beyond a critical value  $\Omega_c$ , the *time-averaged* potential,  $U_{rot}(\mathbf{r})$  eventually develops a local minimum in the center, thus adopting the toroidal shape. For non-interacting gases, the critical frequency coincides with the radial secular frequency,  $\Omega_c = \omega_r$ . Then the radial restoring force of the trap does not balance the centrifugal force, such that atoms can escape from the trap. However, for superfluid gases the critical frequency is reduced,  $\Omega_c < \omega_r$ . Between the rotation frequencies  $\Omega = \Omega_c$  and  $\Omega = \omega_r$ , the state with the lowest energy in the toroidal potential is the vortex, whose filament is pinned to the symmetry axis. For even higher rotation frequencies, we could expect a single vortex with a larger winding number (more than the phase winding of  $2\pi$  for a single turn). However, individual multiple-order vortices in harmonic traps are unstable. Instead, vortex lattices [116] called *Abricosov lattices* will form. For a given trapping potential and mean-field energy, the symmetry of the lattice and the number of vortices depend on the rotation frequency  $\Omega$ . Counter-intuitively, the angular momentum of individual particles  $l_z$  is *not quantized*. When we vary  $\Omega$ , regimes of forbidden  $l_z$  (i.e. when no vortex pattern is formed) alternate with allowed regimes. The discontinuous transition from one vortex pattern to another is a first-order phase transition, which spontaneously breaks one symmetry to form another. An upper limit for the rotation speed is given by the equilibrium between the centrifugal force and the radial restoring force of the trapping potential at  $\Omega = \omega_r$ .



Figure 27.4: Abricosov vortex lattice.

These patterns of vortex lattices were observed in experiments using the *stirring method*, which consists in brushing a far-detuned focused laser ('optical spoon') around the rim of a condensate [448] at a certain frequency  $\Omega$ . In this experiment, the ratio of the mean-field energy to the kinetic energy was  $gn_0/\hbar\omega_z = a_{trap}^2/2\xi^2 > 100$ . Beyond a certain critical rotation frequency,  $\Omega_c \approx 2\pi \times 150$  Hz, a single central vortex

was formed. At even higher frequency, a symmetrical vortex lattice appeared in a transverse plane (see Fig. 27.4). Finally, at rotation frequencies near the radial trap frequency  $\omega_r$ , the condensate wavefunction became turbulent and finally disappeared. As soon as the optical spoon was removed, the vortex lattice gradually decayed losing the vortices one by one.

### 27.2.3 Solitons

Work on solitons has been done by [748, 722, 463, 723, 502, 578, 359, 513, 114, 35, 216, 110, 191].

#### 27.2.3.1 Dark solitons

Solitons are non-singular solutions of any equation satisfying,

$$|\psi(\mathbf{r}, t)| = |\psi(\mathbf{r} - \mathbf{v}t)|. \quad (27.22)$$

Solitons are well known to occur in non-linear optical media, for example in optical fibers, when dispersion is counterbalanced by self-phase modulation, such that optical signals propagate without spreading. The Gross-Pitaevskii equation is another example for a nonlinear wave equation supporting soliton-like solutions. States called *dark soliton* or *twisted state* with a dynamically stable density dip are expected in condensates with repulsive interactions [502, 578, 359, 513]. In contrast to topologically stable states, for example, vortices, dark solitons are pseudo-defects, the decay of which, even though it may be slow, is topologically trivial. Due of the greater freedom of movement of their wavefunctions, solitons can be distorted by complex deformations [114]. Soliton-like matter wave states were initially observed in superfluid  $^3\text{He-B}$  [35]. In dilute gases, the size of the solitons is of the order of healing length.

The first dark solitons in dilute gases were created by applying an inhomogeneous phase shift to a condensate [110, 191]. One half of the condensate was irradiated by a far-detuned laser pulse (detuning  $\Delta$ , Rabi frequency  $\Omega$ , duration  $\tau \ll \hbar/gn_0$ ) in order to advance the phase of this part of the condensate by  $\varphi = \Omega^2\tau/4\Delta$ . When the phase shift was set to  $\pi$ , an abrupt phase gradient developed at the boundary delimiting the two halves. The condensate reacted to the phase gradient by developing a deep density minimum all along the boundary corresponding to a soliton (see Fig. 27.5). The phase distribution can also be imaged by interferometric techniques based on Bragg diffraction (see Sec. 28.2). In one dimension, the density dip of the soliton corresponds to a node of the dipolar topological mode [723, 502, 513].

The abrupt phase gradient at the boundary plane exerts a force trying to increase the gap, while repulsive interactions work to heal it. At zero temperature, this balance ensures the dynamic stability of the soliton. While a perfect dark soliton should be stationary, experiments [110, 191] revealed that solitons with finite contrast propagate along the direction of the plane's normal vector with a velocity, which must always be less than the local sound velocity,

$$v_{sol} = c_s \sqrt{\frac{n_{sol}}{n}}, \quad (27.23)$$

where  $n$  is the peak density of the condensate and  $n_{sol}$  the density at the bottom of the dark soliton [578, 359]. Fig. 27.5 shows that the soliton develops a curvature

when it propagates. One reason for this is a slower sound velocity,  $c_s = \sqrt{gn_0/m}$ , on the edges of the condensate, where the density is lower. The second reason is, that the density in the dip,  $n_{sol}$ , goes to zero at the edges. In the presence of a thermal cloud, dissipation reduces the contrast of the density dip and accelerates the soliton, until it reaches the sound velocity  $c_s$  and finally disappears.

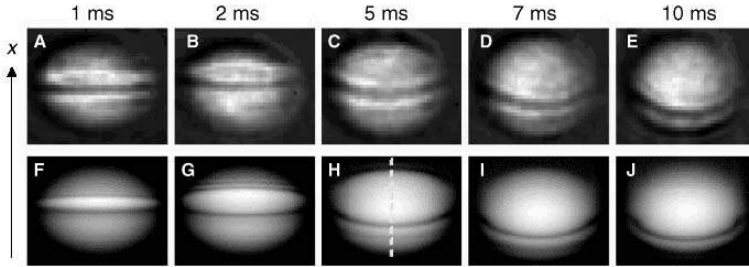


Figure 27.5: Solitons.

### 27.2.3.2 Bright solitons

In condensates with attractive interactions *bright solitons* have been observed, as well [393, 381].

### 27.2.4 Description of general topological modes

A coherent *topological mode* is a stationary solution of the *Gross-Pitaevskii equation*,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U_{tr}(\mathbf{r}) + \frac{4\pi\hbar^2 a_s}{m} N |\phi_n|^2 \right] \phi_n(\mathbf{r}) = E_n \Phi(\mathbf{r}) . \quad (27.24)$$

These modes can be calculated using an *optimized perturbation theory* [152]. We separate the Hamiltonian into an unperturbed part and a perturbed part,  $\hat{H} = \hat{H}_0 + \Delta\hat{H}$ , where the unperturbed part now depends on variational parameters,

$$\hat{H} = \hat{H}_0(u, v, ..) + \Delta H . \quad (27.25)$$

As usual, the first-order energy correction is,

$$E_n^{(1)}(u, v, ..) = E_n^{(0)}(u, v, ..) + \langle \Phi_n^{(0)} | \Delta\hat{H} | \Phi_n^{(0)} \rangle , \quad (27.26)$$

where the  $\Phi_n^{(0)} = \Phi_n^{(0)}(u, v, ..)$  are the solutions of the unperturbed Hamiltonian  $\hat{H}_0$ . Once the energies are found, we must minimize them in terms of the variational parameters,

$$\frac{\partial E_n}{\partial u} = 0 \quad , \quad \frac{\partial E_n}{\partial v} = 0 \dots . \quad (27.27)$$

With these parameters, we obtain the energies and the wavefunctions <sup>2</sup>.

<sup>2</sup>Excited modes can be understood stationary matter waves with the trap serving as a cavity.

### 27.2.4.1 Creation of topological modes

One possibility of creating topological modes is to apply a temporal modulation to the trapping potential [748]. The modulation frequency must be resonant with the energy difference between the excited mode and the ground state. Another possibility is to vary the interaction energy via a modulation of the scattering length in the vicinity of a *Feshbach resonance* [156].

The steady-state situation of a cloud in a stationary trap is *thermal equilibrium*, that is, inversion is not possible. At a time-dependent (e.g. shaking) potential however, for example, transitions to excited vibrational levels can be driven. These can generate inversion, provided collision-induced relaxation is not too fast <sup>3</sup>.

### 27.2.5 Turbulence

The issue of turbulence is one of the most important problems of classical physics yet to be solved [236]. In superfluids, restrictions imposed by quantum mechanics constrain the emergence of turbulence, which is then called *quantum turbulence*. On the other hand, the study of quantum turbulence can improve our understanding of *classical turbulence* [209]. Recently, the study of the dynamics of an ensemble of vortices in a Bose-Einstein condensate allowed the identification of signatures of quantum turbulence [326, 310].

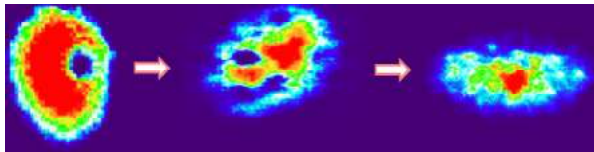


Figure 27.6: Turbulence.

### 27.2.6 Exercises

#### 27.2.6.1 Ex: Comparison between the quantum and the classical vortex

Consider a vortex around a straight line along the  $z$ -axis at  $r = 0$ . Compare the radial velocity variation of a quantum vortex with that of a classical one.

#### 27.2.6.2 Ex: Singularity in vortices

Show for the above simple example,

$$\nabla \times \mathbf{v}_s(\mathbf{r}, t) = \hat{\mathbf{z}} \frac{\ell \hbar}{m} \delta(x) \delta(y) .$$

<sup>3</sup>The dynamics of atoms trapped in a harmonic potential is similar to the Jaynes-Cummings dynamics of an optical mode. However, the non-linear condensate self-interaction changes the situation and makes the collisions being collective.

### 27.2.6.3 Ex: Phase-engineering of a vortex state

The first vortex in a dilute gas was created at the JILA [464]. Study the paper and explain in detail, how the vortex was created.

## 27.3 Atom optics

Unlike the photons [421], there is no doubt about the fact that atoms are particles. On the other hand, the deep analogy between light and matter, resulting from the particle-wave duality, prompted de Broglie in 1924 to ascribe a *wave* to each massive particle, whose wavelength would be a function of the particle's momentum. Whether an atom behaves more like a particle or a wave depends on the specific experimental situation. For example, interferometers emphasize its wave nature: Atoms are able to interfere with *themselves*, when their Broglie wavelength is coherently split and then recombined. (Bosonic) atoms are able to interfere with other atoms, if their de Broglie wavelengths are greater than their distances. For this to happen, it requires high densities and very low temperatures, that is, high phase space densities. When the phase space densities are so high that the Broglie waves come into contact, effects of quantum statistics begin to influence the dynamics of the atoms, and fermions will behave differently from bosons.

Analogously to the distinction between classical and laser optics, we can separate the area of conventional atomic optics working with individual, mutually incoherent atoms, from the area of coherent atomic optics working with Bose-Einstein condensates. Unlike for the study of phenomena related to superfluidity, gases with weak interatomic interactions are generally more useful for the study of the coherent properties of condensates and for application in atomic optics. Nevertheless, interatomic collisions increase the complexity of the dynamics of matter waves interacting with atom optical devices, by introducing non-linearities analogous to those known from nonlinear optics and thus raising the field of *nonlinear atom optics*.

### 27.3.1 Atomic optical tools

The basic equipment of an atomic optics laboratory [491, 3, 548, 246, 564] comprises atomic beams, atom traps, lenses and waveguides, various types of mirrors and resonators, Stern-Gerlach type matter wave polarizers, de Broglie wave phase shifters based on Bragg diffraction, and a multitude of atomic beam gratings. Obviously, gratings allow the construction of atom interferometers, which are used in experiments and high precision devices, for example, atomic gyroscopes and gravimeters. Other applications for atomic beams controlled by atom optical elements are in atomic holography for the projection of complex pattern into integrated semiconductor circuits [503], in lithography [687], and in microscopy [202].

An important feature of atoms (as compared to light) is the existence of a rich internal structure providing a wealth of additional degrees of freedom, whose dynamics (of the Bloch vector) is frequently entangled with the motional dynamics (of the de Broglie wave). This allows to monitor (e.g. in matter wave interferometers) the evolution of the motional state of the matter wave via an observation of the internal



excitation. Moreover, in some interferometers, the de Broglie wave is not even split, and one does interferometry with completely immobile atoms or ions [347].

The epitome of a coherent light source is the laser, and we may ask whether there is a material analogue, which would be a source of coherent matter [728, 95, 649, 338, 510, 400] serving for *coherent atom optics*. In fact, we may already consider a trapped condensate as a stationary *atom laser* pulse with the trapping potential playing the role of the laser resonator. While most atom optical devices (including conventional atomic interferometers) do not require mutual coherence of atoms, certain applications take advantage of an intense, highly directional, monochromatic, and coherent atom source. In this respect, atom lasers are much superior to thermal atomic beams. While a thermal beam contains about  $10^{-12}$  atoms per mode and a magneto-optical trap about  $10^{-6}$ , a condensed mode may contain more than  $10^6$  atoms. Condensates offer the advantage of large de Broglie wave amplitudes and de Broglie wavelengths as long as their actual size (which can be much longer than optical wavelengths). And for an atom laser, the coherence length can even be longer than that of the condensate from which it emerged. This obviously has a major impact on the sensitivity and resolution of atom optical elements, in particular those, where atomic coherence is important, for example, atom interferometers. Without doubt atom lasers will replace conventional atomic beams in precision measurement of fundamental constants and tests of fundamental symmetries ([Phys. World (mar,97) p.43]). Finally, atom lasers are crucial for nonlinear optics.

Also of interest are the references [648, 503, 570, 423, 590, 41, 325, 213, 563, 190, 335, 579, 358, 612, 67, 202, 716].

## 27.3.2 The atom laser

A large number of techniques for making an *atom laser* has already been developed [476, 20, 482, 15, 80, 300, 458] and theories on atom lasers have been formulated [298, 508, 727, 706, 348]. The following sections are devoted to explaining, why the term atom laser is justified. For the reasoning we will let as guide by the optical laser.

We already mentioned the *trapping potential* (replacing the resonator in lasers) as a major ingredients of an atom laser <sup>4</sup>. Another necessary feature would be the availability of an *output coupling* mechanism, which we still need to discuss in the following. Apart from these more practical aspects, we need to prove, that atom lasers are indeed *phase-coherent*, and we have to clarify the role of *bosonic stimulation* and of *irreversibility* in the production process of a BEC.

### 27.3.2.1 Bosonic stimulation and irreversibility

The gain mechanism for optical lasers is photonic stimulation of atoms inciting them to emit other photons into the stimulating mode. The atomic laser operates in a similar way. Atoms trapped in a potential constitute a thermal reservoir. Binary collisions redistribute the atoms among the vibrational energy levels of the potential. If a vibrational level already contains an atomic population, Bose-Einstein quantum

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<sup>4</sup>Coherent reflection of atom laser beams has been demonstrated [88, 22, ?], and an atom laser cavity with efficient transverse focusing has been built [82]

statistics will encourage atoms involved in a collision process to join this level. Ultimately, this comes down to an irreversible pumping of a single level, where the atoms accumulate to build a single degenerate quantum state. Bose condensation is always the result of *bosonic stimulation*. However, the dynamics and time scale for the formation of a condensate have been controversially discussed, until some experiments [482] could directly visualize *in vivo* the process of nucleation and the exponential amplification at the center of a thermal cloud (see Fig. 27.7).

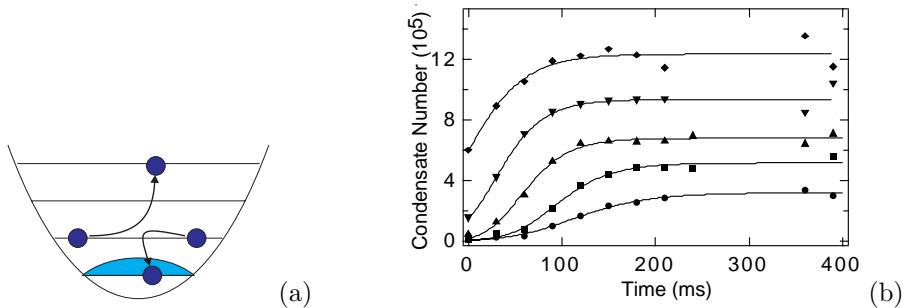


Figure 27.7: (a) Illustration of the idea of bosonic stimulation. (b) The curves show the growth of a condensate toward thermal equilibrium for different initial numbers of condensed atoms.

The very high concentration of population in a single phase space cell during the creation of a condensate represents a dramatic reduction of entropy. Since the total entropy can not decrease, the condensate must be coupled to a thermal reservoir receiving the excess entropy. This coupling is necessarily irreversible. In practice, the reservoir is the cloud of thermal atoms, whose energy is spread over many vibrational states. Irreversibility is introduced by collisions and the subsequent removal of the hottest atoms.

### 27.3.2.2 Phase of a condensate and first and higher-order coherences

First-order coherence and long-range order are necessary conditions for assigning a single global phase to the condensate. The existence of a single phase, and the possibility of measuring it, were questioned in the past. Certainly, the phase of a BEC is not observable *by itself*, but only *the relative phase* of two condensates.

The intrinsic phase-coherence of condensates has demonstrated in many experiments. An early example [304] employed internal state interferometry by splitting and remixing  $^{87}\text{Rb}$  condensates trapped in the different Zeeman states  $|F, m_F\rangle = |1, -1\rangle$  and  $|2, 1\rangle$ . They found that the phase was remembered for times longer than 150 ms. In another experiment [17, 390, 706], illustrated in Fig. 27.8, a condensate was spatially split in two halves and then recombined. The interpenetration of the two halves at a well-defined relative velocity gave rise to a clear matter wave interference pattern. This ability of ballistically expanding condensates to interfere demonstrated the absence of a random phase lag during the expansion process and that the preservation of the condensates' long range order. However, under the repulsive influence of the mean-field energy, the phase profile of a released condensate evolves in a non-uniform

but well-defined manner [636].

The homogeneity of the phase of a *confined* condensate was also confirmed experimentally [660, 299, 81] through interferometric techniques based on Bragg diffraction (see Sec. 28.2.2). The spatial coherence of an output coupled atom laser has been verified with a double-slit experiment [81]. And the temporal coherence of an atom laser beam was shown to be Fourier-limited by the finite output coupling time [?].

Similar to Young's double slit experiment in optics, the observation of matter wave interference only indicates first-order coherence, i.e. amplitude fluctuations in the matter field. Signatures for the presence of higher-order coherences in condensates were discovered in other experiments: The second-order correlation function, which represents a measure for intensity fluctuations (number of particles) in the matter field, was derived from measurements of the condensate's release energy [392]. And the third-order coherence can be deduced from a comparison of the three-body recombination rates for condensed and thermal clouds [113].

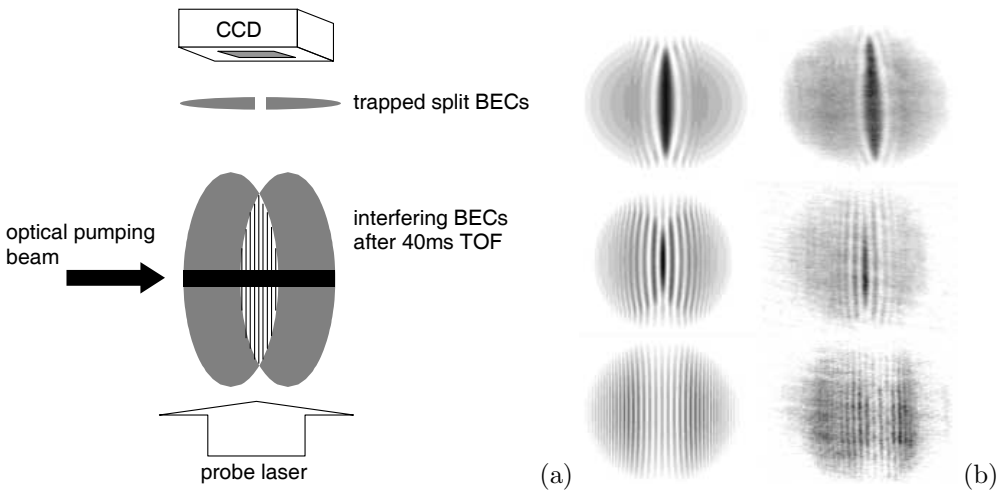


Figure 27.8: (a) Scheme for observation of matter wave interference. (b) Interference fringes.

A reliable characterization of atom number fluctuations and matter wave phase fluctuations in condensates is important for the simple reason, that these fluctuations will limit ultimately the resolution of atom interferometers, analogous to the *Schawlow-Townes limit* in lasers.

### 27.3.2.3 Output coupling

The *output coupler* for a trapped condensate plays a role similar to that of the partially reflecting mirror of a laser resonator. It transfers a fraction of condensed atoms out of the trapping potential through a coherent coupling to untrapped states. The coupling can be conveniently implemented via adiabatic potentials (see 18.1.3 and 24.4.3) generated by radiation (e.g. radiofrequency pulses [476] or continuous radiofrequency [80]). Also, pairs of laser beams in Raman configuration can create a coherent quasi-

continuous and well-collimated atomic beam [300] and tunneling can give rise to a pulsed mode-locked atom laser (*mode-locked laser*) [15].

A trapped condensate represents a *finite reservoir* from which an atom laser can be fed. For a really cw atom laser, an incoherent pumping mechanism, continuously feeding the BEC, while it delivers atoms to the atom laser, is still lacking [451].

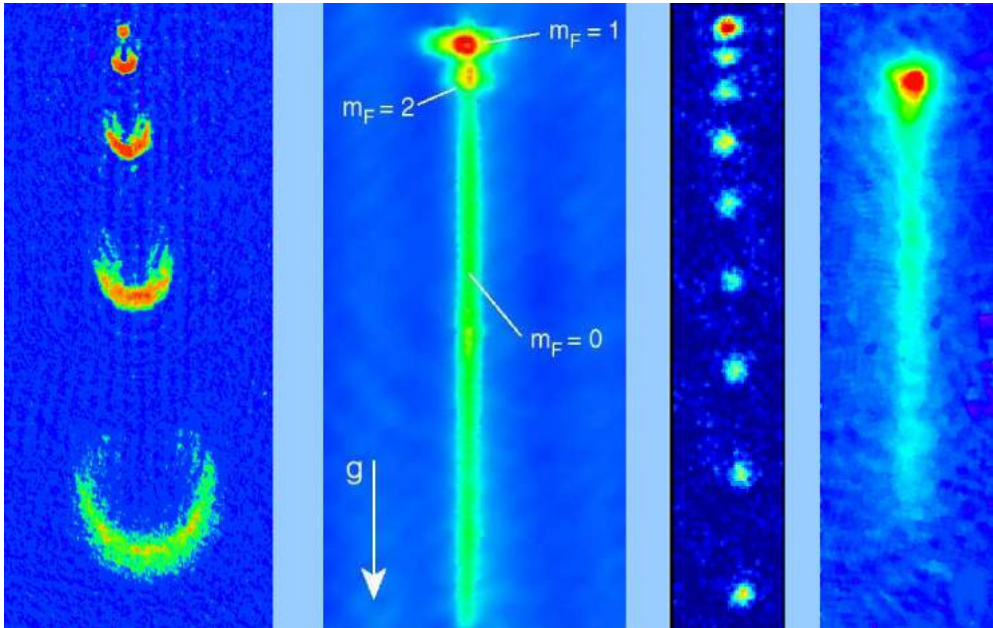


Figure 27.9: Several types of atomic lasers realized, from left to right at the MIT in 1997, in Munich in 1999, at Yale in 1998, and at NIST in 1999. The vertical sizes of the images are, from left to right: 5, 2, 0.5, and 1 mm.

### 27.3.3 Atomic interferometry with Bose-Einstein condensates

The most obvious use of an atom laser is within an atomic interferometer [661, 651, 89, 299, 81, 636, 392, 113, 533, 188, 489, 505]. Many types of interferometers have been developed over the years. First of all, we note that the interferometric idea can be realized in the spatial domain (e.g. an atomic beam passing through a light wave) or in the time domain (e.g. a trapped atomic cloud or an immobile trapped ion irradiated by a pulsed light) [94, 347, 571, 267].

Furthermore, depending on the involved degree of freedom (kinetic or internal excitation), we may distinguish two types of interferometers. Matter wave interferometers operating with the kinetic degree of freedom often use beam splitters based on Bragg diffraction [409, 533, 299, 636]. Matter wave interferometers involving internal degrees of freedom generally couple two species of condensates, that is, two condensates in different states of internal excitation, for example, in different Zeeman [662], hyperfine [514, 304, 489], or dressed states [427]. The phases of two BECs in different internal states, which we will call  $|\pm\rangle$ , evolve according to their respective chemical

potentials,  $\varphi_{|\pm\rangle}(t) = \mu_{|\pm\rangle}t$ . The accumulated phases are not directly observable, but their difference,  $\Delta\varphi(t)$ , can be measured by *Ramsey interferometry*.

### 27.3.4 Non-linear atomic optics

In classical nonlinear optics, the interaction between matter (e.g. dilute gases) and light is described by Maxwell's equations. The electromagnetic field  $\mathbf{E}$  creates a macroscopic polarization,

$$\mathbf{P}(\mathbf{r}, t) = \chi(\mathbf{E})\mathbf{E}(\mathbf{r}, t) = \chi^{(1)} \cdot \mathbf{E} + \chi^{(3)} : \mathbf{E}\mathbf{E}\mathbf{E} + \dots \quad (27.28)$$

which in turn acts back onto the field. Higher-order processes, such as *self-focusing*, *second-harmonic generation*, *four-wave mixing*, etc. are described by the non-linear susceptibility  $\chi^{(3)}$ . These processes require the presence of a non-linear medium (the vacuum polarization itself being too small [382, 290]).

The role of binary collisions in coherent matter wave optics, as described by the nonlinear term in the Gross-Pitaevskii equation (26.21), is very similar to the role of the third-order nonlinear susceptibility in quantum optics [428, 409, 189, 272, 690, 383, 312, 384, 430, 165, 314]. For example, if the atomic interaction is repulsive, the nonlinear term tries to increase the size of the condensate as much as possible within the limits imposed by the trapping potential. This behavior is analogous to the phenomenon of *self-defocusing* known in non-linear optics.

Small-amplitude elementary oscillations are well described by the *Bogolubov-de Gennes equations*, which are a linearized version of the Gross-Pitaevskii equation [152]. On the other hand, large-amplitude oscillations, which are sensitive to the nonlinear mean-field interaction [644], showed a splitting of the frequency for quasi-particle excitation, in analogy with the generation of the second-harmonic (*SHG*) in quantum optics [314].

Other phenomena, such as matter wave *phase conjugation* and four waves mixing (*4WM*) [272] have been observed in experiments [189]. The three matter wave modes for the nonlinear mixing were produced out of a single condensate by applying two short consecutive sequences of Bragg diffraction pulses. The condensates are created in the same spatial region, but at different times. The nonlinear mixing during the process of spatial separation was observed by time-of-flight images.

The geometry of the laser beams is shown in Fig. 27.10(a) in the laboratory system. A first standing wave light pulse is generated by lasers  $\mathbf{k}_1$  and  $\mathbf{k}_2$  detuned from each other by an amount, such that the Bragg condition is satisfied and the momentum  $\mathbf{p}_2 = \hbar\mathbf{k}_1 - \hbar\mathbf{k}_2$  is transmitted to the diffracted atoms. Then, a second standing wave light pulse formed by lasers  $\mathbf{k}_1$  and  $\mathbf{k}_3 = -\mathbf{k}_1$  transmits to the diffracted atoms the momentum  $\mathbf{p}_3 = 2\hbar\mathbf{k}_1$ . The duration and intensity of the standing waves are adjusted such as to create an approximately equal distribution of  $N_j^0$  atoms in all three condensate momentum modes, each mode having a different momentum,  $\mathbf{p}_1 = 0$ ,  $\mathbf{p}_2$ , and  $\mathbf{p}_3$ . Initially, the three wavepackets  $\hat{\psi}_j \equiv \psi_0(\mathbf{r})e^{i\mathbf{p}_j\mathbf{r}/\hbar}$  overlap. The nonlinear term in the Gross-Pitaevskii equation mixes the wavepackets while they separate to

form other wavepackets,  $\hat{\psi}_4 \sim g\hat{\psi}_j^+\hat{\psi}_m\hat{\psi}_n e^{i\mathbf{p}_4\cdot\mathbf{r}/\hbar}$ , where,

$$N_4 = -N_j + N_j^0 = N_m - N_m^0 = N_n - N_n^0 = \sum_{\kappa=1}^3 (N_\kappa^0 - N_\kappa) \quad (27.29)$$

$$\mathbf{p}_4 = -\mathbf{p}_j + \mathbf{p}_m + \mathbf{p}_n$$

$$p_4^2 = -p_j^2 + p_m^2 + p_n^2 .$$

To produce the new momenta,  $\mathbf{p}_4 \neq \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ , the corresponding wavepackets must gather atoms from all three initial packets  $\mathbf{p}_1 \neq \mathbf{p}_2 \neq \mathbf{p}_3$ .

The experimental observation of a newly emerging wavepacket  $\hat{\psi}_4$  has two complementary interpretations: In the inertial system defined by  $\mathbf{p}_1 = -\mathbf{p}_3$  [see Fig. 27.10(b)], the wavepackets  $\hat{\psi}_1$  and  $\hat{\psi}_3$  suffer elastic collisions. The direction in which the condensates are scattered is, a priori, isotropic. The injection of a third condensate  $\hat{\psi}_2$  bosonically stimulates the formation of a fourth one,  $\hat{\psi}_4$ , in a predefined direction  $\mathbf{p}_4 = -\mathbf{p}_2$ . The laws of conservation for the particle numbers, momenta, and energies (27.29) only allow processes, which can be interpreted as degenerate 4WM in this inertial system. Each of the wavepackets  $\hat{\psi}_1$  and  $\hat{\psi}_3$  sacrifice  $N_4$  atoms to create a new wavepacket  $\hat{\psi}_4$  and to amplify the wavepacket  $\hat{\psi}_2$ . The redistribution of atoms is a coherent process.

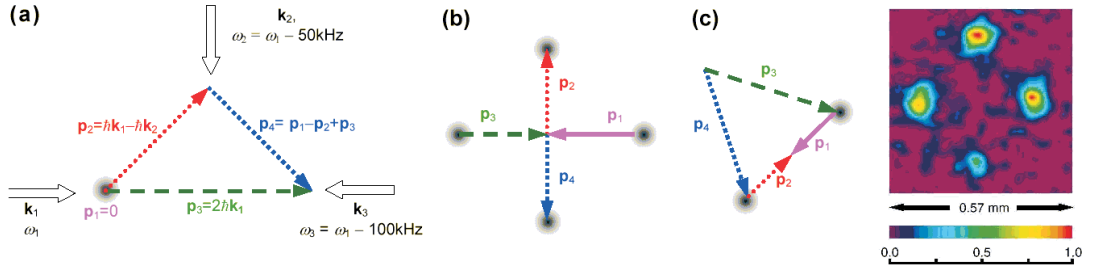


Figure 27.10: Matter wave 4WM can be illustrated (a) in the laboratory system, or (b) in the inertial system defined by  $p_1 = -p_3$ , or (c) in the system defined by  $p_1 = -p_2$ . In each system the process has a different physical interpretation (see text). The right image shows the experimental result.

The second interpretation becomes clear in the inertial system, in which  $\mathbf{p}_1 = -\mathbf{p}_2$  [see Fig. 27.10(c)]. The conservation of energy only allows scattering products satisfying  $p_4 = p_3$ , that is,  $\hat{\psi}_1^+\hat{\psi}_2\hat{\psi}_3$  and  $\hat{\psi}_2^+\hat{\psi}_1\hat{\psi}_3$ . In this system, the process can be interpreted as Bragg diffraction of the wavepacket  $\hat{\psi}_3$  by the matter wave lattice formed by  $\hat{\psi}_1$  and  $\hat{\psi}_2$ . The wavepacket  $\hat{\psi}_4$  is nothing more than the first diffraction order. Unlike the Bragg diffraction in an optical lattice (see Sec. 28.2), the Bragg diffraction by a matter wave lattice requires nonlinear mixing through binary atomic collisions. Thus, the number of redistributed atoms depends on parameters such as the interatomic interaction strength, the size of the condensate, and the collision time between the wavepackets, i.e. the time that the wavepackets spend together before separating.

Despite the similarity with the optical counterpart, matter wave 4WM is fundamentally different: The number of particles must be conserved and the energy-momentum dispersion relation is not linear. Furthermore, while photons require the

presence of a nonlinear medium in order to participate in higher-order processes, atomic matter waves mix through binary collisions.

## 27.4 Quantum atom optics

When describing a condensate by the Gross-Pitaevskii equation, we specify a phase and an atom number. However, both are conjugate quantities, which can not be specified without uncertainty. So, what does the BEC really look like: a Glauber state or rather a Fock state? We need to be careful. Certainly, it makes no sense talking about the absolute phase of a single BEC. Only the *relative phase* between *two* BECs matters. The condition for interference is, that we do not know, from which condensate the interfering atom came  $\Delta N \Delta \varphi \geq 1$ . So, the relative atom number must be uncertain.

### 27.4.1 Quantum transport

Now, let us imagine two BECs in a double-well potential. Atoms may be move between the wells via *Josephson tunneling*, even if the height of the barrier is higher than the atomic energy. Hence, the motion is a type of *quantum transport*. Be  $\psi(\mathbf{r}, t) = \psi_1(\mathbf{r})e^{i\mu_1 t/\hbar} + \psi_2(\mathbf{r})e^{i\mu_2 t/\hbar}$ . In elongated traps the Josephson current is obtained as the expectation value of the *flux operator*,

$$I(z, t) = \frac{i\hbar}{2m} \int \left( \psi(\mathbf{r}, t) \frac{d}{dz} \psi^*(\mathbf{r}, t) - c.c. \right) dx dy . \quad (27.30)$$

One obtains,

$$I(z, t) = \frac{i\hbar}{2m} \int \left( \psi_1 \frac{d\psi_1^*}{dz} + \psi_1 \frac{d\psi_1^*}{dz} + \psi_1 \frac{d\psi_1^*}{dz} e^{i(\mu_1 - \mu_2)t/\hbar} + \psi_1 \frac{d\psi_1^*}{dz} e^{i(\mu_1 - \mu_2)t/\hbar} - c.c. \right) dx dy . \quad (27.31)$$

Choosing the original phase of the two condensates equal to zero, the time-independent terms are real and cancel each other, leaving,

$$\begin{aligned} I(z, t) &= \frac{i\hbar}{2m} \int \left( \psi_1 \frac{d\psi_2}{dz} - \psi_2 \frac{d\psi_1}{dz} \right) 2i \sin \frac{(\mu_1 - \mu_2)t}{\hbar} dx dy \\ &\equiv I_0 \sin \frac{(\mu_1 - \mu_2)t}{\hbar} . \end{aligned} \quad (27.32)$$

This shows that the current oscillates in time. This feature is well-known for *Josephson junction* in superconductors.

The question is now, what will be the steady-state of the two BECs [530]. Experiments have shown, that the BECs will gradually evolve into a superposition of number states, until they are coherent. The time scale is set by Josephson tunneling. The same interference pattern would result from BECs initially having well-defined phases<sup>5,6</sup>

<sup>5</sup>Also, a *spin-squeezed state* i.e. a state with sub-Poissonian number statistics approaching pure number states have been compared to coherent states. Superposition of the first ones exhibited no interference while superposition of the second ones lead to observable interference.

<sup>6</sup>If two Josephson-coupled BECs are initially in Fock-states, the current must initially be a quan-



## 27.4.2 Optical lattices and the Mott insulator

We have already pointed out in Sec. 24.3.2, that laser beams tuned far away from resonances serve to construct trapping potentials for atoms. Laser beams incident on the atomic cloud under various angles allow the engineering of a large diversity of geometries for attractive potentials (with red tuned lasers) or repulsive potentials (with blue tuned lasers). Various cooling methods can be combined with dipolar traps, for example, Doppler cooling [350], Raman cooling [306], evaporative cooling [2], or gravitational Sisyphus cooling [519]. A particularly interesting geometry is that of an optical lattice, which we will discuss in the following sections.

### 27.4.2.1 Bragg scattering from optical lattices

In solid state physics the structure of crystal is studied by Bragg or von Laue scattering with X-ray radiation. Similar techniques can be used in optical lattices [72, 613, 711, 712, 640]. Under certain conditions, we can even expect to open a *photonic band gap* [21, 193, 614], which draws an analogy between optical lattices and *photonic crystal*.

A great advantage of optical lattices is the possibility of directly visualizing the momentum distribution of the confined atoms, that is, the distribution of atoms over the *Brillouin zone*.

### 27.4.2.2 Bloch bands with mean field interaction

The Gross-Pitaevski equation is,

$$H\psi = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi + v \cos Kx + c|\psi|^2 \psi = \mu\psi . \quad (27.33)$$

We have a periodic potential,  $U(x) = U(x+X)$ . In the following, we restrict ourselves to 1D. Assume e.g. a sine wave potential,

$$U(x) = U_0 \cos(2Kx) . \quad (27.34)$$

The Gross-Pitaevskii equation is rescaled via  $k/K \rightarrow k$ ,  $2Kx \rightarrow x$ ,  $4\epsilon t \rightarrow t$ ,  $\psi/\sqrt{n} \rightarrow \psi$  and  $C = \pi n a_s / K^2$ . All frequencies are scaled like  $U/4\epsilon \rightarrow U$ . Then,

$$-\frac{1}{2} \frac{\partial^2 \psi}{\partial x^2} + (U \cos x - U) \psi + C|\psi|^2 \psi = \mu\psi . \quad (27.35)$$

The Bloch-theorem says that the Schrödinger equation can be solved by any Bloch state. Those are superpositions of plane-wave momentum states [?],

$$\psi(x) = e^{ikx} u_k(x) , \quad (27.36)$$

with  $u_k(x) = u_k(x+X)$ . We obtain,

$$-\frac{1}{2} \left( \frac{\partial}{\partial x} + ik \right)^2 u_k + U \cos x u_k + C|u_k|^2 u_k = [\mu(k) + U] u_k . \quad (27.37)$$

---

sum superposition of all currents corresponding to all possible atom number differences. This quantum superposition decoheres rapidly, leaving behind a semi-classical oscillation.



Inserting the plane-wave expansions  $u_k(x) = \sum_{q=-N}^N a_q(k)e^{iqx}$  into the Schrödinger equation, we get,

$$\begin{aligned} & \sum_{q=-N}^N \left[ \frac{1}{2}(q+k)^2 a_q e^{iqx} + \frac{1}{2} U a_q (e^{i(q+1)x} + e^{i(q-1)x}) \right. \\ & \quad \left. + C \sum_{m,n=-N}^N a_m a_n^* a_q e^{i(m-n+q)x} - [\mu(k) + U] a_q e^{iqx} \right] = 0 \\ & \frac{1}{2}(q+k)^2 a_q + \frac{1}{2} U (a_{q-1} + a_{q+1}) + C a_q \sum_{n=-N}^N |a_n|^2 - [\mu(k) + U] a_q = 0 . \end{aligned} \quad (27.38)$$

We choose a cut-off  $q_0$  so that  $a_{q>q_0} = 0$ . For a given  $k$  the coefficients  $a_q$  and the chemical potential  $\mu$ , and thus the Bloch wave  $u_k(x)$  can easily be calculated by minimizing the left hand side of the above equation. Note that for  $C = 0$  we have we linear set of differential equation that can be solved as an eigenvalue problem (see Sec. ??).

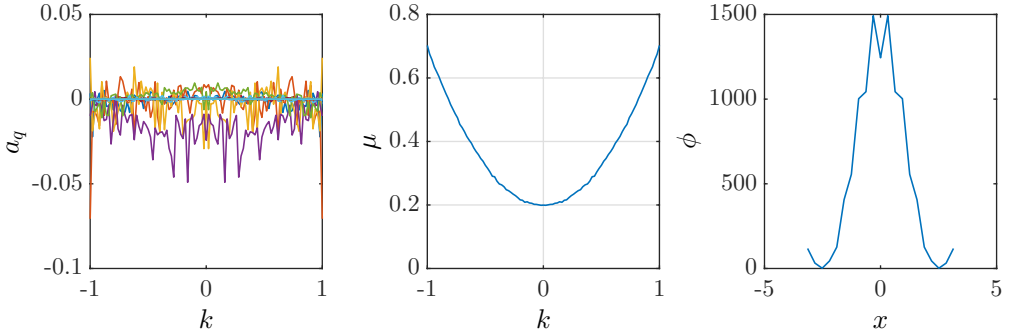


Figure 27.11: (code) Nonlinear interaction matrix finds just one minimum, dependence on  $k$ , [731, 733].

If we only consider the two lowest Bloch bands

$$u_k(x) = e^{ikx} a(x) + e^{i(k-K)x} b(x) \quad (27.39)$$

with  $|a|^2 + |b|^2 = 1$ , so that

$$|u_k|^2 = \left( e^{ikx} a + e^{i(k-K)x} b \right) \left( a e^{ikx} + b e^{i(k-K)x} \right) = 1 + 2ab \cos Kx , \quad (27.40)$$

and insert this into the Gross-Pitaevski equation Eq. (27.37), we find that the system of differential equations Eq. (27.38) simplifies to,

$$\begin{pmatrix} \frac{\hbar^2 k^2}{2m} + c & \frac{v}{2} + abc \\ \frac{v}{2} + abc & \frac{\hbar^2 (k-K)^2}{2m} + c \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \mu \begin{pmatrix} a \\ b \end{pmatrix} . \quad (27.41)$$

For  $-2ab = \frac{v}{c}$  the off-diagonal elements vanish, and because the interacting BEC shields the potential. Since  $|2ab| \leq 1$ , this is only possible for  $c \geq v$ .

If we substitute  $\mu = \tilde{\mu} + \frac{1}{2} \frac{\hbar^2 k^2}{2m} + \frac{1}{2} \frac{\hbar^2 (k-K)^2}{2m} + \frac{3}{2} c$ , multiply the first row with  $b$ , the second with  $a$  and add both rows, we obtain,

$$2\tilde{\mu} = \frac{v}{2ab}. \quad (27.42)$$

**Example 116 (Estimations):** Estimated radial BEC size  $r_t \simeq 10 \mu\text{m}$ , estimated number of atoms per antinode  $n_{1D} \simeq 1000 \mu\text{m}^{-1}$ ,

$$\omega_r = \frac{\hbar k^2}{2m} = 2\pi \cdot 3.8 \text{ kHz} \quad (27.43)$$

$$g_{1D} = \frac{4\pi \hbar^2 a_s}{mr_t^2} \quad (27.44)$$

$$g_{1D} n_{1D} = h \cdot 77 \text{ Hz} \quad (27.45)$$

Since we need at least two Bloch bands to see interesting effects, we must arrange for much stronger mean fields.

### 27.4.2.3 The Mott insulator

In the Mott insulating state, the atoms are *localized* at individual sites of an optical lattice. On one hand, the localization impedes any phase relation between atoms at different sites, that is, at a given site the phase uncertainty  $\Delta\phi$  is complete. But at the same time, there is a perfect correlation of the atom number at each site known as *spin squeezing*<sup>7</sup>, because (in a homogeneous lattice) every site contains exactly the same number of atoms, that is, the atom number uncertainty  $\Delta N$  tends to zero. At a given lattice site, the number of atoms and the phase of the wavefunction can not be simultaneously fixed:  $\Delta N \Delta\phi > 1$ .

The absence of relative coherence between different sites and of the ability to interfere prohibits the description of the system by a single global wavefunction and the use of the Gross-Pitaevskii equation. Nevertheless, the Mott insulating state is not equivalent to a completely randomized sample. On the contrary, the coherence only changes its character<sup>8</sup>.

The *Mott transition* of a condensate from a superfluid state and to state of a *Mott insulator* occurs as a *quantum phase transition*, because it is driven by quantum fluctuations rather than of thermal noise. Therefore, it is a direct result of Heisenberg's uncertainty relation.

### 27.4.2.4 The Bose-Hubbard model

The *Bose-Hubbard model* gives an approximate description of the physics of interacting *bosons* in a lattice. The model is closely related to the fermionic Hubbard model, used in solid state physics for the description of superconducting systems and the hopping of electrons between the atoms of a solid crystalline lattice.

<sup>7</sup>The spin squeezing feature makes the Mott insulator interesting for spectroscopy at the *Heisenberg limit* and for quantum computation.

<sup>8</sup>Remember, that the Fock state is a complicated superposition of Glauber states. The disappearance and reappearance of coherence is reminiscent to the phenomenon of collapse and revival in the Jaynes-Cummings model.

The Bose-Hubbard model starts from the following Hamiltonian [530, 280],

$$\hat{H} = -J \sum_{(i,j)} \hat{a}_i^\dagger \hat{a}_j + \sum_i \varepsilon_i \hat{n}_i + \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1), \quad (27.46)$$

where

$$J \equiv \int d^3 \mathbf{x} w^*(\mathbf{x} - \mathbf{x}_i) \left[ -\frac{\hbar}{2m} \nabla^2 + V_0(\mathbf{x}) \right] w^*(\mathbf{x} - \mathbf{x}_i), \quad (27.47)$$

and

$$U \equiv \frac{4\pi a_s \hbar^2}{m} \int d^3 \mathbf{x} |w^*(\mathbf{x})|^4, \quad (27.48)$$

with  $\varepsilon_i \equiv \frac{4\pi a_s \hbar^2}{m} \int d^3 \mathbf{x} V_{trap}(\mathbf{x}) |w(\mathbf{x} - \mathbf{x}_i)|^2 \approx V_{trap}(\mathbf{x}_i)$  and  $w(\mathbf{x}) = w(x)w(y)w(z)$  are the *Wannier functions* for an individual particle. We assume for the moment a homogeneous condensate.

The Hilbert space dimension of the Bose-Hubbard model grows exponentially with the number of atoms  $N$  and the number of sites  $L$ ,

$$D_b = \frac{(N_b + L + 1)!}{N_b!(L - 1)!}. \quad (27.49)$$

For the Fermi-Hubbard model, the Pauli exclusion principle leads to the Hilbert space dimension,

$$D_f = \binom{L}{N_f}. \quad (27.50)$$

In three dimensional lattices the Hilbert space grows even faster. Therefore, it is a difficult computational task to model or simulate such systems, and generally not possible for more than 20 atoms and 20 lattice sites.

At zero temperature, the Bose-Hubbard model (in the absence of disorder) predicts the atomic ensemble to be an a Mott insulating state (MI) when  $J \ll U$ , a superfluid state (SF) when  $J \gg U$ , or a *supersolid phase* (SS), where both solid and superfluid phases (diagonal and off-diagonal) coexist. Mott insulation phases are characterized by integer site occupation numbers, by the existence of an energy gap for particle-hole excitations, and zero compressibility. In the presence of disorder, a third phase, the *Bose glass* exists. This phase is insulation because of the Anderson localization effects. Bose glass is characterized by a finite compressibility, the absence of a gap, and an infinite superfluid susceptibility [239]. See also (watch talk).

In the limit of strong tunneling and weak interactions,  $J \gg U$ , the matter wave function looks like a *Bloch state*,

$$|\psi_{SF}\rangle \sim \left( \sum_{i=1}^M \hat{a}_i^\dagger \right)^N |0\rangle. \quad (27.51)$$

The variance of the number of particles per site is Poissonian,  $\sigma_{SF} \sim \sqrt{N_i}$ , that is, the wavefunction per lattice site is (quasi)-coherent. However, the total wavefunction is delocalized over all lattice sites, the local wavefunctions have a rigid phase relationship

and no long-range coherence. Otherwise, the matter wave function is an independent product of *Fock states*,

$$|\psi_{MI}\rangle \sim \prod_{i=1}^M (\hat{a}_i^\dagger)^n |0\rangle. \quad (27.52)$$

The momentum distribution in terms of Wannier functions is [294, 732],

$$n(\mathbf{k}) = |w(\mathbf{k})|^2 \sum_{i,j} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \langle \hat{a}_i^\dagger \hat{a}_j \rangle. \quad (27.53)$$

### 27.4.3 Schrödinger cats

Ruostekoski *et al.* [589] proposed a double BEC system consisting of two momentum sidemodes and a far-off resonance laser beam that constantly spontaneously redistributes the atoms between the sidemodes. Homodyne detection of the scattered photons established *relative phase* information in such a way, that the relative number information is blurred in such a way that both sidemodes evolve into a simultaneous superposition of phase and number states. They disregard thermal excitations and two-body collisions. The cats are very sensitive to decoherence.

Cirac *et al.* [135] and Gordon *et al.* [273] consider Josephson double species condensates. The relative atom numbers Rabi flop. Mediated by the mean-field the systems may evolve into cats. The proposals have been reexamined by Dalvit *et al.* [170]. Other contributions come from [271, 333, 595, 572, 362]. First experiments on spin-squeezed states have been made by [530].

### 27.4.4 Exercises

#### 27.4.4.1 Ex: Superfluid to Mott insulator transition

Consider a condensate trapped in a 3D *simple cubic* optical lattice with lattice spacing  $l$ . The Hamiltonian can be written as,

$$\hat{H} = -J \sum_{i,j} \delta_{ij}^{(1)} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i,$$

where  $\hat{a}_i$  ( $\hat{a}_i^\dagger$ ) is the operator annihilating (creating) one boson in the lattice site  $i$ ;  $\delta_{ij}^{(1)} = 1$  only when  $i$  and  $j$  are nearest neighbors, otherwise it is zero. Assume a total of  $M \gg 1$  sites, periodic boundary conditions in the  $x$ ,  $y$ , and  $z$  directions, and  $U > 0$ . On this lattice we consider the construction operator  $\hat{b}_s^\dagger$  defined in the following way:

$$\hat{b}_s^\dagger = \frac{1}{\sqrt{M}} \sum_i \hat{a}_i^\dagger.$$

- Describe the action of this construction operator.
- Derive the commutation relation,

$$[\hat{a}_\alpha, \hat{b}_s^\dagger] = \frac{1}{\sqrt{M}}.$$

- Derive the commutation relation,

$$[\hat{a}_\alpha, (\hat{b}_s^\dagger)^N] = \frac{N}{\sqrt{M}} (\hat{b}_s^\dagger)^{N-1}.$$

d. Suppose that the following  $N$ -atom state exists:

$$|N, SF\rangle \equiv \frac{1}{\sqrt{N!}} (\hat{b}_s^\dagger)^N |0\rangle ,$$

where  $SF$  stands for a name label (and not for quantum numbers). Show that for  $N = M$  we have  $\hat{a}_\alpha |N, SF\rangle = |N - 1, SF\rangle$ .

e. Define the density operator for the site  $i$  as  $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ . Calculate the density fluctuation,

$$\Delta n_i = \sqrt{\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2}$$

of the state  $|N, SF\rangle$  with  $N = M$ .

f. Calculate the total energy  $\langle H \rangle$  with the state  $|N, SF\rangle$ .

g. Next consider the state,

$$|N, MI\rangle \equiv \prod_j \hat{a}_j^\dagger |0\rangle .$$

Calculate  $\langle \hat{a}_i^\dagger \hat{a}_j \rangle$  and the density fluctuations  $\Delta n_i$  for this state.

h. Calculate the total energy  $\langle H \rangle$  with the state  $|N, MI\rangle$ .

i. Discuss the energy for the states  $|N, SF\rangle$  and  $|N, MI\rangle$ . Which one is the ground state? How to make a ground state change from  $|N, SF\rangle$  to  $|N, MI\rangle$ ?

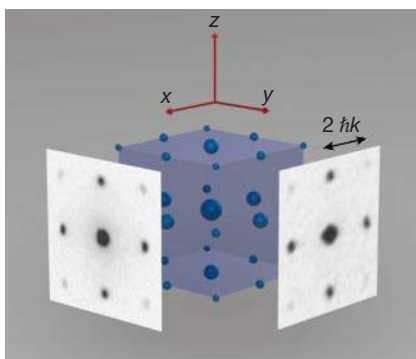
## 27.5 Further reading

M.R. Matthews et al., *Vortices in a Bose-Einstein Condensate* [DOI]

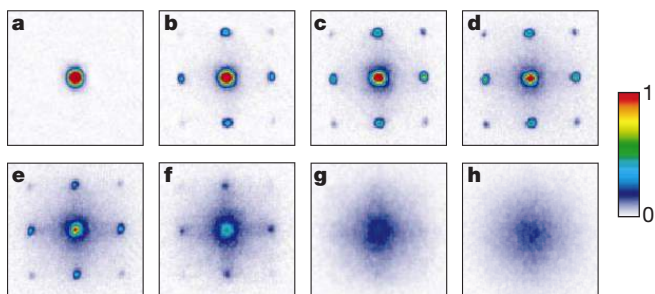
K.M. Mertes et al., *Nonequilibrium Dynamics and Superfluid Ring Excitations in Binary Bose-Einstein Condensates* [DOI]

I. Bloch, *Ultracold quantum gases in optical lattices* [DOI]

J. Estève et al., *Squeezing and entanglement in a Bose-Einstein condensate* [DOI]



**Figure 1** Schematic three-dimensional interference pattern with measured absorption images taken along two orthogonal directions. The absorption images were obtained after ballistic expansion from a lattice with a potential depth of  $V_0 = 10E_r$  and a time of flight of 15 ms.



**Figure 2** Absorption images of multiple matter wave interference patterns. These were obtained after suddenly releasing the atoms from an optical lattice potential with different potential depths  $V_0$  after a time of flight of 15 ms. Values of  $V_0$  were: **a**,  $0 E_r$ ; **b**,  $3 E_r$ ; **c**,  $7 E_r$ ; **d**,  $10 E_r$ ; **e**,  $13 E_r$ ; **f**,  $14 E_r$ ; **g**,  $16 E_r$ ; and **h**,  $20 E_r$ .

Figure 27.12: Signature of the Mott phase.



# Chapter 28

## Interaction of Bose-Einstein condensates with light

Light can essentially be used in two ways for the manipulation of matter waves: 1. Tuned *far from resonance*, light serves to create conservative optical dipole potentials (see Secs. 24.3.2 and 27.4.2). In such circumstances the states of internal atomic excitation can be adiabatically eliminated from the description of the center-of-mass dynamics. 2. *Close to resonance* the situation is quite different, but even then, the coherent excitation of internal states may allow for a controlled manipulation of the atomic motion. Among the examples discussed in the following sections are the adiabatic sweeps, the Raman output coupler, Bragg pulses, photoassociation, and matter wave superradiance (see Fig. 28.1).

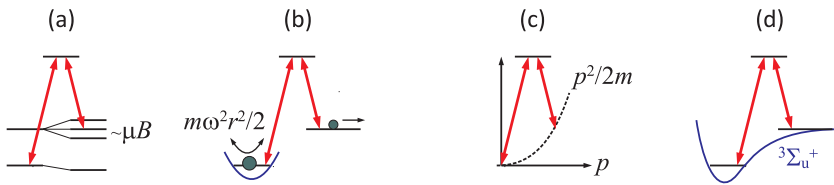


Figure 28.1: Different types of coherent coupling: (a) coherent coupling of hyperfine levels, (b) coupling from a confined state to the continuum of free states, (c) mutual coupling of different velocity states of an atom, and (d) coupling between a (collisional) state of two free atoms with a bound molecular state.

### 28.1 Scattering of light by degenerate gases

#### 28.1.1 The structure factor for degenerate quantum gases

We introduced in Sec. 19.1.1 the notion of the structure factor, where it was used to characterize the scattering of light by thermal distributions of atoms. To characterize the scattering of matter waves, we must generalize the notion of the structure factor. We wrote in (19.3) the Fourier transform of the density distribution, which now becomes, after inserting  $\hat{n}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$  and the plane wave expansion (26.70),

$$\hat{\rho}^\dagger(\mathbf{q}) = \int \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}d^3r = \frac{V}{(2\pi)^3} \iint \hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}}e^{i(\mathbf{k}-\mathbf{k}'+\mathbf{q})\cdot\mathbf{r}}d^3k'd^3kd^3r. \quad (28.1)$$



With (26.76) and assuming sharp momenta (26.71),

$$\hat{\rho}^\dagger(\mathbf{q}) = V^2 \iint \hat{a}_{\mathbf{k}'}^\dagger \hat{a}_{\mathbf{k}} \delta_{\mathbf{k}', \mathbf{k} + \mathbf{q}} d^3 k' d^3 k = \sum_{\mathbf{k}', \mathbf{k}} \hat{a}_{\mathbf{k}'}^\dagger \hat{a}_{\mathbf{k}} \delta_{\mathbf{k}', \mathbf{k} + \mathbf{q}} . \quad (28.2)$$

Finally,

$$\boxed{\hat{\rho}^\dagger(\mathbf{q}) = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k} + \mathbf{q}}^\dagger \hat{a}_{\mathbf{k}} = \sum_{\mathbf{k}} |\mathbf{k} + \mathbf{q}\rangle \langle \mathbf{k}|} . \quad (28.3)$$

Hence,  $\hat{\rho}^\dagger(\mathbf{q})$  describes the scattering of an atom with the momentum  $\mathbf{k}$  to  $\mathbf{k} + \mathbf{q}$ . We also find,

$$\hat{\rho}^\dagger(\mathbf{q}) = \hat{\rho}(-\mathbf{q}) . \quad (28.4)$$

Understanding the fundamental state  $|g\rangle$  as the state without excitations, we define the *static structure factor* (19.5) now normalized to the number of particles [651],

$$\boxed{S(\mathbf{q}) \equiv \frac{1}{N} \langle g | \hat{\rho}(\mathbf{q}) \hat{\rho}^\dagger(\mathbf{q}) | g \rangle} , \quad (28.5)$$

as a generalization of the classical structure factor. The static structure factor describes the probability to excite a condensate by creating a quasi-particle with momentum  $\mathbf{k}$ . We will need these notions in the Sec. 28.2.3.

The *dynamic structure factor* is obtained from  $S(\mathbf{q}) = \int S(\mathbf{q}, \omega) d\omega$  and measures the density of correlations in the ground state with 0 momentum. The formula describes, how an atom probes its environment by scattering quasi-particles back and forth,

$$S(\mathbf{q}, \omega) = \frac{1}{N} \sum_f \langle g | \hat{\rho}(\mathbf{q}) | f \rangle \langle f | \hat{\rho}(\mathbf{q}) | g \rangle \hbar \delta(\hbar\omega - E_f + E_g) . \quad (28.6)$$

Solve the Excs. 28.1.6.1 to 28.1.6.5.

**Example 117 (Spatial coherence and the correlation function):** The *spatial coherence* can be defined by [CCT & Aspect],

$$\boxed{F(\mathbf{x}) \equiv \int \langle \mathbf{r} | \hat{\rho} | \mathbf{r} + \mathbf{x} \rangle d^3 r = \int e^{i\mathbf{k} \cdot \mathbf{x}} \langle \mathbf{k} | \hat{\rho} | \mathbf{k} \rangle d^3 k} . \quad (28.7)$$

We will demonstrate this relationship in Exc. 28.1.6.6. The *coherence length*  $\xi$  is given by  $F(\xi) = \frac{1}{e} F(0) = \frac{1}{e}$ . A *second order correlation function* is defined by,

$$\boxed{\begin{aligned} g^{(2)}(\mathbf{r}_1, \mathbf{r}_2) &= \frac{\langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) \rangle}{\langle \hat{n}(\mathbf{r}_1) \rangle \langle \hat{n}_2(\mathbf{r}) \rangle} . \\ g^{(2)}(\mathbf{r}) &\equiv g^{(2)}(\mathbf{r}_1, \mathbf{r}_1 + \mathbf{r}) \end{aligned}}$$

## 28.1.2 The structure factor in Bragg spectroscopy

### 28.1.2.1 The Hamiltonian of the Rayleigh scattering process

In Sec. 2.5.2 we saw the Galilei-boost (2.190),

$$|\mathbf{k} + \mathbf{q}\rangle = e^{i\mathbf{q} \cdot \hat{\mathbf{r}}} |\mathbf{k}\rangle . \quad (28.8)$$

In the second quantization we generalize to,

$$|\mathbf{k} + \mathbf{q}\rangle = \int \hat{\psi}^\dagger(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} \hat{\psi}(\mathbf{r}) d^3r |\mathbf{k}\rangle = \hat{\rho}^\dagger(\mathbf{q}) |\mathbf{k}\rangle. \quad (28.9)$$

Thus, we can implement the second quantization by simply replacing  $e^{i\mathbf{q}\cdot\mathbf{r}}$  by  $\hat{\rho}^\dagger(\mathbf{q})$ . Now, the Hamiltonian for the process of a photon absorption from the mode  $\hat{c}_{\mathbf{k}_i}$ , taking into account the photonic recoil, was introduced in (18.6),

$$\hat{H}_{int} = \hbar\Omega(\hat{\mathbf{r}}) e^{-i\mathbf{k}_i\cdot\hat{\mathbf{r}}} \hat{c}_{\mathbf{k}_i} \hat{\sigma}^+ + c.c. \quad (28.10)$$

If the process is followed by the reemission of a photon to the mode  $\hat{c}_{\mathbf{k}_f}$ ,

$$\boxed{\hat{H}_{int} = \hbar\Omega(\hat{\mathbf{r}}) e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot\hat{\mathbf{r}}} \hat{c}_{\mathbf{k}_f}^\dagger \hat{c}_{\mathbf{k}_i}}. \quad (28.11)$$

Going to second quantization, as done in (28.9), and doing the Fourier transform <sup>1</sup>,

$$\tilde{H}_{int} = C \sum_{\mathbf{p}_f, \mathbf{p}_i} \hat{c}_{\mathbf{k}_f}^\dagger \hat{c}_{\mathbf{k}_i} \hat{a}_{\mathbf{p}_f}^\dagger \hat{a}_{\mathbf{p}_i} \delta_{\mathbf{k}_f - \mathbf{k}_i + \mathbf{p}_f - \mathbf{p}_i}. \quad (28.12)$$

We assume here, that the light modes  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are predefined, but the velocities  $\mathbf{p}_i$  are distributed. Otherwise, in the expression (28.12), we must also sum over light modes <sup>2</sup>,

$$\boxed{\tilde{H}_{int} = C \sum_{\mathbf{k}_i, \mathbf{k}_f, \mathbf{p}_i, \mathbf{p}_f} \hat{c}_{\mathbf{k}_f}^\dagger \hat{c}_{\mathbf{k}_i} \hat{a}_{\mathbf{p}_f}^\dagger \hat{a}_{\mathbf{p}_i} \delta_{\mathbf{k}_f - \mathbf{k}_i + \mathbf{p}_f - \mathbf{p}_i}}, \quad (28.13)$$

where  $C$  is a normalization constant. This Hamiltonian describes the elementary scattering process as a process of four wave mixing (4WM) [390, 652]. The light and the atoms are treated on equal footings as modes which can receive (quasi-)particle populations, and the scattering corresponds to a redistribution of populations between the modes <sup>3</sup>.

The Hamiltonian (28.13) can be applied to various situations, such as spontaneous or stimulated Rayleigh scattering or Bragg scattering, depending on which ones of the modes  $\mathbf{k}_f$ ,  $\mathbf{k}_i$ ,  $\mathbf{p}_f$ , and  $\mathbf{p}_i$  are populated or filtered by imposed boundary conditions.

Using momentum conservation  $\mathbf{q} \equiv \mathbf{k}_f - \mathbf{k}_i = -\mathbf{p}_f + \mathbf{p}_i$ , we obtain the cross section,

$$\left( \frac{d\sigma}{d\Omega} \right)_{\mathbf{k}_i \rightarrow \mathbf{k}_f} = C^2 \sum_f |\langle f | \hat{H}_{int} | i \rangle|^2 = C^2 \sum_f |\langle f | \sum_{\mathbf{p}_i} \hat{c}_{\mathbf{k}_i + \mathbf{q}}^\dagger \hat{c}_{\mathbf{k}_i} \hat{a}_{\mathbf{p}_i - \mathbf{q}}^\dagger \hat{a}_{\mathbf{p}_i} | i \rangle|^2, \quad (28.14)$$

**Example 118 (Description of Bragg scattering via the structure factor):** In this example we irradiate two plane waves in directions  $\mathbf{k}_1$  and  $\mathbf{k}_2$  into a Bose-Einstein condensate. The total intensity will be,

$$I_{mod}(\mathbf{r}, t) = I \cos(\mathbf{q} \cdot \mathbf{r} - \omega t) \quad \text{with} \quad \mathbf{q} = \mathbf{k}_1 - \mathbf{k}_2. \quad (28.15)$$

<sup>1</sup> $\hat{a}_{\mathbf{p}}$  and  $\hat{a}_{\mathbf{p}}^\dagger$  are the operators of the quantized atomic field, while  $\hat{c}_{\mathbf{k}}$  and  $\hat{c}_{\mathbf{k}}^\dagger$  are the operators of the light fields.

<sup>2</sup>Note the different form of this Hamiltonian as compared to (19.10).

<sup>3</sup>This is analogous to the way, in which a 'collision' redistributes atomic populations between momentum modes. We will discuss this general concept of 4WM in Secs. 28.3.4 and 27.3.4.

and the optical potential,

$$V_{mod} = \frac{\hbar\Gamma^2}{8\Delta} I \cos(\mathbf{q} \cdot \mathbf{r} - \omega t) = \frac{\hbar\Gamma^2}{8\Delta} \frac{I}{2I_{sat}} (e^{i\mathbf{q} \cdot \mathbf{r} - i\omega t} + e^{-i\mathbf{q} \cdot \mathbf{r} + i\omega t}) \quad (28.16)$$

$$\rightarrow \hat{V}_{mod} = \frac{V}{2} [\hat{\rho}^\dagger(\mathbf{q})e^{-i\omega t} + \hat{\rho}^\dagger(-\mathbf{q})e^{i\omega t}] .$$

Now, the transition rate is [652],

$$\frac{W}{N} = 2\pi\Omega_R^2 S(\mathbf{q}, \omega) = \frac{2\pi}{N\hbar} \left(\frac{V}{2}\right)^2 \sum_f |\langle f | \hat{\rho}^\dagger(\mathbf{q}) | g \rangle|^2 \delta(\hbar\omega - (E_f - E_g)) , \quad (28.17)$$

with  $\frac{V}{2} = \hbar\Omega_R$ .

Resolve Exc. 28.1.6.7.

### 28.1.3 Bosonic stimulation

We assume in the following weak light intensities (and hence a negligible contribution of the Mollow fluorescence spectrum). That is, without cooperative effects the light would be elastically scattered by Rayleigh scattering. Now, we adopt a notation labeling the multimodal state by the numbers of photons and atoms distributed over the available light and momentum modes. That is, the initial state consists of  $n_{\mathbf{p}}$  atoms distributed over momentum atomic states  $\mathbf{p}$  and  $N_{\mathbf{k}}$  photons distributed over wave vector modes  $\mathbf{k}$  denoted by  $|\dots N_{\mathbf{k}} \dots\rangle_{rad} \otimes |\dots n_{\mathbf{p}} \dots\rangle_{at}$ :

$$|i\rangle \equiv |\dots n_{\mathbf{p}_i} \dots n_{\mathbf{p}_f} \dots\rangle_{at} \otimes |\dots N_{\mathbf{k}_i} \dots N_{\mathbf{k}_f} \dots\rangle_{rad} \equiv \left| \begin{array}{c} \dots n_{\mathbf{p}_i} \dots n_{\mathbf{p}_f} \dots \\ \dots N_{\mathbf{k}_i} \dots N_{\mathbf{k}_f} \dots \end{array} \right\rangle , \quad (28.18)$$

where we introduced the vector-like notation for notational compactness.

A particular scattering process can be treated like a 'collision' by redistributing the initial populations to final populations:

$$|f\rangle = \left| \begin{array}{c} \dots n_{\mathbf{p}_i} - 1 \dots n_{\mathbf{p}_f} + 1 \dots \\ \dots N_{\mathbf{k}_i} - 1 \dots N_{\mathbf{k}_f} + 1 \dots \end{array} \right\rangle . \quad (28.19)$$

We write the matrix element,

$$\langle f | \hat{H}_{int} | i \rangle \propto \left\langle \begin{array}{c} \dots n_{\mathbf{p}'_i} \dots n_{\mathbf{p}'_f} \dots \\ \dots N_{\mathbf{k}'_i} \dots N_{\mathbf{k}'_f} \dots \end{array} \right| C \sum_{\mathbf{k}'_i, \mathbf{k}'_f, \mathbf{p}'_i, \mathbf{p}'_f} \hat{c}_{\mathbf{k}'_f}^\dagger \hat{c}_{\mathbf{k}'_i} \hat{a}_{\mathbf{p}'_f}^\dagger \hat{a}_{\mathbf{p}'_i} \delta_{\mathbf{k}'_f - \mathbf{k}'_i + \mathbf{p}'_f - \mathbf{p}'_i} \left| \begin{array}{c} \dots n_{\mathbf{p}_i} \dots n_{\mathbf{p}_f} \dots \\ \dots N_{\mathbf{k}_i} \dots N_{\mathbf{k}_f} \dots \end{array} \right\rangle . \quad (28.20)$$

Assuming that all modes are not degenerate, such that  $[\hat{a}_{\mathbf{p}_f}, \hat{a}_{\mathbf{p}_i}^\dagger] = \delta_{\mathbf{p}_f, \mathbf{p}_i}$ , that is,  $\hat{a}_{\mathbf{p}_f}^\dagger$  and  $\hat{a}_{\mathbf{p}_f}$  only act on the mode  $|n_{\mathbf{p}_f}\rangle_{at}$ , etc.,

$$\sum_{\mathbf{p}'_i} \hat{a}_{\mathbf{p}'_i} |\dots n_{\mathbf{p}_i} \dots\rangle_{at} = \sum_{\mathbf{p}_i} \sqrt{n_{\mathbf{p}_i}} |\dots n_{\mathbf{p}_i} - 1 \dots\rangle_{at} \quad (28.21)$$

and

$$\sum_{\mathbf{p}'_f} \hat{a}_{\mathbf{p}'_f}^\dagger |\dots n_{\mathbf{p}_f} \dots\rangle_{at} = \sum_{\mathbf{p}_f} \sqrt{n_{\mathbf{p}_f} + 1} |\dots n_{\mathbf{p}_f} + 1 \dots\rangle_{at} ,$$

as well as,

$$\begin{aligned} \sum_{\mathbf{k}'_i} \hat{c}_{\mathbf{k}'_i} | \dots N_{\mathbf{k}_i} \dots \rangle_{rad} &= \sum_{\mathbf{k}_i} \sqrt{N_{\mathbf{k}_i}} | \dots N_{\mathbf{k}_i} - 1 \dots \rangle_{rad} \\ \text{and } \sum_{\mathbf{k}'_f} \hat{c}_{\mathbf{k}'_f}^\dagger | \dots N_{\mathbf{k}_f} \dots \rangle_{rad} &= \sum_{\mathbf{k}_f} \sqrt{N_{\mathbf{k}_f} + 1} | \dots N_{\mathbf{k}_f} + 1 \dots \rangle_{rad} . \end{aligned} \quad (28.22)$$

Let us now assume for a moment, that the photon is scattered to the vacuum, that is, the final mode of light is initially empty,  $N_{\mathbf{k}_f} = 0$ <sup>4</sup>,

$$\begin{aligned} \langle f | \hat{H}_{int} | i \rangle_{inel} & \\ \propto \left\langle \begin{array}{c} \dots n_{\mathbf{p}'_i} \dots n_{\mathbf{p}'_f} \dots \\ \dots N_{\mathbf{k}'_i} \dots N_{\mathbf{k}'_f} \dots \end{array} \middle| \sum_{\mathbf{p}_f, \mathbf{p}_i, \mathbf{k}_f, \mathbf{k}_i} \sqrt{N_{\mathbf{k}_i}} \sqrt{n_{\mathbf{p}_f} + 1} \sqrt{n_{\mathbf{p}_i}} \begin{array}{c} \dots n_{\mathbf{p}_i} - 1 \dots n_{\mathbf{p}_f} + 1 \dots \\ \dots N_{\mathbf{k}_i} - 1 \dots 1_{\mathbf{k}_f} \dots \end{array} \right\rangle & \\ = \sum_{\mathbf{p}_f, \mathbf{p}_i, \mathbf{k}_f, \mathbf{k}_i} \sqrt{N_{\mathbf{k}_i}} \sqrt{n_{\mathbf{p}_f} + 1} \sqrt{n_{\mathbf{p}_i}} \delta_{N_{\mathbf{k}'_i}, N_{\mathbf{k}_i} - 1} \delta_{N_{\mathbf{k}'_f}, N_{\mathbf{k}_f} + 1} \delta_{n_{\mathbf{p}'_i}, n_{\mathbf{p}_i} - 1} \delta_{n_{\mathbf{p}'_f}, n_{\mathbf{p}_f} + 1} & \\ = \sqrt{N_{\mathbf{k}_i}} \sqrt{n_{\mathbf{p}_f} + 1} \sqrt{n_{\mathbf{p}_i}} . & \end{aligned} \quad (28.23)$$

Obviously, the differential scattering cross-section,

$$\boxed{\left( \frac{d\sigma}{d\Omega} \right)_{inel} \propto N_{\mathbf{k}_i} (n_{\mathbf{p}_f} + 1) n_{\mathbf{p}_i}} . \quad (28.24)$$

depends, in addition to the numbers of provided photons  $N_{\mathbf{k}_i}$  and atoms  $n_{\mathbf{p}_i}$  in the initial mode, also on the *number of atoms in the final mode*  $n_{\mathbf{p}_f}$ . This amplification of the probability of the scattering process is called *bosonic stimulation*.

Now, we consider the degenerate case, where the initial atomic momentum mode coincides with the final mode,  $n_{\mathbf{p}_f} = n_{\mathbf{p}_i}$ . In this case,

$$\sum_{\mathbf{p}'_f = \mathbf{p}'_i} \hat{a}_{\mathbf{p}'_f}^\dagger \hat{a}_{\mathbf{p}'_i} | \dots n_{\mathbf{p}_i} \dots n_{\mathbf{p}_f} \dots \rangle_{at} = \sum_{\mathbf{p}'_i} \hat{a}_{\mathbf{p}'_i}^\dagger \hat{a}_{\mathbf{p}'_i} | \dots n_{\mathbf{p}_i} \dots n_{\mathbf{p}_i} \dots \rangle_{at} = \sum_{\mathbf{p}_i} n_{\mathbf{p}_i} | \dots n_{\mathbf{p}_i} \dots n_{\mathbf{p}_i} \dots \rangle_{at} , \quad (28.25)$$

and a calculus analogous to (28.23) yields,

$$\begin{aligned} \langle f | \hat{H}_{int} | i \rangle_{el} &\propto \left\langle \begin{array}{c} \dots n_{\mathbf{p}'_i} \dots n_{\mathbf{p}'_f} \dots \\ \dots N_{\mathbf{k}'_i} \dots N_{\mathbf{k}'_f} \dots \end{array} \middle| \sum_{\mathbf{p}_i, \mathbf{k}_f, \mathbf{k}_i} \sqrt{N_{\mathbf{k}_i}} n_{\mathbf{p}_i} \begin{array}{c} \dots n_{\mathbf{p}_i} \dots n_{\mathbf{p}_i} \dots \\ \dots N_{\mathbf{k}_i} - 1 \dots 1_{\mathbf{k}_f} \dots \end{array} \right\rangle \\ = \sum_{\mathbf{p}_i, \mathbf{k}_f, \mathbf{k}_i} \sqrt{N_{\mathbf{k}_i}} n_{\mathbf{p}_i} \text{rad} \langle \dots N_{\mathbf{k}'_i} \dots N_{\mathbf{k}'_f} \dots | \dots N_{\mathbf{k}_i} - 1 \dots 1_{\mathbf{k}_f} \dots \rangle_{rad} \text{at} \langle \dots n_{\mathbf{p}'_i} \dots n_{\mathbf{p}'_f} \dots | \dots n_{\mathbf{p}_i} \dots n_{\mathbf{p}_i} \dots \rangle_{at} & \\ = \sum_{\mathbf{p}_i, \mathbf{k}_f, \mathbf{k}_i} \sqrt{N_{\mathbf{k}_i}} n_{\mathbf{p}_i} \delta_{N_{\mathbf{k}'_i}, N_{\mathbf{k}_i} - 1} \delta_{N_{\mathbf{k}'_f}, N_{\mathbf{k}_f} + 1} \delta_{n_{\mathbf{p}'_i}, n_{\mathbf{p}_i}} \delta_{n_{\mathbf{p}'_f}, n_{\mathbf{p}_i}} = \sqrt{N_{\mathbf{k}_i}} n_{\mathbf{p}_i} . & \end{aligned} \quad (28.26)$$

Now, the differential scattering cross-section,

$$\boxed{\left( \frac{d\sigma}{d\Omega} \right)_{el} \propto N_{\mathbf{k}_i} n_{\mathbf{p}_i}^2} , \quad (28.27)$$

<sup>4</sup>We will discuss later the case, where the scattering is (bosonically) stimulated by the number of photons already present in the final mode prior to the scattering process.

only depends on the number of provided photons  $N_{\mathbf{k}_i}$  and the number of atoms  $n_{\mathbf{p}_i}$  in the initial mode.

### 28.1.3.1 Elastic and inelastic scattering

The interpretation of the result is the following: Light can be scattered in two ways: (i) with or (ii) without change of atomic moment distribution. The event of a photon scattering (28.19) then it consists of two terms (28.24) and (28.27) [553],

$$\frac{d\sigma}{d\Omega} = \left( \frac{d\sigma}{d\Omega} \right)_{el} + \left( \frac{d\sigma}{d\Omega} \right)_{inel}. \quad (28.28)$$

The first term of (28.28) occurs when the momentum of the scattering atom does not change,  $\mathbf{p} = \mathbf{q}$ , that is, when the populations of the momentum states  $n_{\mathbf{p}}$  and  $n_{\mathbf{q}}$  do not change. The corresponding term (28.27) describes elastic Rayleigh scattering. This process is coherent, that is, the phase relationship between the incident wave and the outgoing wave is fixed, because the photon emission is self-stimulated. I.e. it decays to the original mode via *forward scattering* within the angle defined by the *phase matching condition*  $\vartheta < \lambda/d$ , where  $d$  is the size of the atomic sample [390]. This contribution is dispersive, reversible, and conservative, and it is at the origin of the dipole force.

The second term of (28.28) is the inelastic part of Rayleigh scattering, where an atom with the initial momentum  $n_{\mathbf{p}}$  is scattered to the momentum state  $n_{\mathbf{q}}$ . This term is absorptive, dissipative, and spontaneous. The frequency of the photons is shifted, a momentum is imparted to the atom, such that the process is incoherent. Hence, a suggestive way of expressing the differential scattering cross-section (28.19) is,

$$\frac{d\sigma}{d\Omega} \propto \left| \sum_i n_i \langle i | \hat{H}_{int} | i \rangle \right|^2 + \sum_{i \neq f} n_i (1 + n_f) |\langle i | \hat{H}_{int} | f \rangle|^2, \quad (28.29)$$

where  $|i\rangle$  and  $|f\rangle$  denote momentum states of the atomic sample.

The bosonic stimulation of inelastic Rayleigh scattering represents a way to overcome, on one hand the restrictive phase matching condition, and on the other the incoherence of the scattering into large angles. For non-interacting systems of localized bosons  $S(\mathbf{q}, \omega)$  can be expressed using single particle states  $|i\rangle$  with energy  $E_i$  and population  $N_i$  [see (19.3) and (19.6)],

$$S(\mathbf{q}, \omega) = N \left| \sum_i n_i \langle i | \hat{H}_{int} | i \rangle \right|^2 \delta(\omega) + N \sum_{i \neq f} |\langle f | \hat{H}_{int} | i \rangle|^2 n_i (n_f + 1) \delta[\omega - (E_f - E_i)/\hbar], \quad (28.30)$$

with  $S_0(\mathbf{q}) = |\langle \hat{\rho}^\dagger(\mathbf{q}) \rangle|^2 = \left| \sum_i n_i \langle i | \hat{H}_{int} | i \rangle \right|^2$ .

### 28.1.4 Playing with bosonic and fermionic states

Here, we want to address the question, whether scattering processes are influenced by bosonic stimulation or cooperative enhancement. Let us consider the case of  $N$  atoms (bosons or fermions) generated from vacuum by operators  $\hat{a}_m^\dagger(\mathbf{q})|0\rangle$ , where  $m$

indicates some additional quantum number (for example, the vibrational state of a loose trapping potential) helping us to enumerate fermionic states, and  $\mathbf{q}$  indicates the momentum (considered independent from the trapping potential for short enough times). The operators respect the rules,

$$\begin{aligned} [\hat{a}_m(\mathbf{0}), \hat{a}_n(\mathbf{q})]_{\mp} &= 0 = [\hat{a}_m^{\dagger}(\mathbf{0}), \hat{a}_n^{\dagger}(\mathbf{q})]_{\mp} \\ \text{and} \quad [\hat{a}_m(\mathbf{0}), \hat{a}_n^{\dagger}(\mathbf{q})]_{\mp} &= \delta_{m,n} \delta_{\mathbf{0},\mathbf{q}} \quad \text{and} \quad \hat{a}_m(\mathbf{q})|0\rangle = 0, \end{aligned} \quad (28.31)$$

where upper signs hold for bosons and lower signs for fermions. Initially the  $N$  atoms are in the bosonic, respectively, fermionic many-body state [500],

$$\boxed{|\Psi_b^{(N)}(\mathbf{0})\rangle = \frac{1}{\sqrt{N!}} \hat{a}_0^{\dagger}(\mathbf{0})^N |0\rangle \quad \text{resp.} \quad |\Psi_f^{(N)}(\mathbf{0})\rangle = \prod_{n=0}^{N-1} \hat{a}_n^{\dagger}(\mathbf{0}) |0\rangle}. \quad (28.32)$$

Note that  $|\Psi_b^{(N)}(\mathbf{0})\rangle = |N\rangle$  is a Fock state satisfying  $\langle \Psi_b^{(N)}(\mathbf{0}) | \Psi_b^{(N)}(\mathbf{0}) \rangle = 1$ , while  $|\Psi_f^{(N)}(\mathbf{0})\rangle$  is a product state being normalized as well,  $\langle \Psi_f^{(N)}(\mathbf{0}) | \Psi_f^{(N)}(\mathbf{0}) \rangle = 1$ .

Probing the number of atoms in a many-body state is done by,

$$N = \langle \Psi | \hat{N} | \Psi \rangle \quad \text{where} \quad \hat{N} = \int \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}(\mathbf{r}) d^3r = \sum_{m,\mathbf{k}} \hat{a}_m^{\dagger}(\mathbf{k}) \hat{a}_m(\mathbf{k}), \quad (28.33)$$

or if we are only interested in a particular momentum state  $\mathbf{k}$  and vibrational state  $m$ ,

$$\langle \Psi | \hat{N}_m(\mathbf{k}) | \Psi \rangle = \langle \Psi | \hat{a}_m^{\dagger}(\mathbf{k}) \hat{a}_m(\mathbf{k}) | \Psi \rangle = \|\hat{a}_m(\mathbf{k}) | \Psi \rangle\|^2. \quad (28.34)$$

Other possible many-body states are bosonic or fermionic product states,

$$\boxed{|\Psi^{(N_1)}(\mathbf{0})\rangle |\Psi^{(N_2)}(\mathbf{q})\rangle}. \quad (28.35)$$

We will see in 28.1.6.9 that product states are normalized if the partial states are normalized. Explicitly,

$$\begin{aligned} |\Psi_b^{(N_1)}(\mathbf{0})\rangle |\Psi_b^{(N_2)}(\mathbf{q})\rangle &= \frac{1}{\sqrt{N_1! N_2!}} \hat{a}_0^{\dagger}(\mathbf{0})^{N_1} \hat{a}_0^{\dagger}(\mathbf{q})^{N_2} |0\rangle \\ |\Psi_f^{(N_1)}(\mathbf{0})\rangle |\Psi_f^{(N_2)}(\mathbf{q})\rangle &= \prod_{n=0}^{N_1-1} \hat{a}_n^{\dagger}(\mathbf{0}) \prod_{n=0}^{N_2-1} \hat{a}_n^{\dagger}(\mathbf{q}) |0\rangle. \end{aligned} \quad (28.36)$$

Note, that product states in the same mode need renormalization when merged,

$$|\Psi_b^{(N_1)}(\mathbf{0})\rangle |\Psi_b^{(N_2)}(\mathbf{0})\rangle = \frac{1}{\sqrt{N_1! N_2!}} \hat{a}_0^{\dagger}(\mathbf{0})^{N_1+N_2} |0\rangle = \sqrt{\binom{N_1+N_2}{N_1}} |\Psi_b^{(N_1+N_2)}(\mathbf{0})\rangle, \quad (28.37)$$

for example,  $|\Psi_b^{(N)}(\mathbf{0})\rangle |\Psi_b^{(1)}(\mathbf{0})\rangle = \sqrt{N+1} |\Psi_b^{(N+1)}(\mathbf{0})\rangle$ .

A  $\pi/2$ -Bragg pulse has the faculty to transfer 50% of the atoms into a momentum mode  $\mathbf{q}$ , thus creating a new state where every single atom lives in a coherent

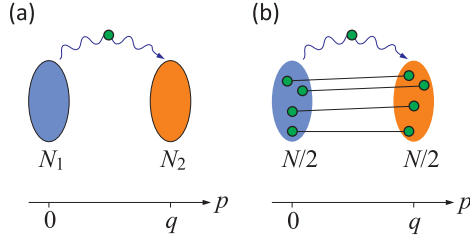


Figure 28.2: Cartoon of (a,b) bosonic stimulation and (c,d) cooperative enhancement.

superposition of two momenta,

$$\begin{aligned}
 |\Psi_b^{(brgg,N)}(\mathbf{0}, \mathbf{q})\rangle &= \frac{[\hat{a}_0^\dagger(\mathbf{0}) + \hat{a}_0^\dagger(\mathbf{q})]^N}{\sqrt{2^N N!}} |0\rangle = \sum_{n=0}^N \binom{N}{n} \frac{\hat{a}_0^\dagger(\mathbf{0})^n \hat{a}_0^\dagger(\mathbf{q})^{N-n}}{\sqrt{2^N N!}} |0\rangle \\
 |\Psi_f^{(brgg,N)}(\mathbf{0}, \mathbf{q})\rangle &= \prod_{n=0}^{N-1} \frac{[\hat{a}_n^\dagger(\mathbf{0}) + \hat{a}_n^\dagger(\mathbf{q})]}{\sqrt{2}} |0\rangle
 \end{aligned} \quad (28.38)$$

In the following, we will study scattering processes, that is, fluctuations, in the presence of the states (28.35) or (28.38).

#### 28.1.4.1 Bosonic stimulation versus cooperative enhancement by a Bragg grating

Now, we scatter a photon, whose fate is not of interest here, but which triggers possible transitions of an atom sitting together with  $N_1$  atoms in the momentum state  $\mathbf{0}|0\rangle$  towards another momentum state  $\mathbf{q}|0\rangle$  initially populated with  $N_2$  atoms via the operator,

$$\hat{H} = \sum_m \hat{a}_m^\dagger(\mathbf{k}) \hat{a}_m(\mathbf{0}) , \quad (28.39)$$

which in fact is nothing else than the static structure factor. Applying this process to bosonic or fermionic clouds, as defined in (28.32), we find *bosonic stimulation* only in the case of bosons,

$$\langle \Psi^{(N_1-1)}(\mathbf{0}) \Psi^{(N_2)}(\mathbf{q}) | \hat{H} | \Psi^{(N_1)}(\mathbf{0}) \Psi^{(N_2-1)}(\mathbf{q}) \rangle = \delta_{\mathbf{k}, \mathbf{q}} \begin{cases} \sqrt{N_1 N_2} & \text{for bosons} \\ 1 & \text{for fermions} \end{cases} , \quad (28.40)$$

as will be shown in Exc. 28.1.6.10(a). The transition probabilities are then,

$$\frac{d\sigma}{d\Omega} = |\langle f | \hat{H} | i \rangle|^2 = \delta_{\mathbf{k}, \mathbf{q}} \begin{cases} N_1 N_2 & \text{for bosons} \\ 1 & \text{for fermions} \end{cases} . \quad (28.41)$$

Note, that these results does not change in the presence of a Bragg grating not participating in the dynamics:

$$\langle \Psi_b^{(M-1)}(\mathbf{0}) \Psi_b^{(brgg, N+1)}(\mathbf{0}, \mathbf{q}) | \hat{H} | \Psi_b^{(M)}(\mathbf{0}) \Psi_b^{(brgg, N)}(\mathbf{0}, \mathbf{q}) \rangle = 1 . \quad (28.42)$$

However, applying the same scattering process between a BEC with  $M$  atoms and the Bragg state defined in (28.38) consisting of  $N$  atoms, we identify two interesting possibilities for which we find,

$$\boxed{\begin{aligned} \langle \Psi_b^{(M-1)}(\mathbf{0}) \Psi_b^{(brgg,N)}(\mathbf{0}, \mathbf{q}) | \hat{H} | \Psi_b^{(M)}(\mathbf{0}) \Psi_b^{(brgg,N-1)}(\mathbf{0}, \mathbf{q}) \rangle &= (\delta_{\mathbf{k},\mathbf{0}} + \delta_{\mathbf{k},\mathbf{q}}) \sqrt{MN} \\ \langle \Psi_b^{(M)}(\mathbf{q}) \Psi_b^{(brgg,N-1)}(\mathbf{0}, \mathbf{q}) | \hat{H} | \Psi_b^{(M-1)}(\mathbf{q}) \Psi_b^{(brgg,N)}(\mathbf{0}, \mathbf{q}) \rangle &= \delta_{\mathbf{k},\mathbf{q}} \sqrt{MN} \end{aligned}} \quad (28.43)$$

Interestingly, we find the same expression for bosons and for fermions,

$$\boxed{\langle \Psi_{b,f}^{(brgg,N-1)}(\mathbf{0}, \mathbf{q}) \Psi_{b,f}^{(1)}(\mathbf{q}) | \hat{H} | \Psi_{b,f}^{(brgg,N)}(\mathbf{0}, \mathbf{q}) \rangle = \sqrt{\frac{N}{2}} \left[ \delta_{\mathbf{k},\mathbf{0}} \pm \frac{N-1}{2} (\delta_{\mathbf{k},\mathbf{0}} + \delta_{\mathbf{k},\mathbf{q}}) \right]} \quad (28.44)$$

as will be shown in Exc. 28.1.6.10(b). The transition probabilities are then for boson and for fermions,

$$\frac{d\sigma}{d\Omega} = |\langle f | \hat{H} | i \rangle|^2 = \delta_{\mathbf{k},\mathbf{q}} \frac{N(N-1)^2}{4} \quad (28.45)$$

This means that, if  $\mathbf{k} = \mathbf{0}$  or  $\mathbf{k} = \mathbf{q}$ , the scattering is subject to *cooperative enhancement* by a factor of  $N/2$  (which is the number of atoms in each of the momentum state  $\mathbf{0}$  and  $\mathbf{q}$ ) independently on the quantum nature of the atom (boson or fermion). That is, the probability that the scattered atoms joins one of the two momentum goes, for large  $N$ , like  $N^2$ , but for  $N = 1$  there is no enhancement possible. Do Exc. 28.1.6.11.

### 28.1.4.2 Interpretation of bosonic stimulation as cooperative enhancement

The distinction between spontaneous and stimulated processes is not always obvious, as there is a whole world of cooperative processes in between those two concepts, for instance, superradiance, Bragg scattering, and enhanced spontaneous emission into a resonant cavity. All those processes have in common that they are amplified by fluctuations.

**Example 119 (Stimulated emission versus spontaneous emission: Cooperativity in a cavity):** Let us first discuss the case of a cavity. Vacuum fluctuations (VF) are structured by a cavity (finesse  $F$ ) leading to a modified DOS becoming anisotropic and developing spectral resonances. In resonance the VFs are enhanced (we get a standing wave of VFs), while off resonance they are suppressed. Therefore, an excited atom placed inside a cavity will suffer 'spontaneous stimulation' to decay into the cavity mode. Alternatively, we may say that the atom not only reacts to the local VFs but to all VFs reflected  $F$  times by the cavity mirrors provided these VFs are in phase (which is the case when the cavity is resonant). That is, *cavity-enhanced VFs amplify scattering into cavity modes* and, as we argued in Sec. 20.1.4 the VFs are measured by the structure factor (20.42).

Note, that the presence of photons in the cavity does not stimulate 'additionally', because stimulated emission and absorption are reversible processes.

**Example 120 (Bragg scattering: Cooperativity in a lattice):**



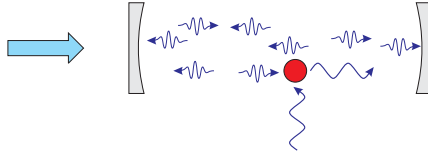


Figure 28.3: Cartoon of cooperative enhancement in a cavity.

**Example 121 (Matter wave superradiance and CARL: Cooperativity in a BEC):** We have seen that the stimulated processes mentioned above do not rely on quantum statistics, but rather on symmetry and coherence. Let us start with a naive picture of bosonic stimulation, a concept which can be applied to matter waves [391]. The physical process behind bosonically stimulated scattering is, that the presence of a macroscopically occupied state increases the density fluctuations of the system, and bosonically enhanced scattering is simply the diffraction of particles from these density fluctuations measured by  $S(\mathbf{q}, \omega)$ .

### 28.1.5 Collective scattering for condensates with interactions

Until now we totally disregarded interactions between particles. Correlations are introduced in a BEC by interactions between the atoms. Therefore, collective scattering effects are influenced by interactions, while on the other hand an ideal gas ( $gn \rightarrow 0$ ) scatters like an ultra-cool non-degenerate thermal cloud. In this sense, particle-like excitations ( $\mathbf{p}^2/2m \gg gn$ ) in an interacting BEC behave like thermal atoms. The mean-field energy can be seen as resulting from excitations of phonon pairs. These pairwise excitations populate the momentum modes, which modify the scattering of light via bosonic stimulation. That is, an interacting condensate ( $gn > 0$ ) gives a collective response to an incident light beam. Note that  $\mu > 0$  is possible when  $V(\mathbf{r}) \neq 0$  and  $gn \neq 0$  even if  $T \rightarrow 0$ , which is the case here considered.

What is the nature of the collective behavior? 1. The Bogolubov spectrum is modified. In the phononic regime, the absence of dispersion allows the definition of a speed of sound. 2. The scattering of light can be suppressed by excitation of phonon pairs. This effect is anisotropic and more pronounced in forward direction. That is, the resonance at which the light is scattered is shifted and broadened. The latter effect is understood via destructive interference of two processes: Scattering from a BEC to the momentum mode  $\mathbf{k}$  and from the momentum mode  $-\mathbf{k}$  to a BEC.

It is important to be aware that the notion of *bosonic stimulation*  $\sim n_i(1+n_f)$  and *fermionic inhibition*  $\sim n_i(1-n_f)$  also has its limitations, when interatomic interactions are not negligible, that is, when the quantum depletion is remarkable [275, 467]. The effect of interatomic collisions can be taken into account as contributions of pair correlations to the ground state of the BEC,

$$|\psi_0, n_0\rangle = |n_0, 0, 0\rangle - \sum_{\mathbf{k}} (v_{\mathbf{k}}^2/u_{\mathbf{k}}^2) |n_0 - 2, 1, 1\rangle + \sum_{\mathbf{k}} (v_{\mathbf{k}}^2/u_{\mathbf{k}}^2)^2 |n_0 - 4, 2, 2\rangle - \dots, \quad (28.46)$$

where  $|n_0, n_{\mathbf{k}}, n_{-\mathbf{k}}\rangle$  denotes the state with  $n_0$  atoms in the trap's ground state and  $n_{\pm\mathbf{k}}$  atoms in the momentum mode  $\mathbf{k}$ , where  $v_{\mathbf{k}}^2$  is the average population of momentum

mode  $\mathbf{k}$ . The populated recoil modes result in a increase of spontaneous emission by a factor of  $v_{\mathbf{k}}^2 = 1 + u_{\mathbf{k}}^2$ . We can also understand the modification of the scattering rate as resulting from small scale inhomogeneities generated by pair correlations. The effect is strongest at small scattering angles, that is in forward direction.

## 28.1.6 Exercises

### 28.1.6.1 Ex: Sum rules for the dynamic structure factor

Derive the following sum rules for the norm, the kinetic energy, and the compressibility,

$$\begin{aligned} S(\mathbf{q}) &= \int S(\mathbf{q}, \omega) d\omega \\ \frac{\hbar^2 q^2}{2m} &= \int \hbar\omega S(\mathbf{q}, \omega) d\omega \\ \frac{\kappa^2}{2} &= \int \frac{S(\mathbf{q}, \omega)}{\hbar\omega} d\omega \Big|_{\mathbf{q} \rightarrow 0} . \end{aligned}$$

### 28.1.6.2 Ex: Interaction energy of a condensate via spatial coherence

Show that the total energy of a condensate is given by  $\langle U \rangle = \frac{1}{2} \int n(\mathbf{r}_1) U(\mathbf{r}_1 - \mathbf{r}_2) g^{(2)}(\mathbf{r}_1, \mathbf{r}_2) n(\mathbf{r}_2) d^3 r_1 d^3 r_2$ .

### 28.1.6.3 Ex: Structure factor of a condensate in the local density approximation

Calculate the structure factor of a condensate in the local density approximation (LDA) [108, 651].

### 28.1.6.4 Ex: Structure structure of a Fermi gas

Calculate the structure factor for Bragg scattering on a Fermi gas.

### 28.1.6.5 Ex: Structure factor of a heteronuclear mixture

In this exercise we discuss the structure factor of a heteronuclear mixture (specifically contemplating  ${}^6\text{Li}$  mixed with  ${}^{87}\text{Rb}$ ) generalizing the available theory for Li spin mixtures to heteronuclear mixtures [149, 252, 253, 696]. The total dynamic structure factor is,

$$S(q, \omega) = S_{87,87}(q, \omega) + S_{6,6}(q, \omega) + S_{6,87}(q, \omega) + S_{87,6}(q, \omega) .$$

Exciting the Bragg resonance for Li, the Rb cloud would stay unaffected, the such that around  $\omega/2\pi = 295$  kHz,  $S_{87,87}(q, \omega) = 0$ , as well as,  $S_{6,87}(q, \omega) = S_{87,6}(q, \omega) = 0$ . For Fermi gas  $S_{6,6}(q, \delta) \rightarrow 1$ , except if Bose gas induces Li-Li correlations, as in the case of BCS-pairing of phonon-mediated Efimov states.

How does Rb influence the Bragg scattering of Li? Via a variation of the apparent

mass as a displacement of the Bragg resonance or as a second peak appearing at a specific detuning of the Bragg beams at  $\omega_{6,6} * 6/(6 + 87)$ ?

### 28.1.6.6 Ex: Spatial coherence of a condensate

Derive the relationship (28.7).

### 28.1.6.7 Ex: Structure factor for Bragg scattering

Demonstrate the following relationships,

$$\frac{dp_{cm}(\mathbf{q}, \omega)}{dt} = -m\omega_z^2 z_{cm} + \hbar q \frac{\Omega_{br}^2}{2} \int d\delta' [S(\mathbf{q}, \omega') - S(-\mathbf{q}, -\omega')] \frac{\sin(\omega - \omega')t_{br}}{\omega - \omega'}$$

$$\ddot{p}_{cm}(q, \omega) + \omega_z^2 p_{cm} = \hbar q \frac{\Omega_{br}^2}{2} \int d\omega' [S(\mathbf{q}, \omega') - S(-\mathbf{q}, -\omega')] \cos(\omega - \omega')t_{br} \longrightarrow 0 .$$

### 28.1.6.8 Ex: Commutation expressions for bosons and fermions

Verify the following useful commutation relations:

a. For bosons,

$$\hat{a}_m(\mathbf{k})\hat{a}_n^\dagger(\mathbf{q})^N = N\delta_{m,n}\delta_{\mathbf{k},\mathbf{q}}\hat{a}_n^\dagger(\mathbf{q})^{N-1} + \hat{a}_n^\dagger(\mathbf{q})^N\hat{a}_m(\mathbf{k}) , \quad (28.47)$$

which can be generalized to,

$$\hat{a}_m(\mathbf{k})[\hat{a}_n^\dagger(\mathbf{q}_1) + \hat{a}_n^\dagger(\mathbf{q}_2)]^N \quad (28.48)$$

$$= N\delta_{m,n}(\delta_{\mathbf{k},\mathbf{q}_1} + \delta_{\mathbf{k},\mathbf{q}_2})[\hat{a}_n^\dagger(\mathbf{q}_1) + \hat{a}_n^\dagger(\mathbf{q}_2)]^{N-1} + [\hat{a}_n^\dagger(\mathbf{q}_1) + \hat{a}_n^\dagger(\mathbf{q}_2)]^N\hat{a}_m(\mathbf{k}) .$$

b. For fermions do not support macroscopic populations of the type  $\hat{a}_n^\dagger(\mathbf{q})^N$ . Performing a number  $P$  of permutations of the operators and assuming that one fermion of the product state is in the internal state  $n$ , we calculate,

$$\hat{a}_n(\mathbf{k}) \prod_{m=0}^{N-1} \hat{a}_m^\dagger(\mathbf{q}) = (-1)^P \left[ \delta_{\mathbf{k},\mathbf{q}} \prod_{m \neq n}^{N-1} \hat{a}_m^\dagger(\mathbf{q}) - \prod_{m=0}^{N-1} \hat{a}_m^\dagger(\mathbf{q})\hat{a}_n(\mathbf{k}) \right] . \quad (28.49)$$

If none of the fermions of the product state is in state  $n$  the first part of the sum simply vanishes. This expression can also be generalized to,

$$\hat{a}_n(\mathbf{k}) \prod_{m=0}^{N-1} [\hat{a}_m^\dagger(\mathbf{q}_1) + \hat{a}_m^\dagger(\mathbf{q}_2)] = (-1)^P \prod_{m \neq n}^{N-1} [\hat{a}_m^\dagger(\mathbf{q}_1) + \hat{a}_m^\dagger(\mathbf{q}_2)]\hat{a}_n(\mathbf{k})[\hat{a}_n^\dagger(\mathbf{q}_1) + \hat{a}_n^\dagger(\mathbf{q}_2)]$$

$$= (-1)^P \left[ (\delta_{\mathbf{k},\mathbf{q}_1} + \delta_{\mathbf{k},\mathbf{q}_2}) \prod_{m \neq n}^{N-1} [\hat{a}_m^\dagger(\mathbf{q}_1) + \hat{a}_m^\dagger(\mathbf{q}_2)] - \prod_{m=0}^{N-1} [\hat{a}_m^\dagger(\mathbf{q}_1) + \hat{a}_m^\dagger(\mathbf{q}_2)]\hat{a}_n(\mathbf{k}) \right] . \quad (28.50)$$

**28.1.6.9 Ex: Extracting the atom number from many-body states**

Verify the normalization of (a) the bosonic Fock state (28.32), (b) the fermionic product state (28.32), (c) the bosonic product state (28.35), (d) the bosonic Bragg grating state (28.37), and (e) the fermionic Bragg grating state (28.37). **Help:** Speed up the calculations by using the results of 28.1.6.8.

**28.1.6.10 Ex: Bosonic stimulation and cooperative enhancement by lattices of bosons and fermions**

Compare bosons and fermions with respect to (a) bosonic stimulation and (b) cooperative enhancement.

**28.1.6.11 Ex: Cooperative enhancement versus bosonic stimulation**

CARL amplification comes from cooperativity not from bosonic stimulation [500, 391, 617], that is, it should work for fermions and boltzons. To demonstrate this proceed as follows:

a. Set up the single-atom Hamiltonian for a 3D harmonic potential in which the atoms (bosons or fermions) are initially placed allowing for the possibility of momentum recoil by photon scattering. This disregards the trap's inhomogeneity, but is a good assumption for short times. What are the eigenfunction of this Hamiltonian? Calculate the expectation value for the density distribution. Express the field operators in momentum space. Express the lowest energy states for a bosonic/fermionic cloud in momentum representation.

b. Now apply a  $\pi/2$ -Bragg-pulse imparting the recoil  $\mathbf{K}$  to the cloud. What is the resulting state? Recalculate the expectation value for the density distribution.

c. Now, assume the presence of another free (test) atom (or photon). Write down the Hamiltonian and the wavefunction for this atom. It is supposed to interact with the atomic cloud via the (perturbatively treated) interaction potential,

$$\hat{V} = \lambda \int d^3r \hat{\psi}_1^\dagger(\mathbf{r}) \hat{\psi}_2^\dagger(\mathbf{r}) \hat{\psi}_2(\mathbf{r}) \hat{\psi}_1(\mathbf{r}) .$$

Calculate the probability that the atom is scattered at a particular wavevector, i.e. determine the cooperative enhancement factor.

d. Is cooperative enhancement possible with just one atom?

e. How about cooperative enhancement in a cavity, when cooperativity is ensured by a single atom plus all its mirror images?

**28.2 Bragg diffraction**

An important technique for manipulating the atomic motion is by *Bragg diffraction*<sup>5</sup>. It allows the coherent transfer of atoms to other states of motion or to superpositions of motional states, and is extremely useful for applications, such as the realization of

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<sup>5</sup>The idea is analogous to the manipulation of the  $\mathbf{k}$ -vector of light waves by acousto-optic modulators.

matter wave beamsplitters [409] and atomic lasers, or for the targeted excitation of quasi-particles [409, 660, 651].

To implement Bragg diffraction, we consider two laser pulses with different frequencies and propagation directions  $\omega, \mathbf{k}_\omega$  and  $\omega - \Delta\omega, \mathbf{k}_{\omega-\Delta\omega}$ , detuned from an atomic resonance and intersecting at the position of atoms under an angle  $\vartheta$ , as shown in Fig. 28.4(a). The superposition of the electric fields of the light beams,

$$\begin{aligned} E &= E_0 e^{i(\mathbf{k}_\omega \cdot \mathbf{r} - \omega t)} + E_0 e^{i[\mathbf{k}_{\omega-\Delta\omega} \cdot \mathbf{r} - (\omega - \Delta\omega)t]} = E_0 e^{i(\mathbf{k}_\omega \cdot \mathbf{r} - \omega t)} \left( 1 + e^{-i(\mathbf{q} \cdot \mathbf{r} - \Delta\omega t)} \right) \\ &= 2E_0 e^{i(\mathbf{k}_\omega \cdot \mathbf{r} - \omega t)} e^{-\frac{i}{2}(\mathbf{q} \cdot \mathbf{r} - \Delta\omega t)} \cos \frac{\mathbf{q} \cdot \mathbf{r} - \Delta\omega t}{2}, \end{aligned} \quad (28.51)$$

where  $\mathbf{q} \equiv \mathbf{k}_\omega - \mathbf{k}_{\omega-\Delta\omega}$ , produces a standing light wave with an intensity proportional to,

$$|E|^2 = 4E_0^2 \cos^2 \frac{\mathbf{q} \cdot \mathbf{r} - \Delta\omega t}{2} = 2E_0^2 [1 + \cos(\mathbf{q} \cdot \mathbf{r} - \Delta\omega t)], \quad (28.52)$$

with which the atoms interact.

The Bragg diffraction technique has proven extremely efficient: up to 100% of the atoms can be transferred to well-defined momentum sidemodes. In general, the components of a cloud with different momentum modes overlap during the time scale of the Bragg pulses. They only separate spatially after a ballistic flight time, which then allows their identification via absorption imaging.

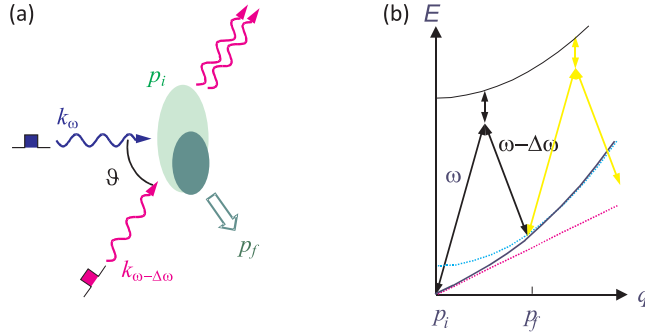


Figure 28.4: Bragg scattering of atoms at a standing light wave. (a) Geometric layout: Short pulses of two laser beams in Raman configuration enclosing an angle of  $\vartheta$  and detuned from each other by  $\Delta\omega$  are simultaneously irradiated into the cloud. (b) Bogolubov dispersion relation for interacting condensates (blue line). The quadratic dispersion relation (cyan) holds for free particles, and the linear dispersion relation (magenta) for phonon excitations.

## 28.2.1 Interpretations of the Bragg diffraction process

Bragg's diffraction can be treated within the formalism developed in Sec. 28.1.2, as will be shown later, in Sec. 28.2.3. But before that, let us present a simplified approach and several simple pictures illustrating the dynamics of Bragg diffraction.

### 28.2.1.1 Bragg diffraction picture

The *first interpretation* of this phenomenon is as *matter wave Bragg diffraction* at a standing light wave (i.e. an one-dimensional optical lattice) formed by two crossing

pulsed laser beams <sup>6</sup>. We consider atoms initially at rest exposed to the standing wave (28.51) with  $\Delta\omega = 0$  and  $\mathbf{q} \equiv q\hat{\mathbf{e}}_z$ , such that the dipolar potential  $U \propto |E|^2$  is, with (28.52),

$$U(z) = U_0 \cos^2 \frac{qz}{2} . \quad (28.53)$$

Assuming a given finite interaction time  $\tau$ , the modulation of the local phase of the atoms becomes <sup>7</sup>,

$$\psi_\tau(z) = \psi_0(z) e^{iU(z)\tau/\hbar} = \psi_0(z) e^{\frac{i}{2\hbar} U_0 \tau (\cos qz + 1)} = \psi_0(z) e^{iU_0 \tau / 2\hbar} \sum_n i^n J_n \left( \frac{U_0 \tau}{2\hbar} \right) e^{inqz} , \quad (28.54)$$

where  $J_n$  are the Bessel functions of the first kind <sup>8</sup>.

The condensed wavefunction evolves into a superposition of motional modes, which correspond to the diffraction orders of Bragg scattering and their amplitudes through the Bessel functions  $J_n$ . The diffraction efficiency increases with laser intensity and with time.

Now, we need to generalize this result to the propagating standing wave of the expression (28.52). The intensity generates a dipole potential,

$$U(z, t) \approx U_0 \cos^2 \frac{q_z z - \Delta\omega t}{2} , \quad (28.55)$$

so that the condensate now evolves according to,

$$\psi(z, t) = \psi_0(z) e^{i/\hbar \int_{t_0}^{t_0+\tau} U(z, t) dt} = \psi_0(z) e^{i/\hbar \int_{t_0}^{t_0+\tau} U_0 \cos^2 \frac{q_z z - \Delta\omega t}{2} dt} . \quad (28.56)$$

For short interaction times,  $\tau \ll 2\pi/\Delta\omega$ , ...

### 28.2.1.2 Compton scattering picture

The *second interpretation* is that of *Compton scattering*: Spontaneous Rayleigh scattering of a photon from a mode  $\mathbf{k}_\omega$  into a solid angle around  $\mathbf{k}_\omega - \Delta\omega$  leaves an atom with the recoil momentum  $\hbar\mathbf{q} \equiv \mathbf{p}_f \cdot \mathbf{p}_i$ . Of course, one can *stimulate* the Rayleigh scattering process by providing the laser mode  $\mathbf{k}_\omega - \Delta\omega$  at the entrance. By replacing the spontaneous output mode with a stimulated input mode, we increase the probability for an atomic recoil in the momentum mode  $\hbar\mathbf{q}$ , which is thus pre-selected by the choice of  $\mathbf{k}_\omega - \Delta\omega$ . Since the elementary scattering process must conserve energy and total momentum,

$$\begin{aligned} \hbar\omega + \frac{p_i^2}{2m} &= \hbar(\omega - \Delta\omega) + \frac{p_f^2}{2m} \\ \hbar\mathbf{k}_i + \mathbf{p}_i &= \hbar\mathbf{k}_f + \mathbf{p}_f , \end{aligned} \quad (28.57)$$

we obtain the *Bragg condition*,

$$E = \Delta\omega = \frac{p_f^2}{2m} - \frac{p_i^2}{2m} = \frac{(\mathbf{p}_f - \mathbf{p}_i)^2}{2m} + \frac{(\mathbf{p}_f - \mathbf{p}_i) \cdot \mathbf{p}_i}{m} = \frac{q^2}{2m} + \frac{\mathbf{q} \cdot \mathbf{p}_i}{m} . \quad (28.58)$$

<sup>6</sup>Note, that the initial population of the recoil mode should be small. Otherwise, since Bragg diffraction is a coherent and thus reversible process, atoms initially in the recoil mode are transferred back to the original matter wave mode.

<sup>7</sup>Using the Jacobi-Anger expansion,  $e^{i\beta \cos x} = \sum_n i^n J_n(\beta) e^{inx}$ .

<sup>8</sup>Andreas got  $\psi_0(z) \sum_n J_n^2(U_0\tau/2\hbar) e^{inqz/2}$ .

Expressed by the Bragg angle, the condition reads,

$$q = \sqrt{(\mathbf{p}_f - \mathbf{p}_i)^2} = \sqrt{\hbar^2 \mathbf{k}_i^2 + \hbar^2 \mathbf{k}_f^2 - 2\hbar^2 \mathbf{k}_i \mathbf{k}_f} \simeq \hbar k_i \sqrt{2 - 2 \cos \theta} = 2\hbar k_i \sin \vartheta / 2. \quad (28.59)$$

The efficiency for transferring atoms to the recoil mode depends on the fulfillment of this condition. The Bragg condition can be employed to select higher diffraction orders.

### 28.2.1.3 Stimulated Raman scattering picture

A *third interpretation* is as *stimulated Raman scattering* between two different kinetic states of the atom [see 28.4(b)]. In fact, the momentum modes  $\mathbf{p}_i$  and  $\mathbf{p}_f$  have different energies, which, for a condensate, are determined by the Bogolubov spectrum [268]. By varying the angle  $\vartheta$  in the Bragg condition (28.58), we can choose the amount of energy to be transferred and thus probe the spectrum, i.e. measure the excitation energy  $E(\mathbf{q}, \mu)$  as a function of the momentum  $\mathbf{q}$  and the chemical potential  $\mu$  in the particle regime  $\mathbf{q}^2/2m \gg \mu$ , as well as in the phonon regime  $\mathbf{q}^2/2m \ll \mu$ . On the other hand, varying the detuning  $\Delta\omega$  in the Bragg condition (28.58), we selectively address different velocity classes of a gas or condensate, which allows us to probe its velocity distribution. This procedure is called spectroscopy of *recoil-induced resonances* (RIR) [157, 660]. RIR spectroscopy also provides detailed information on the mean-field energy and the (inhomogeneous) density distribution of a condensate. Note, finally, that Bragg scattering is closely related to *Kapitza-Dirac* scattering of atomic beams, well-known in conventional atom optics [380, 276].

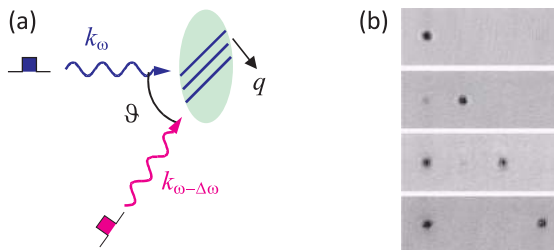


Figure 28.5: Bragg scattering of atomic clouds. (a) Geometric layout as in 28.4. Here, we assume  $p_i = 0$ . (b) Experiment showing coherent splitting by a Bragg pulse.

### 28.2.1.4 Coherent splitting

There is a general interest in the possibility of dividing phase space by coherent coupling of otherwise independent modes. We are talking, of course, about double slits or beamsplitters, which represent an essential tool of quantum mechanics. Bragg diffraction realizes a beamsplitter for atomic clouds analogous to the optical beamsplitter. In fact, Bragg diffraction has been used for the realization of output couplers for atom lasers and for atom interferometers. A suggestion that is sometimes made is the following: 'A condensate is a macroscopically populated momentum mode. The Bragg beamsplitter divides the phase space into two entangled output modes. Shouldn't it

be possible to generate a macroscopic superposition of two condensates, i.e. a really macroscopic Schrödinger cat?’ of the type

$$(|\Psi_+\rangle + |\Psi_-\rangle) . \quad (28.60)$$

There is an obvious fundamental interest to study such states and the mechanisms leading to their decoherence (see Sec. 16.1.1).

To clarify the situation, we first have to say, what we mean by *Schrödinger cat*. A Schrödinger cat is a quantum superposition of many-body states. A perfect cat made of  $N$  two-level atoms can be expressed as  $|+\dots\rangle \pm |-\dots\rangle$ . The Einstein-Podolsky-Rosen (EPR) and the Greenberger-Horne-Zeilinger states (GHZ) belong to this category. The degree of entanglement of the cat is measured by the information entropy defined as  $S = -\langle \log_2 \hat{\rho} \rangle$ , where  $\hat{\rho}$  is the density operator. The information entropy measures the amount of classical information that can be encoded in the quantum state. For example, the entropy of a perfect cat state is  $S = 1$  bit, because if we find one of the atoms in the state  $|+\rangle$ , we know that all others are in the same state.

Second, we have to explain, what we mean by a *beamsplitter*. Subject to a beam splitting process, every individual atom has the choice between one of two output ports. However, if the process is coherent, every atom will evolve into a coherent superposition, but it does so independently from the other atoms. That is, we can write the state of the atomic cloud as a product state of *Schrödinger kittens*  $(|+\rangle \pm |-\rangle)^N$ , but no real cat. The information entropy is  $S = N$  bit, as for independent atoms. *Clearly, the state (28.60) is NOT the state generated by a beamsplitter!* Nevertheless, the beamsplitter creates a certain correlation between the two modes (see Sec.15.6).

It may come as a surprise, that a condensate composed of totally delocalized atoms coherently interacting with a homogeneous light field (the photons of the Bragg beams are totally delocalized over the field mode including the condensate volume) increases its entropy from 1 to  $N$  bits. This argument, however, would be the same for a non-condensed *thermal* cloud being sufficiently cold that the thermal de Broglie wavelengths exceeds the size of the cloud. That is, even in condensates the photons are scattered by individual atoms. The interaction with the light *localizes* one atom in the condensate before removing it from there by recoil. Nevertheless, cooperative interaction of several atoms with a light mode is possible, e.g. in superradiance or when the photons are recycled by means of an optical cavity, as in the Jaynes-Cummings model.

## 28.2.2 Bragg interferometry of a thermal gas

Even above the critical temperature the momentum distribution of a dilute thermal gas is (slightly) modified by quantum statistics, i.e. by the classical, bosonic or fermionic nature of the gas. The momentum distributions have been calculated in Chp. 25.3. We have already emphasized that Bragg interferometry can be used to measure the momentum distribution of a gas via RIR spectroscopy, whether the gas is condensed or thermal. Now, let us discuss Bragg interferometry on a thermal gas, based on the articles [461][DOI](#) and [180][DOI](#).



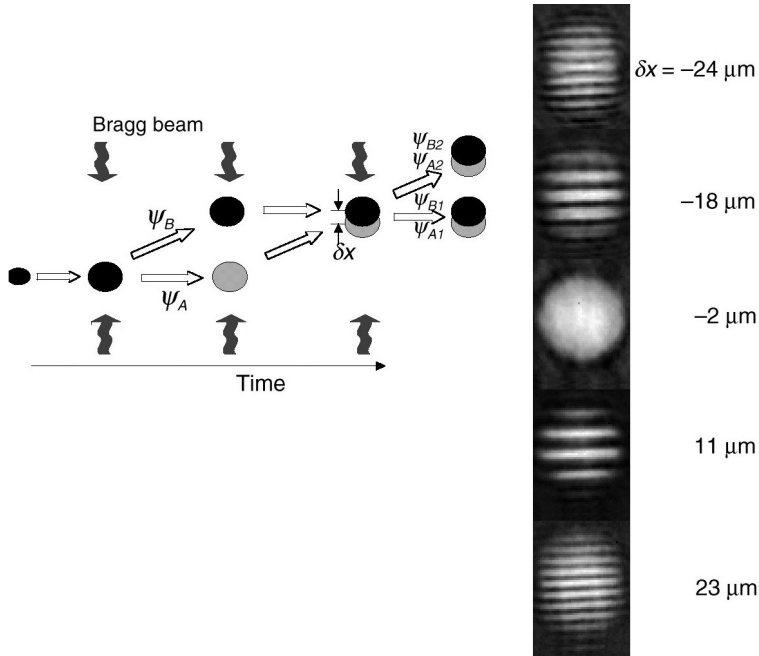


Figure 28.6: Bragg interferometer.

### 28.2.2.1 Free evolution of a thermal cloud

To describe the Bragg scattering process quantitatively, we interpret it as a *Raman transition between discrete atomic momentum states governed by a Schrödinger equation*. On the other hand, as long as no radiation is incident the atomic center-of-mass wavefunctions evolve freely or under the constraint of an external potential. That is, both processes concern the same motional degree of freedom. In order to derive a complete quantum model, let us first develop the formalism for the description of the free evolution of a thermal cloud, then we explain how a resonant radiation can be included.

We consider a thermal atomic cloud initially distributed over many momentum classes according to the Maxwell-Boltzmann velocity distribution,

$$D(k_z) = \frac{\hbar}{(2\pi m k_B T)^{1/2}} e^{-\hbar^2 k_z^2 / 2m k_B T} = \frac{e^{-\pi k_z^2 / k_{therm}^2}}{k_{therm}}, \quad (28.61)$$

using  $k_{therm} \equiv 2\pi/\lambda_{therm}$  and (24.9). Because of the inhomogeneity of the distribution, any evolution of atoms belonging to specific momentum classes caused by velocity-selective radiation pulses, must be calculated with individual atoms. The final momentum distribution (e.g. after a pulse sequence) can then be obtained by weighing with the individual evolution with the initial momentum distribution<sup>9</sup>.

<sup>9</sup>The procedure neglects interatomic interactions, which is always a good presumption, for example, for an ultracold Fermi gas [183] or for <sup>88</sup>Sr atoms, which have a very small scattering length.

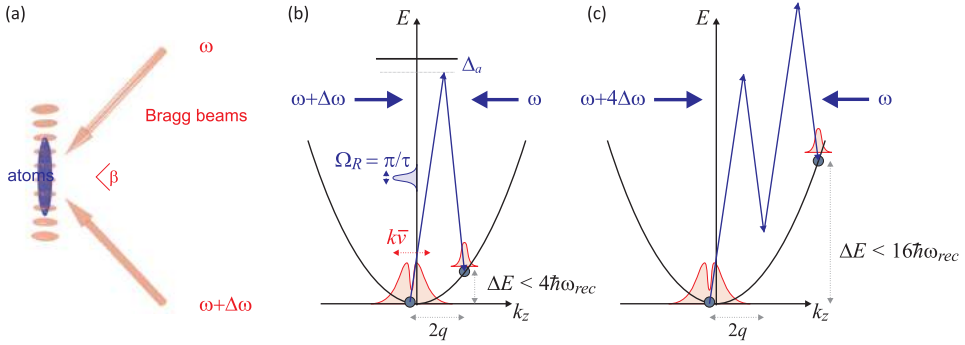


Figure 28.7: (a) Geometry for Bragg diffraction. (b) Illustration of a Raman transition between two points of the free-particle dispersion curve, when the atoms are initially thermally distributed. (c) Same as (a), but now the detuning  $\Delta\omega$  is adjusted for second-order Bragg diffraction.

We describe the quantum state of a thermal atom  $|\psi\rangle$  as a plane wave,  $\langle z|\psi\rangle \propto e^{ik_z z}$ , which in momentum space corresponds to a Dirac distribution,  $\langle k_z|\psi\rangle \propto \delta(z - z_0)$ . Without radiative coupling, we describe the evolution in momentum space by the solution of the Schrödinger equation (or propagator),

$$\langle k_z|\psi(t)\rangle = e^{i\hat{H}t/\hbar}\langle k_z|\psi(0)\rangle. \quad (28.62)$$

In free space, with the Hamiltonian  $\hat{H}_{free} = \hbar^2 k_z^2 / 2m$ , the wavefunction is obviously constant.

In order to couple two intervals of momentum distribution by resonant radiation, we first need to duplicate the Hilbert space,

$$a_{i,k_z}(t) \equiv \langle i|\psi_{k_z}(t)\rangle = \langle i|\langle k_z|\psi(t)\rangle \quad (28.63)$$

with  $i = 1, 2$ . Note that, in this case, the Hilbert spaces are not disjoint.

To obtain the atomic momentum distribution after the application of a pulse sequence, we calculate the evolution of the amplitudes  $a_{j,k_z}$  for a variety of initial momenta and weigh the final populations of the momentum states with the distribution function  $D(k_z)$ . The number of atoms expected in the zeroth and first Bragg diffraction order is, therefore,

$$N_j(t) = \int D(k_z) |a_{j,k_z}(t)|^2 dk_z. \quad (28.64)$$

### 28.2.2.2 Bragg scattering and RIR

For large momentum distributions,  $T \gg T_{rec}$ , the atomic cloud occupies many momentum states, such that the Bragg scattering produces a RIR-like signal. That is, the scattering probability is proportional to the *population difference* of the initial and final momentum states, as discussed in Sec. 22.3.1. The number of scattered atoms/photons is, therefore,

$$\dot{N}_{brg} \propto \Omega_R \left. \frac{\partial D(k_z)}{\partial k_z} \right|_{k_z = \hbar m \Delta\nu / q}. \quad (28.65)$$

where,

$$\Omega_R = \frac{\Omega_1 \Omega_2}{2\Delta_a} = \frac{1}{\Delta_a} \frac{3\lambda^2}{4\pi} \frac{\Gamma}{\hbar\omega} \sqrt{I_1 I_2} = \frac{3\pi c^2 I}{\hbar\omega^3} \frac{\Gamma}{\Delta_a} \quad (28.66)$$

is the two-photon Rabi frequency. For very narrow momentum distributions,  $T \ll T_{rec}$ , we may assume the atomic cloud to occupy only a single momentum state,

$$\dot{N}_{brg} \propto \Omega_R D(k_z). \quad (28.67)$$

The transition rate per atom is then given by [652],

$$\frac{W}{N} = \frac{2\pi\hbar}{N} \Omega_R^2 \sum_f |\langle f | \hat{\rho}^\dagger(\mathbf{k}) | g \rangle|^2 \delta(\hbar\nu - E_f + E_g) \equiv 2\pi\Omega_R^2 S(\mathbf{k}, \nu). \quad (28.68)$$

As illustrated in Fig. 28.7, to scatter an atom with the initial wavevector  $k_z$  to the next higher momentum state  $k_z + 2q$ , the Bragg condition requires,

$$\Delta\nu_R = \nu_{R2} - \nu_{R1} = \frac{\hbar(k_z + 2q)^2}{2m} - \frac{\hbar k_z^2}{2m} = \frac{2\hbar q}{m} (k_z + q). \quad (28.69)$$

If we tune  $\Delta\nu(\pm\Delta k_z)$  until the Bragg signal  $\dot{N}_{brg}$  drops to  $e^{-1/2}$ ,

$$\Delta\nu_R(\Delta k_z) - \Delta\nu_R(-\Delta k_z) = \frac{4\hbar\Delta k_z q}{m} = \frac{4\hbar q}{m} \frac{\sqrt{mk_B T}}{\hbar} = 4q \sqrt{\frac{k_B T}{m}}. \quad (28.70)$$

### 28.2.2.3 Bragg scattering by free atoms

Let us first assume that during the Bragg pulse only two discrete atomic momentum states  $j = 0, 1$  are coupled [74, 461, 180], and that trapping potentials are absent or can be neglected. This is justified for Bragg pulse sequences much shorter than an oscillation period of the trap. We denote the probability amplitudes for the two momentum states by momentum space wavefunctions  $a_{j,k_z}$ . They correspond to atoms with initial momenta  $\hbar k_z$  that are coupled to states with momentum  $\hbar k'_z = \hbar(k_z + 2q)$ . The temporal evolution of the amplitudes under the action of the Bragg light is given by the solutions of the Schrödinger equation [461]<sub>DOI</sub>, [180]<sub>DOI</sub>,

$$\begin{pmatrix} a_{0,k_z}(t) \\ a_{1,k_z}(t) \end{pmatrix} = e^{-i\hat{H}_R t/\hbar} \begin{pmatrix} a_{0,k_z}(0) \\ a_{1,k_z}(0) \end{pmatrix}, \quad (28.71)$$

with the Hamiltonian,

$$\hat{H}_R = \begin{pmatrix} \frac{\hbar^2}{2m} k_z^2 & \frac{1}{2} \hbar \Omega_R \\ \frac{1}{2} \hbar \Omega_R & \frac{\hbar^2}{2m} k_z'^2 - \hbar \delta \end{pmatrix}, \quad (28.72)$$

where  $\Delta = 2\hbar q^2/m - \delta$  is the detuning of the Bragg lasers from the recoil shift. When the Bragg light is switched off, the Hamiltonian simplifies to,

$$\hat{H}_{free} = \begin{pmatrix} \frac{\hbar^2}{2m} k_z^2 & 0 \\ 0 & \frac{\hbar^2}{2m} k_z'^2 - \delta \end{pmatrix}. \quad (28.73)$$

Concatenating temporal evolutions described by  $e^{-i\hat{H}_R t/\hbar}$  and  $e^{-i\hat{H}_{free} t/\hbar}$ , the phase evolution of individual atoms in momentum state superpositions can be calculated for arbitrary sequences of pulses separated by intervals of free evolution, for example, Ramsey-type sequences.

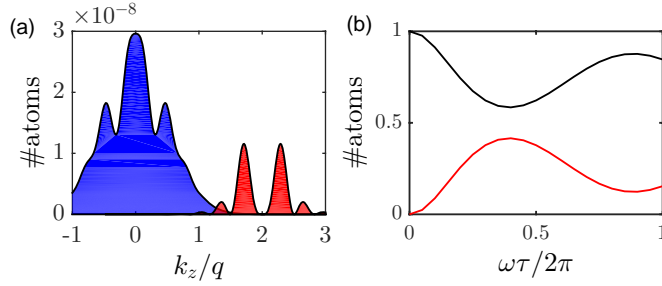


Figure 28.8: (code) (a) Distribution of momentum classes in the direction of  $k_z$  after irradiation of a  $2\pi$  Bragg pulse. The width of the structure is determined by the power broadening of the Raman transition. (b) Temporal evolution of the populations of the momentum states 0 and  $2q$ .

#### 28.2.2.4 Bragg scattering by trapped particles

When trapped atoms are considered, the problem arises that the Hilbert space of momentum states is simultaneously coupled by two interactions: a moving optical lattice (generated by the Bragg lasers) and the (harmonic) trap. However, the situation gets simpler if a separation of the scales is possible. In general, the duration of a pulse is very short,  $\tau \ll 2\pi/\omega_z$ . In contrast, the duration of a free evolution period  $\Delta t$  (e.g. in a Ramsey cycle) may be such, that it is no more negligible compared to a trap oscillation period, so that we need to account for the action of the trapping potential explicitly.

As the trap couples the atomic momenta with the atomic positions ( $E_{kin} + E_{pot} = const$ ), the initial spatial distribution of the atoms must now be considered. For simplicity, we describe it as a thermal Gaussian, similarly to what has been done in Eq. (28.61) for the momentum distribution,

$$G(z) = \sqrt{\frac{m\omega_z^2}{2\pi k_B T}} e^{-m\omega_z^2 z^2 / 2k_B T} = \frac{e^{-\pi z^2 / a_z^4 k_{therm}^2}}{a_z^2 k_{therm}}. \quad (28.74)$$

Beginning with the positions  $z$  and initial momenta  $k_z$ , after a diffraction pulse transferring the recoil  $2q$  to part of the atoms and being short enough not to change their positions, the atoms follow classical trajectories. The atomic momenta (now depending on time) are simply the solution of the equation of motion  $\hbar \dot{k}_z = -m\omega_z^2 z$  with the initial conditions  $z(0) = z$  and  $k_z(0) = k_z$ , respectively,  $k'_z(0) = k_z + 2q$ ,

$$\begin{aligned} \tilde{k}_z(t) &= k_z \cos \omega_z t - \frac{m\omega_z}{\hbar} z \sin \omega_z t \\ \tilde{k}'_z(t) &= (k_z + 2q) \cos \omega_z t - \frac{m\omega_z}{\hbar} z \sin \omega_z t, \end{aligned} \quad (28.75)$$

where the first expression holds for non-diffracted atoms and the second for diffracted atoms. These momenta are substituted for  $k_z$  and  $k'_z$ , respectively, in the Hamiltonians (28.72) and (28.73). As the Bragg pulses are short compared to the oscillation period,  $\tau \ll 2\pi/\omega_z$ , the effect of the trapping potential may be neglected during Bragg scattering. This means that the Hamiltonian  $\hat{H}_R$  depends on  $\tilde{k}_z(t)$ , but can be

treated as time-independent for the short intervals  $\tau$ . In contrast, the Hamiltonian for free propagation  $\hat{H}_{free}$  depends on the time, if  $\Delta t$  is long. In this case, the phase evolution of the atoms in both coupled states can be described by the time evolution operator as,

$$e^{-i\hat{H}_{free}t/\hbar} = \begin{pmatrix} \exp\left(-i\int_0^t dt \frac{\hbar}{2m}\tilde{k}_z^2(t)\right) & 0 \\ 0 & \exp\left(-i\int_0^t dt \left[\frac{\hbar}{2m}\tilde{k}'_z(t) - \delta\right]\right) \end{pmatrix}. \quad (28.76)$$

Since the amplitudes  $a_{j,z,k_z}$  now also depend on the initial atomic positions, the final populations of the momentum states must be additionally weighted with the initial spatial distribution. Therefore, the Eq. (28.64) for the expected the numbers of diffracted and non-diffracted atoms must be replaced by,

$$N_j(t) = \iint D(k_z)G(z) |a_{j,z,k_z}(t)|^2 dk_z dz. \quad (28.77)$$

In practice, however, it might be a good approximation to assume small displacements around a  $\delta$ -shaped position distribution. Note, that the transformation (28.75) must be repeated for every free evolution pulse of a sequence.

**Example 122 (Approximation for small displacements):** In practice, we may neglect the displacements,  $z \simeq 0$ . Then the equations (28.75) simplify to,

$$\tilde{k}_z(t) = k_z \cos \omega_z t \quad \text{and} \quad \tilde{k}'_z(t) = (k_z + 2q) \cos \omega_z t.$$

Inserting them in (28.76) we obtain for the propagator,

$$e^{-i\hat{H}_{free}t/\hbar} = \exp\left(-\frac{i\hbar k_z^2}{4m\omega_z}(\cos \omega_z t \sin \omega_z t + \omega_z t)\right) \begin{pmatrix} 1 & 0 \\ 0 & \exp\left(-\frac{i\hbar q k_z}{2m\omega_z}(\cos \omega_z t \sin \omega_z t + \omega_z t)\right) \end{pmatrix}.$$

In Exc. 28.2.4.1 we will study the behavior of an ultracold atomic cloud subject to a gravitational potential during a Ramsey-Bordé sequence.

### 28.2.2.5 Bloch equations approach

Experimentally, we observe decoherence of the dynamics described above on a very slow time scale. This phenomenon can be included in a description based on Bloch equations,

$$\frac{d}{dt}\vec{\rho}_{k_z}(\tau) = M_j\vec{\rho}_{k_z}(\tau), \quad (28.78)$$

with

$$\vec{\rho}_{k_z}(\tau) = \begin{pmatrix} \rho_{00,k_z}(\tau) \\ \rho_{01,k_z}(\tau) \\ \rho_{10,k_z}(\tau) \\ \rho_{11,k_z}(\tau) \end{pmatrix} \quad \text{and} \quad M_j = \begin{pmatrix} 0 & \Gamma & \frac{i}{2}\Omega_R & -\frac{i}{2}\Omega_R \\ 0 & -\Gamma & -\frac{i}{2}\Omega_R & \frac{i}{2}\Omega_R \\ \frac{i}{2}\Omega_R & -\frac{i}{2}\Omega_R & -\gamma - i\Delta_j & 0 \\ -\frac{i}{2}\Omega_R & \frac{i}{2}\Omega_R & 0 & -\gamma + i\Delta_j \end{pmatrix} \quad (28.79)$$

with the solution,

$$\vec{\rho}_{k_z}(\tau) = e^{M_3 t} e^{M_2 t} e^{M_1 t} \vec{\rho}_{k_z}(0) \quad (28.80)$$

with,

$$\begin{aligned} \Delta_1 &= \frac{\hbar}{2m} (k_z + 2q)^2 - \Delta\nu - \frac{\hbar}{2m} k_z^2 \\ \Delta_3 &= \frac{\hbar}{2m} [(k_z + 2q) \cos \omega_{tr} \tau]^2 - \frac{\hbar}{2m} [(k_z + 2q) \cos \omega_{tr} \tau - 2q]^2 - \Delta\nu . \end{aligned} \quad (28.81)$$

We weigh populations with the initial momentum distribution,

$$N_j(\tau) \equiv \int D(k_z) \rho_{jj,k_z}(\tau) dk_z . \quad (28.82)$$

### 28.2.2.6 Kapitza-Dirac scattering

An atomic beam with longitudinal de Broglie wavelength  $\lambda_{dB} = h/p$  diffracted by a solid periodic grating with a slit distance of  $d$  receives a transverse amplitude modulation. In the far field, this generates focuses at angles defined by  $n\lambda_{dB}/d = \sin \vartheta$ . Alternatively, the grating may consist of a standing light wave detuned from resonances. The standing wave will create a periodic optical potential, which imprints a transverse phase modulation on the atomic beam. In the far field, the result will be the same as for the solid grating. Each atom will evolve into a superposition of momentum sidemodes  $\pm n2\hbar k$ , without any momentum having been transferred to the atoms. The diffraction angle is again  $\sin \vartheta = \pm n2\hbar k/p = \pm n\lambda_{dB}/(\lambda/2)$ , where  $\lambda/2 = d$  is the periodicity of the standing light wave. However, this is only true if the phase shift is much smaller than  $\pi$ . This scheme is called the *Raman-Nath regime* or the regime of *Kapitza-Dirac scattering*. An equivalent condition for this regime is, that the interaction time is less than a period of oscillation in the optical potential,  $\tau \ll \sqrt{\hbar/\omega_{rec}/U}$ , or  $v_{trans}\tau \ll \lambda$ .

The Raman-Nath regime is realized by a very focused optical standing wave. A wave that is not plane can be considered a superposition of many spatial modes. Since (off-resonant) scattering (absorption followed by induced emission) corresponds to a photon redistribution between spatial modes, in a tight waist the phase matching condition is somewhat relaxed and minor corrections to the energy balance are possible. In a certain sense, Kapitza-Dirac scattering is the inverse process of 'forward scattering' of a laser beam passing through an atomic cloud: the roles of light and atoms are exchanged. The requirement that the interaction time be short implies, that the light grating is 'optically dilute' for the atomic beam <sup>10</sup>.

For larger Rabi frequencies,

$$\Omega_R \gg \frac{2\hbar q \sigma_{k_z}}{m} , \quad (28.83)$$

with  $\sigma_{k_z} = \sqrt{mk_B T/\hbar^2}$  being the width of the momentum distribution, the Doppler broadening is dominated by power broadening, meaning that Bragg diffraction occurs

<sup>10</sup>Note, that we usually employ the term of *optical diluteness* the other way round, i.e. an atomic cloud can be optically dilute (or dense) for a laser beam.

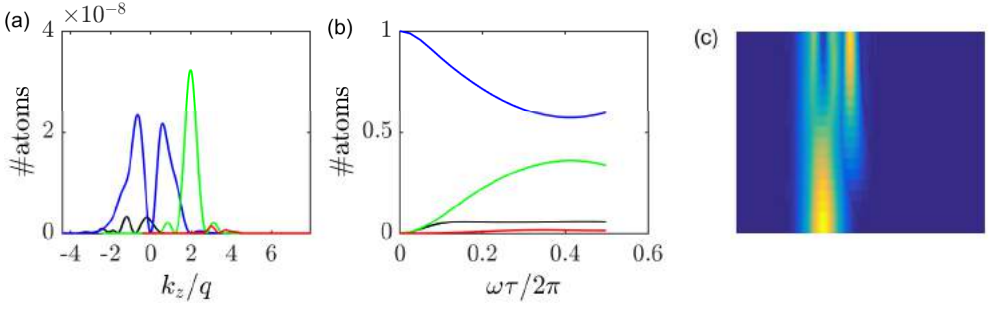


Figure 28.9: (code) (a) Distribution of momentum classes in the direction of  $k_z$  after irradiation of a  $\pi$  Bragg pulse. (b,c) Temporal evolution of the populations of the momentum states  $nq$ .

all over the atomic cloud. At some point, however, the Rabi frequency becomes comparable to the energy difference between adjacent momentum states, and Kapitza-Dirac scattering sets in. According to [74] the scattering will stay two-state like as long as the Rabi frequency fulfills the condition,

$$\Omega_R \ll \frac{\hbar}{m}(4q^2 - 2q\sigma_{k_z}). \quad (28.84)$$

In the Kapitza-Dirac regime, the large energy uncertainty, connected with the fast coupling rate, allows several momentum states to be coupled simultaneously. In particular the Bragg Hamiltonian is replaced by,

$$\hat{H}_\tau = \begin{pmatrix} \ddots & & \ddots & & & & \\ \ddots & & \frac{\hbar(k_z - 2q)^2}{2m} + \delta & \frac{\Omega_R}{2} & & & \\ & & \frac{\Omega_R}{2} & \frac{\hbar k_z^2}{2m} & & & \\ & & & \frac{\Omega_R}{2} & \frac{\hbar(k_z + 2q)^2}{2m} - \delta & \ddots & \\ & & & & & \ddots & \ddots \end{pmatrix}. \quad (28.85)$$

The crossover from the Bragg-diffraction regime to Kapitza-Dirac scattering is a smooth transition. As we will see below, for intermediate Rabi frequencies (here  $1 \text{ MHz} > \Omega_R/2\pi > 100 \text{ kHz}$ ) the neighboring diffraction states, corresponding to momentum shifts of  $4\hbar q$  and  $-2\hbar q$  (second and minus first order), are scarcely populated. For higher and higher Rabi frequencies,  $\Omega_R/2\pi > 1 \text{ MHz}$ , the scattering populates more and more diffraction orders.

### 28.2.2.7 Higher-order Bragg scattering

Higher-order Bragg scattering is possible as well. Then the  $2n$ -photon Rabi frequency must be calculated and inserted in the second diagonal of (28.85).

### 28.2.3 Bragg spectroscopy of a condensate

To measure the Bogolubov spectrum, we need to excite perturbations in a condensate and study its reaction [652].

Let us now imagine that the potential has the form of a standing wave. Technically this can be done by two laser beams having the same frequency crossing at the position of the atoms,

$$V_{trap}(\mathbf{r}, t) \equiv \frac{V}{2} e^{i\mathbf{q}_1 \cdot \mathbf{r} - i\omega t} + \frac{V}{2} e^{i\mathbf{q}_2 \cdot \mathbf{r} - i\omega t} . \quad (28.86)$$

Choosing the coordinate system such that,  $\mathbf{q}_1 \equiv (k_x, 0, k_z)$  and  $\mathbf{q}_2 \equiv (k_x, 0, -k_z)$ ,

$$V_{trap}(\mathbf{r}, t) = \frac{V_x}{2} e^{ik_z z - i\omega t} + \frac{V_x}{2} e^{-ik_z z + i\omega t} , \quad (28.87)$$

with  $V_x \equiv V e^{ik_x x}$ . With this weak perturbation applied to the atoms, we make the ansatz,

$$\psi(\mathbf{r}, t) = e^{-i\mu t/\hbar} (\psi_0(\mathbf{r}, t) + u(t)e^{ik_z z - i\omega t} - v(t)e^{-ik_z z + i\omega t}) , \quad (28.88)$$

where the amplitudes of the perturbation,  $u(t)$  and  $v(t)$ , only vary slowly in time. Assuming that  $\psi_0$  is fairly homogeneous, i.e.  $\langle \psi_0 | \nabla_z | \psi_0 \rangle \simeq 0$ , the momentum transferred to the BEC is,

$$\langle \psi(\mathbf{r}, t) | -i\hbar \nabla_z | \psi(\mathbf{r}, t) \rangle = \hbar k_z (|u|^2 - |v|^2) . \quad (28.89)$$

We can now solve the Gross-Pitaevskii equation (26.20) in the same way as in Sec. ?? inserting the ansatz (28.88). The terms proportional to  $e^{ik_z z - i\omega t}$  are,

$$\frac{\hbar^2 \mathbf{k}_z^2}{2m} u + \frac{V}{2} \psi_0 + g(|\psi_0|^2 + |u|^2 + |v|^2) u + g\psi_0^2 v + g|v|^2 u + g|\psi_0|^2 u = \left( i\hbar \frac{\partial}{\partial t} + \hbar\omega + \mu \right) u , \quad (28.90)$$

and the analogously for  $e^{-ik_z z + i\omega t}$ . Using  $\mu = gn = g|\psi_0|^2$  and assuming that the perturbation is weak,  $|u|, |v| \ll |\psi_0|$ , we obtain,

$$\begin{aligned} \left( \frac{\hbar^2 k^2}{2m} + gn \right) u + \frac{V}{2} \psi_0 - gnv &= \left( i\hbar \frac{\partial}{\partial t} + \hbar\omega \right) u \\ - \left( \frac{\hbar^2 k^2}{2m} + gn \right) v - \frac{V}{2} \psi_0 + gnu &= \left( -i\hbar \frac{\partial}{\partial t} + \hbar\omega \right) v . \end{aligned} \quad (28.91)$$

This effect is called *Bragg diffraction* of atoms by a standing light wave.

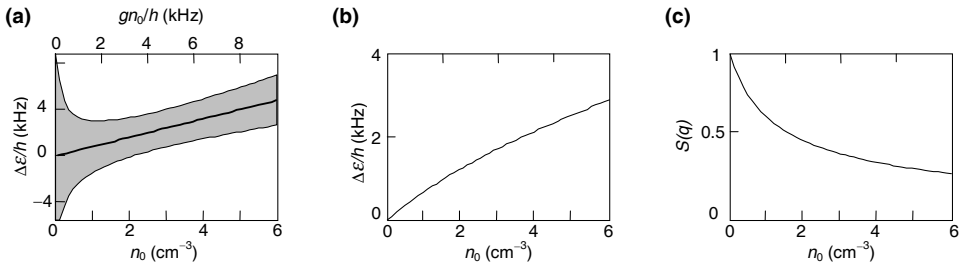


Figure 28.10: Spectrum of elementary excitations.



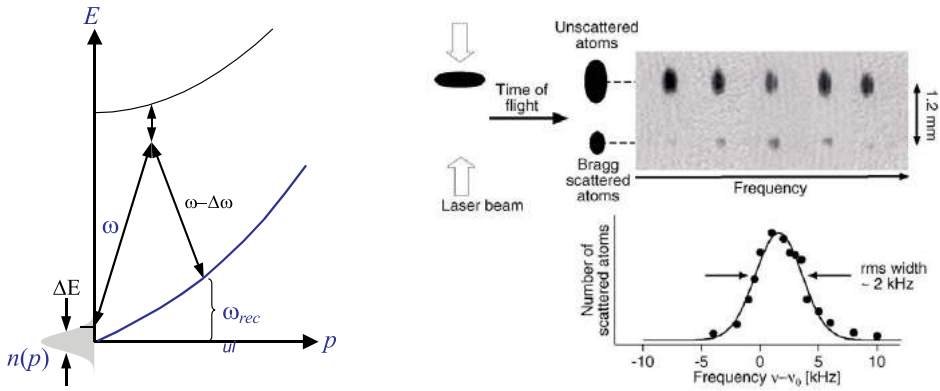


Figure 28.11: Spectrum of elementary excitations.

Using  $\mathcal{L} \equiv \frac{\hbar^2 \mathbf{k}^2}{2m} + V_{trap} + 2gn - \mu - i\hbar \frac{\partial}{\partial t}$ , we can write,

$$\begin{pmatrix} \mathcal{L} - \hbar\omega_{\mathbf{k}} & -gn \\ -gn & \mathcal{L} + \hbar\omega_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} u \\ v^* \end{pmatrix} = 0. \quad (28.92)$$

These equations can be decoupled using the Bogolubov transform.

We calculate the momentum transferred to the BEC, assuming  $\psi_0$  to be fairly homogeneous,

$$\langle \psi(\mathbf{r}, t) | -i\hbar \nabla | \psi(\mathbf{r}, t) \rangle = \hbar \mathbf{q} (|u|^2 - |v|^2). \quad (28.93)$$

## 28.2.4 Exercises

### 28.2.4.1 Ex: Bragg diffraction in a Ramsey-Bordé interferometer

Simulate the behavior of a cold atomic cloud subject to a gravitational potential during a Ramsey-Bordé sequence using the formalism developed in Sec. 28.2.2.

## 28.3 Matter wave superradiance

### 28.3.1 Classical superradiance

The Bragg beam splitter introduced in the last section does not give rise to collective scattering, even when the atoms are as strongly correlated as in a condensate. On the other hand, collective scattering is known to occur in a classical gas: When two atoms excited to an internal energy level,  $\sim hc/\lambda$ , are separated by a distance  $R$  too large to form a molecule, but smaller than the wavelength of the excited transition,  $a_B \ll R \ll \lambda$ , the atoms are coupled to the electromagnetic continuum by the same radiation that they emit (see Fig. 28.12). The dipole moments of the atoms stimulate each other to emit, and we observe a synchronized and accelerated relaxation, resulting in a coherent and directional burst of radiation [196, 574]. The directionality of the radiation is due to a destructive interference of the dipolar radiation patterns emitted by the atoms in all directions except the direction chosen by the first emitted photon. This direction

is random (except when bosonically stimulated). The atomic sample evolves, during this time, to a state of coherent superposition, until all the atoms are deexcited. This phenomenon is called *Dicke superradiance*. A similar effect exists for matter waves, and will be discussed in the following sections [352].

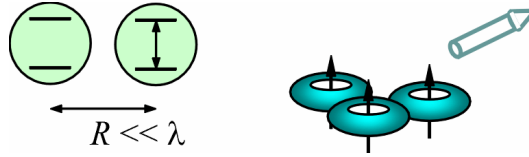


Figure 28.12: Superradiance assumes small interatomic distances compared to the wavelength of the excited dipole. Toroidal interference patterns interfering constructively in only one direction.

### 28.3.2 Matter wave superradiance & CARL

We consider the process of Rayleigh scattering from a condensate. The scattering rate obviously depends on the number of atoms and the laser intensity. The crucial point now is, that this rate can be stimulated by populations in the output modes, that is, the modes of scattered light and the atomic recoil modes. Matter and light participate in the scattering process as equal partners. In Sec. 28.2.1 we showed that Bragg scattering can be interpreted as *optical stimulation of matter wave scattering*. By analogy, it is possible to imagine a process of *wave matter stimulation of light scattering*. We will now discuss such a process, called *superradiant Rayleigh scattering* or *matter wave superradiance* (MWSR) [352], with the help of the small cartoon shown in Fig. 28.13. See also (watch talk).

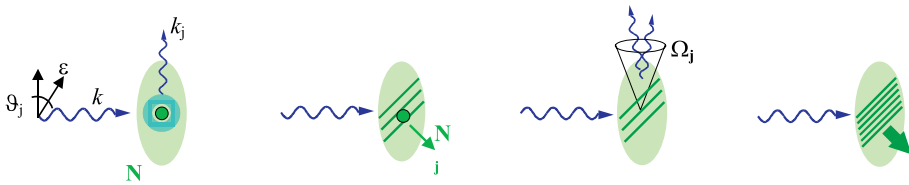


Figure 28.13: Cartoon for MWSR (see text).

Let us imagine an elongated condensate, subject to a magnetic field directed along its long axis and illuminated perpendicularly to the long axis by a linearly polarized laser beam. The scattered light is emitted into a (toroidal) dipolar radiation pattern. The fraction of the light scattered into the solid angle  $\Omega_j$ , which is inclined by angle  $\vartheta_j$  with respect to the polarization of the incident laser is  $\Omega_j \sin^2 \vartheta_j / (8\pi/3)$ . Of course, the number of scattered photons also depends on the optical cross section  $\sigma$  and the number of scattering atoms  $N_0$ . When an atom, recoiling due to the transfer of one unit of photonic momentum, moves with a speed of a few centimeters per second through the condensate, it interferes with other atoms of the condensate, thus forming a wave matter grating. The grating, the lifetime of which is long in comparison to the scattering rate, now stimulates subsequent photons to follow the same path  $\Omega_j$

and receives, in turn, the scattering atoms. In other words, the bosonic stimulation of the scattering process by the  $N_j$  atoms already populating the recoil mode amplifies the photon scattering rate by a factor of  $N_j + 1$ . The differential optical cross section (power  $P_j$  scattered into the direction  $\Omega_j$  divided by the laser intensity  $I$ ) is [352],

$$\frac{d\sigma}{d\Omega_j} = \frac{P_j}{I} = \frac{\Omega_j \sin^2 \vartheta_j}{8\pi/3} \sigma N_0 (N_j + 1) . \quad (28.94)$$

Each scattering event of a photon into the mode  $\Omega_j$  transfers an atom to the recoil mode  $N_j$ :

$$\dot{N}_j = P_j/\hbar\omega \equiv G_j N_j \quad \text{where} \quad G_j = \frac{I}{\hbar\omega} \sigma \frac{\Omega_j \sin^2 \vartheta_j}{8\pi/3} N_0 . \quad (28.95)$$

The phase matching condition is satisfied for a solid angle of approximately  $\Omega_j = \lambda^2/A_j$ , where  $A_j$  is the cross-sectional area of the condensate. If  $l_j$  is the length of condensate, we can write,

$$G_j = \frac{I}{\hbar\omega} \sigma \frac{\sin^2 \vartheta_j}{8\pi/3} n_0 \lambda^2 l_j . \quad (28.96)$$

With the atomic density  $n_0 = N_0/(A_j l_j)$ , the factor  $n_0 \lambda^2 l_j$  describes the optical density of the BEC in the direction of the scattering. Therefore, we obtain *exponential gain* for the atom number  $N_j$ , that is, the process is self-amplifying.

Using the terms of the *dressed atom* picture, we would say that the excited state of our system is formed by the BEC and the laser mode. This state relaxes to a state formed by the recoiled atoms and the scattered photons. The exponential gain occurs, when this system exhibits inversion. The inversion is maintained, until the BEC is completely transferred to the momentum recoil modes <sup>11</sup>.

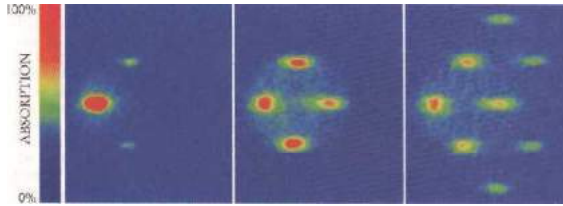


Figure 28.14: Observation of matter wave superradiance.

It is instructive to compare Dicke superradiance and matter wave superradiance. Dicke superradiance is induced by an electronic coherence between adjacent atoms.

<sup>11</sup>Superradiant scattering is due to a nonlinear coupling between two matter waves and two optical waves in a *four-wave mixing* process (4WM) interpreted as scattering of light *from* a wave matter *stimulated* by a wave matter mode. The process does not require nonlinearity due to collisions, but it works with an ideal gas,  $g \rightarrow 0$ . This distinguishes it from the 4WM of four matter waves, studied in Sec. 27.3.4 and interpreted as a scattering of atoms by a matter wave stimulated by matter wave mode, and 4WM in quantum optics involving four photons. But in all cases bosonic stimulation is crucial.

It requires a sufficiently long coherence time for the atomic dipoles. On the other hand, MWSR is a coherence effect between two states of the atomic center-of-mass motion, i.e. the condensed state and a momentum sidemode. A long lifetime of this coherence is necessary to allow for correlations between successive scattering events. The coherence lifetime corresponds to a coherence length, which for a condensate is equal to its physical size, whereas for a thermal cloud, it only corresponds to its thermal Broglie wavelength. This explains why it is difficult to observe MWSR with non-condensed atomic clouds.

Since the scattered photons quickly leave the BEC, there is no feedback or bosonic stimulation by the optical output mode. This can be interpreted as a fast decaying cavity mode, and the regime is called the *bad cavity limit*. Let us now imagine, that the photons were recycled, for example, via an optical cavity constructed around the BEC and reflecting back the photons emitted in the solid angle  $\Omega_j$ <sup>12</sup>. The mirrors of the cavity create reflection images of the radiating atoms, which increase the *density of states*, the scattering rate, and the gain  $G_j$  increase by a factor of  $8F/\pi$ . An interesting question now is, what happens in the limit  $F \rightarrow \infty$ . If the decay of the cavity mode, and therefore the removal of photons from the coherent interaction zone (which is precisely the volume occupied by the BEC) is slow, the MWSR process seems to be doubly stimulated, optically and atomically. However, in this case we also expect the inverse process, where photons are scattered back to the original mode, to occur and to be stimulated by the number of atoms  $N_0$  in the condensate. We see that the simple picture of bosonic stimulation does not work in this case, and a more complete model including the possibility of Rabi oscillations amplified by stimulated emission is necessary<sup>13</sup>.

### 28.3.3 Amplification of matter and light waves

The feedback-induced exponential gain giving rise to the phenomenon of MWSR can be used to construct a phase-coherent amplifier of matter and light waves. After all, the momentum side modes observed in the MWSR process [352] already represent amplified vacuum fluctuations. To experimentally realize a *coherent matter wave amplifier* [412, 354], it is sufficient to replace the vacuum fluctuations of the original MWSR experiment with a small *seed condensate*:  $\sim 0.1\%$  of the 'mother condensate' proved sufficient to stimulate the matter wave amplifier. The seed condensate was created by Bragg diffraction transferring atoms from the mother BEC to another momentum state (see Sec. 28.2). The matter wave grating formed by interference of the seed condensate and the mother BEC was subsequently amplified by a MWSR pulse. The gain for the atom number in the seed condensate was 10 to 100 depending on the intensity and duration of the MWSR pulse. Finally, the coherence of the amplification process was demonstrated by *active atom interferometry* using the Ramsey scheme:

<sup>12</sup>Alternatively, we may imagine a scheme decelerating of the group velocity of the light pulse.

<sup>13</sup>The phenomenon of the matter wave superradiance can be understood without quantization of the atomic motion [?] and, in particular, without quantum degeneracy. A cold and dense thermal cloud can show the phenomenon of MWSR [746]. The scattered light forms together with the pump light, a propagating standing light wave, from which the atoms are scattered by Bragg diffraction. Atoms are accelerated by the CARL effect [157, 91, 424, 499, 498, 412, 354, 353] through a coherent redistribution of photons between the pump and scattered modes. However, as was shown later-on, the different recoil modes of the condensate exhibit phase-coherence, which is not explained by a theories treating the atomic motion semi-classically.

One of the interferometer arms consisted of the amplified seed condensate and the other of a reference condensate (local oscillator) especially created by Bragg diffraction from the mother condensate. The observation of interference between these two matter waves proved the coherence of the amplification process and the existence of a well-defined phase relationship between the input and the output of the matter wave amplifier.

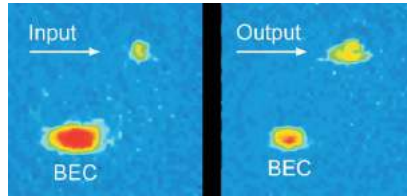


Figure 28.15: Matter wave amplification of a 'seed condensate' at the expense of a 'mother condensate'. Time-of-flight imaging visualizes the condensate's momentum distribution.

In analogy to electronics, we may consider the coherent matter wave amplifier as an *active device* complementing the atom optical toolbox of *passive devices* (see Sec. 27.3.1).

### 28.3.4 Four-wave mixing of optical and matter waves

We will now make an attempt to categorize the various scattering processes involving condensates. Let us first return to the radiation pressure [Fig. 28.16(a)], where an incident photon is spontaneously scattered into a random direction. The isotropy of the scattering process can, however, be broken when certain directions (i.e. spatial modes) are favored by bosonic stimulation. The symmetry of the roles of matter wave modes and light modes allows us to treat both on the same footing, for example, we can stimulate scattered modes either by matter or light waves.

Let us first have a look at stimulation by optical modes [Fig. 28.16(b) and (c)]. Fig. (b) describes optical four-wave mixing (4WM) in nonlinear optical media, i.e. *optically stimulated scattering of photons* from a standing light wave, which is a 4WM process of 4 photons. Fig. (c) describes Bragg scattering, i.e. an *optically stimulated scattering of atoms* by a standing light wave, which is a 4WM process of 2 photons and 2 atoms.

Similarly, a scattering process can also be stimulated by a macroscopic number of atoms in a recoil mode [Fig. 28.16(d) and (f)]. Fig. (d) describes superradiant Rayleigh scattering and matter wave amplification, i.e. scattering of photons *stimulated by a de Broglie wave*, which again corresponds to 4WM of 2 photons and two atoms. Fig. (e) describes amplification of a laser pulse by superradiant Rayleigh scattering, i.e. scattering of photons in a matter wave with *double stimulation by light waves and de Broglie waves*, which once again is a 4WM process of 2 photons and 2 atoms. Finally, Fig. (f) describes the basic process of nonlinear atom optics, i.e. the scattering of atoms by a matter wave *stimulated by de Broglie waves*, which is a 4WM process of 4 atoms.

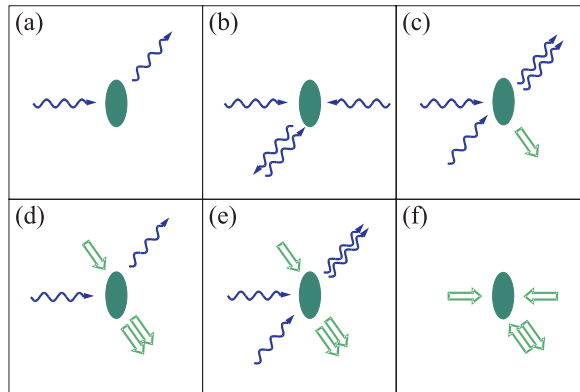


Figure 28.16: Schematic comparison of 4WM processes between light and matter wave modes. (a) Spontaneous emission, (b) classical 4WM of light modes, (c) Bragg scattering, (d) superradiant Rayleigh scattering, respectively, matter wave amplification, (e) optical amplification, and (f) 4WM of matter waves.

## 28.4 Condensates in electronically excited states

The interaction between condensates and light has, so far, been treated in the limit where the *population of excited states can be neglected or adiabatically eliminated*. An example was the coherent coupling of different kinetic states of an atom by a method called *Bragg diffraction* discussed in Sec. 28.2.

On the other hand, atoms can have metastable excited states, which can introduce new degrees of freedom, and a whole world of new problems emerges that need to be addressed: How do condensed atoms move, when they are in different states of internal excitation (or superposition of states), and how do atoms in different states interact with each other? We will now turn our attention to coherent coupling of internal states<sup>14</sup>.

In Sec. 28.4.1 we will show how to generalize the second-quantized formalism introduced in 26.2.1 in order to deal with coupled condensates in different states of internal excitation.

In Sec. 28.4.2 we will discuss examples of how coherent coupling of two states can be accomplished either by radiofrequency/microwave radiation or by two laser beams in Raman configuration. In order to avoid spontaneous relaxation, we often choose state with low excitation energy, for example, within the hyperfine structure ( $\hat{H} \sim \mathbf{I} \cdot \mathbf{J}$ ) or the Zeeman structure ( $\hat{H} \sim \mu \cdot B$ ) of the electronic ground state. But one can also consider the coupling between different *kinetic states* of free atoms  $\hat{H} \sim \mathbf{p}^2/2m$ , or the *output coupling* of atoms confined to a trapping potential ( $\hat{H} \sim \frac{m}{2}\omega^2\mathbf{r}^2$ ), or even a chemical coupling between a vibrational state of two atoms bound together to form

<sup>14</sup>We will disregard, for the moment, possible effects due to inhomogeneous broadening caused by the finite volume of the cloud inside the potential (Zeeman shift in magnetic traps or dynamic Stark shift optical traps) or effects due to interatomic interactions. But we have to keep in mind, that interatomic interaction can have a big impact on the dynamics, because the chemical potential of each condensate depends on its number of atoms. Thus, in view of the inhomogeneity of the trapping potential, the transfer of atoms can excite oscillations and sound waves in the condensates.

a molecular and a state, where the same two atoms are free and involved in an elastic collision.

Finally, in Sec. 28.4.3 we will show how to harness the forces induced by atom-light coupling in order to design new geometries of trapping potentials.

### 28.4.1 Theory of the interaction of condensates with light

Let us consider two Bose-Einstein condensates in the mean-field approximation consistent of atoms in two different internal excitation states,  $\psi_1$  and  $\psi_2$ , separated by the energy  $\hbar\omega_0$ . We illuminate the BEC by a plane wave of monochromatic light with the frequency  $\omega$ . The formal procedure consists of constructing the Hamiltonian of individual atoms, as done in Eq. (18.2), and then quantizing the field of matter [550],

$$\hat{H}_{atom} = |1\rangle\hat{H}_{cm}^{(1)}\langle 1| + |2\rangle(\hat{H}_{cm}^{(2)} + \hbar\omega_0)\langle 2| \quad \text{where} \quad \hat{H}_{cm}^{(j)} = \frac{\hat{\mathbf{P}}^2}{2m} + V_{trap}^{(j)}(\hat{\mathbf{r}}), \quad (28.97)$$

where we allow for the fact that the trapping potentials can be different for the two excitation states. We assume that atoms in different states of excitation are distinguishable, such that their respective wavefunctions commute:

$$\hat{\psi}_j(\mathbf{r}) \equiv |j\rangle\langle j|\hat{\psi}(\mathbf{r}) \quad , \quad [\hat{\psi}_j(\mathbf{r}), \hat{\psi}_{j'}(\mathbf{r}')] = \delta_{jj'}\delta^3(\mathbf{r} - \mathbf{r}'). \quad (28.98)$$

However, we need to consider interatomic collisions which, in the mean-field approximation (26.19) are described by,

$$\hat{H}_{mf}^{(j)} = \int \hat{\psi}_j^\dagger(\mathbf{r}) \frac{2\pi\hbar^2 a_s}{m} \hat{\psi}_j(\mathbf{r}) d^3r. \quad (28.99)$$

The total atomic Hamiltonian is then a generalization of the many-body Hamiltonian (26.6),

$$\boxed{\mathcal{H}_{atom} = \int \hat{\psi}_1^\dagger(\mathbf{r}) \left( \hat{H}_{cm}^{(1)} + \hat{H}_{mf}^{(1)} \right) \hat{\psi}_1(\mathbf{r}) d^3r + \int \hat{\psi}_2^\dagger(\mathbf{r}) \left( \hat{H}_{cm}^{(2)} + \hat{H}_{mf}^{(2)} + \hbar\omega_0 \right) \hat{\psi}_2(\mathbf{r}) d^3r}. \quad (28.100)$$

#### 28.4.1.1 Interaction with a single light mode

The normalized annihilation operator for a photon in mode  $\mathbf{k}$  is,

$$\vec{\mathcal{E}}^+(\mathbf{r}) = \sqrt{\frac{\hbar\omega}{2\epsilon_0 V}} \vec{\epsilon} \hat{a} e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (28.101)$$

The semi-classical Hamiltonian (the light not being quantized) of individual particles is, in the rotating wave approximation,

$$\hat{H}_{field} = \hbar\omega \hat{a}^\dagger \hat{a} \quad \text{and} \quad \hat{H}_{int} = -\hat{\mathbf{d}} \cdot \vec{\mathcal{E}} = -|2\rangle\hat{\mathbf{d}}^+ \cdot \vec{\mathcal{E}}^+ \langle 1| - |1\rangle\hat{\mathbf{d}}^- \cdot \vec{\mathcal{E}}^- \langle 2|. \quad (28.102)$$

For a condensate we still need to second-quantize the interaction part of the Hamiltonian which, disregarding collisions gives <sup>15</sup>,

$$\mathcal{H} = \hat{H}_{field} + \mathcal{H}_{atom} - \int \left( \hat{\mathbf{d}}^+ \cdot \hat{\mathcal{E}}^+ \hat{\psi}_2^\dagger(\mathbf{r}) \hat{\psi}_1(\mathbf{r}) + \hat{\mathbf{d}}^- \cdot \hat{\mathcal{E}}^- \hat{\psi}_1^\dagger(\mathbf{r}) \hat{\psi}_2(\mathbf{r}) \right) d^3r . \quad (28.103)$$

With the Hamiltonian (28.103) we derive the Heisenberg equations for the condensate respecting the commutation rules (28.98) <sup>16</sup>,

$$\begin{aligned} \dot{\hat{\psi}}_2 &= -\frac{\imath}{\hbar} (\hat{H}_{cm} + \hbar\omega_0) \hat{\psi}_2 + \frac{\imath}{\hbar} \hat{\mathbf{d}}^+ \cdot \hat{\mathcal{E}}^+ \hat{\psi}_1 \\ \dot{\hat{\psi}}_1 &= -\frac{\imath}{\hbar} \hat{H}_{cm} \hat{\psi}_1 + \frac{\imath}{\hbar} \hat{\mathbf{d}}^- \cdot \hat{\mathcal{E}}^- \hat{\psi}_2 . \end{aligned} \quad (28.104)$$

We transform to the non-rotating coordinate system by  $\tilde{\psi}_2 \equiv \psi_2 e^{i\omega t}$  and  $\tilde{\mathcal{E}}^+ \equiv \hat{\mathcal{E}}^+ e^{i\omega t}$  introducing the detuning  $\Delta \equiv \omega - \omega_0$ :

$$\partial_t \tilde{\psi}_2 = \imath (\Delta - \frac{1}{\hbar} \hat{H}_{cm}) \tilde{\psi}_2 + \frac{\imath}{\hbar} \hat{\mathbf{d}}^+ \cdot \tilde{\mathcal{E}}^+ \tilde{\psi}_1 . \quad (28.105)$$

Making the adiabatic approximation  $\partial_t \tilde{\psi}_2 = 0$  and disregarding the external degree of freedom,  $\hat{H}_{cm} = 0$ , we obtain,

$$\tilde{\psi}_2 = \frac{\imath \hat{\mathbf{d}}^+ \cdot \tilde{\mathcal{E}}^+}{\hbar \Delta} \tilde{\psi}_1 . \quad (28.106)$$

### 28.4.1.2 Heisenberg equation for the light field

Similarly, we can write the Heisenberg equation for the light mode,

$$\frac{d\hat{a}}{dt} = \frac{\imath}{\hbar} [\mathcal{H}, \hat{a}] = -i\omega \hat{a} + \imath \sqrt{\frac{\omega}{2\epsilon_0 V}} \int \hat{\mathbf{e}}_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \cdot \left( \hat{\mathbf{d}}^+ \hat{\psi}_2^\dagger \hat{\psi}_1 + \hat{\mathbf{d}}^+ \hat{\psi}_1^\dagger \hat{\psi}_2 \right) d^3r . \quad (28.107)$$

The integration of this gives the distribution of the fields (incident and scattered), such that,

$$\tilde{\mathcal{E}}^+(\mathbf{r}) = \tilde{\mathcal{E}}_{in}^+(\mathbf{r}) + \int K(\mathbf{d}, \mathbf{r} - \mathbf{r}') \hat{\psi}_1^+(\mathbf{r}') \hat{\psi}_1(\mathbf{r}') d^3r' , \quad (28.108)$$

with the kernel:

$$K(\mathbf{d}, \mathbf{r}) = \frac{1}{4\pi\epsilon_0} \left[ k^2 (\mathbf{R} \times \mathbf{d}) \times R \frac{e^{i\mathbf{k}R}}{R} + [3\mathbf{R}(\mathbf{R} \cdot \mathbf{d} - \mathbf{d})] \left( \frac{1}{R^3} - \frac{i\mathbf{k}}{R^2} \right) e^{i\mathbf{k}R} \right] . \quad (28.109)$$

We focus on the first term dominating in the far-field, and neglect the second term by letting  $R \approx r - \hat{\mathbf{e}}_R \cdot \mathbf{r}'$  and  $\hat{R} \approx r$ . We also define  $\mathbf{k}_s \equiv k\hat{\mathbf{e}}_R$ , and we only retain the term of order  $1/R$ . In this Born approximation for optically thin media, we obtain,

$$K(\mathbf{d}, \mathbf{r}) \simeq \frac{1}{4\pi\epsilon_0} \frac{e^{i\mathbf{k}R}}{r} k^2 (\mathbf{r} \times \mathbf{r}) \times \mathbf{d} e^{-i\mathbf{k}_s \mathbf{r}'} . \quad (28.110)$$

<sup>15</sup>Or, by defining the Rabi frequency  $g_1$  generated by a single photon,  $\mathcal{H}_{int} = -i\hbar g_1 \hat{a} \int d^3\mathbf{r} \hat{\psi}_2^\dagger(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\psi}_1(\mathbf{r}) + h.c.$

<sup>16</sup>In the first quantization, these equations would simply be the equations of motion for the amplitudes of the fundamental and excited states.



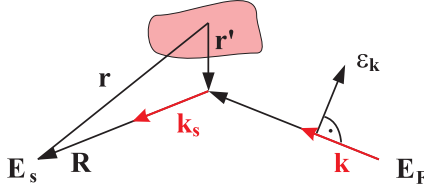


Figure 28.17: Scheme for the light scattering off a condensate.

### 28.4.1.3 Incident plane waves

When we now excite the condensate by a plane wave,

$$\hat{\mathcal{E}}_{in}^+(\mathbf{r}) = \frac{1}{2}\tilde{\epsilon}\vec{e}^{i\mathbf{k}\cdot\mathbf{r}}, \quad (28.111)$$

we derive in the Born approximation of the equation (28.108):

$$\tilde{\mathcal{E}}_s^+(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{r} k^2 \mathbf{r} \times (\mathbf{r} \times \hat{\mathbf{d}}^-) \int e^{-i\mathbf{k}_s\cdot\mathbf{r}'} \hat{\psi}_1^\dagger(\mathbf{r}') \hat{\psi}_2(\mathbf{r}') d^3r', \quad (28.112)$$

and from this the fluorescence spectrum.

## 28.4.2 STIRAP & adiabatic sweep

A frequent problem for experimenters is the need to transfer a magnetically trapped atomic cloud from one Zeeman or hyperfine state to another. We will present here two techniques called STImulated Raman Adiabatic Passage and *adiabatic sweep*.

### 28.4.2.1 Adiabatic sweep

To discuss the adiabatic sweep, we consider the example of a  $^{87}\text{Rb}$  cloud trapped in the state  $|F, m_F\rangle = |2, -2\rangle$ . The application of resonant radiofrequency radiation to the transition  $|2, -2\rangle - |2, -1\rangle$  also couples all other  $m_F$  states and causes a diffusion of the atomic populations toward an uncontrollable mixture of states. An alternative is the application of a ramp sweeping the radiofrequency from red to blue (or vice versa). Such a ramp is able to transfer the entire population toward the opposite Zeeman state  $|2, +2\rangle$ . To see this, we solve the Schrödinger equation,  $|\psi(t+dt)\rangle = e^{iH dt}|\psi(t)\rangle$ , iteratively,

$$H = \begin{pmatrix} 0 & \frac{1}{2}\Omega & 0 & 0 & 0 \\ \frac{1}{2}\Omega & -\Delta & \frac{1}{2}\Omega & 0 & 0 \\ 0 & \frac{1}{2}\Omega & -2\Delta & \frac{1}{2}\Omega & 0 \\ 0 & 0 & \frac{1}{2}\Omega & -3\Delta & \frac{1}{2}\Omega \\ 0 & 0 & 0 & \frac{1}{2}\Omega & -4\Delta \end{pmatrix}. \quad (28.113)$$

The initial population distribution is  $|\psi(t)\rangle = (1 \ 0 \ 0 \ 0 \ 0)^t$ .  $\Omega$  is the Rabi frequency generated by the radiofrequency,  $\Delta(t)$  is the instantaneous detuning. The curves of Fig. 28.18 show the temporal evolution of populations  $|\langle k|\psi(t)\rangle|^2$ .

The disadvantage of this method is that only the external (fully stretched) states  $|m_F| = F$  can be interconverted.

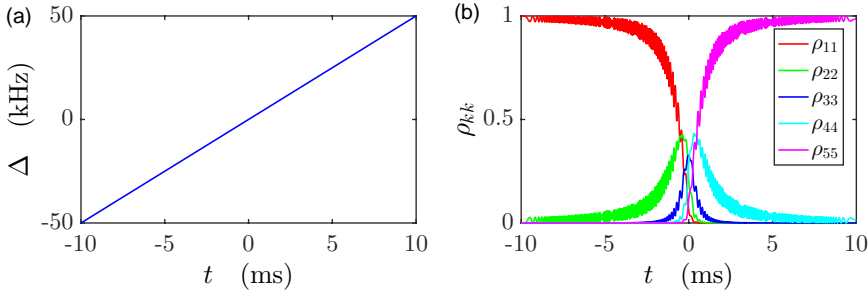


Figure 28.18: (code) Adiabatic sweep through the ground state  $^{87}\text{Rb } F = 2$ . The Rabi frequency is  $\Omega = (2\pi)8$  kHz. The frequency ramp is  $\Delta(t) = \frac{t}{t_m} (2\pi)50$  kHz with  $t_m = 10$  ms. The red line shows the evolution of the population in the state  $|2, -2\rangle$ , the green line of state  $|2, +2\rangle$ , and the blue line is the sum of the populations of all other states.

### 28.4.2.2 Sweep through a dark resonance

To discuss STIRAP, let us think of how to transfer atoms from the state  $|1\rangle \equiv |2, 2\rangle$  to  $|2\rangle \equiv |2, 1\rangle$ . The general idea consists in applying two radiation fields with Rabi frequencies  $\Omega_{13}$  and  $\Omega_{23}$ , tuned a bit out of resonance with an intermediate state  $|3\rangle$ ,  $\Delta_{13} = \Delta_{23} \neq 0$ , in a counterintuitive pulse sequence. That is, the field  $\Omega_{23}$  is applied first and then adiabatically turned down, while the field  $\Omega_{13}$  is ramped up. This method is capable of transferring all atoms.

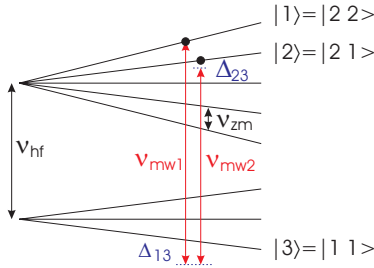


Figure 28.19: STIRAP.

Considering the example of the preceding section, we will discuss here another option (see Fig. 28.19). We consider continuous microwave fields with fixed tunings  $\Delta_{13}$  to the red of the state  $|3\rangle \equiv |1, 1\rangle$  state. Now, we apply a ramp to the second microwave field  $\Delta_{23}$ , such that the two radiation fields, at some point, cross the Raman resonance, for example,

$$\nu_{mw1} = \nu_{hf} + 3\nu_{zm} + \Delta_{13} \quad \text{and} \quad \nu_{mw2}(t) = \nu_{hf} + 2\nu_{zm} + \Delta_{23}(t). \quad (28.114)$$

The evolution of the populations can be simulated by iterative solution of the Schrödinger

equation,  $|\psi(t + dt)\rangle = e^{iH dt}|\psi(t)\rangle$  with,

$$\hat{H} = \begin{pmatrix} 0 & 0 & \frac{1}{2}\Omega_{13} \\ 0 & \Delta_{23} - \Delta_{12}(t) & \frac{1}{2}\Omega_{23} \\ \frac{1}{2}\Omega_{13} & \frac{1}{2}\Omega_{23} & \Delta_{23} \end{pmatrix}. \quad (28.115)$$

The initial population distribution is  $|\psi(t)\rangle = (1 \ 0 \ 0)^t$ . The curves of Fig. 28.20 show the temporal evolution of the populations  $|\langle k|\psi(t)\rangle|^2$ .

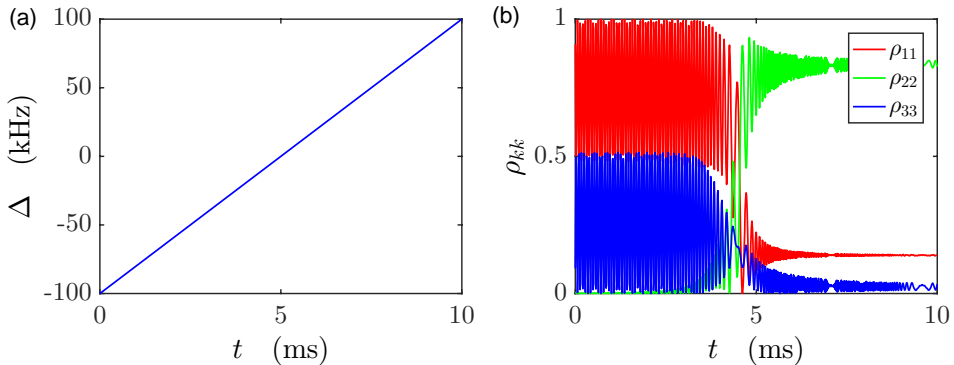


Figure 28.20: (code) STIRAP ramp through a dark resonance. Here, the Rabi frequencies are  $\Omega_{13} = \Omega_{23} = 2\pi 10$  kHz. The frequency of the first microwave is  $\Delta_{13} = (2\pi)10$  kHz and the frequency ramp of the second microwave is given by  $\Delta_{23}(t) = \frac{2t-t_m}{t_m} (2\pi)100$  kHz, where  $t_m = 10$  ms.

### 28.4.3 Condensate in adiabatic potentials

Adiabatic potentials have already been introduced in Secs. 18.1.3 and 24.4.3. Here, we will focus on the dynamics of condensed atoms in different states of electronic excitation, when these states are subject to different potentials and radiation fields that can induce transitions between the states. In particular, we consider paramagnetic atoms in different Zeeman states placed in inhomogeneous static magnetic fields and subject to single-mode or multi-mode radiofrequency radiation fields [154]<sub>DOI</sub>. To simplify the problem, let us concentrate on two-level systems, e.g. a system with the total spin  $F = \frac{1}{2}$  [751]<sub>DOI</sub>, and only consider the one-dimensional case.

#### 28.4.3.1 Coupled Gross-Pitaevskii equations

For a single atom the Hamiltonian is the one given in (18.12),

$$\hat{H}(\mathbf{r}) = |1\rangle \left( \frac{1}{2}\mu_B g_F B(\mathbf{r}) - \frac{1}{2}\hbar\omega \right) \langle 1| + |2\rangle \left( -\frac{1}{2}\mu_B g_F B(\mathbf{r}) + \frac{1}{2}\hbar\omega \right) \langle 2| + |1\rangle \frac{1}{2}\hbar\Omega \langle 2| + |2\rangle \frac{1}{2}\hbar\Omega \langle 1|. \quad (28.116)$$

With the definition,

$$\hat{\psi}_k(\mathbf{r}) \equiv \langle k|\hat{\psi}(\mathbf{r})\rangle, \quad (28.117)$$

and the abbreviation  $\hbar\Delta(\mathbf{r}) \equiv \mu_B g_F B(\mathbf{r}) - \hbar\omega(\mathbf{r})$  we proceed to the second quantization via,

$$\mathcal{H} = \sum_{k \neq m} \int d^3r \hat{\psi}_k^\dagger \left[ \frac{-\hbar^2 \nabla^2}{2m} + \frac{1}{2} u_{kk} \hat{\psi}_k^\dagger \hat{\psi}_k + \frac{1}{2} u_{k,m} \hat{\psi}_m^\dagger \hat{\psi}_m \right] \hat{\psi}_k + \left[ (-1)^k \frac{\hbar}{2} \Delta(\mathbf{r}) \hat{\psi}_k^\dagger \hat{\psi}_k + \frac{\hbar}{2} \Omega(\mathbf{r}) (\hat{\psi}_k^\dagger \hat{\psi}_m + \hat{\psi}_m^\dagger \hat{\psi}_k) \right] \quad (28.118)$$

The total energy of the system is the sum of the energies of the individual condensates (kinetic, potential, and collisional interaction) *plus* the interspecies collisional interaction energy. The coefficients  $u_{kl} = 4\pi\hbar^2 a_{kl}/m$  with the scattering lengths  $a_{kl}$  govern the impact of the collisions.

The interaction with the radiofrequency field leads to Rabi oscillations with frequency  $\Omega$ <sup>17</sup> The tuning of the radiofrequency depends on the position, due to the non-homogeneous Zeeman shift  $\Delta$ . Also, to simplify the model, we assume  $u_{kl} = 0$  for  $k \neq l$ ,

$$\hat{H} = \sum_{k \neq m} \int d^3r \hat{\psi}_k^\dagger \left[ \frac{-\hbar^2 \nabla^2}{2m} + \frac{1}{2} u_{kk} \hat{\psi}_k^\dagger \hat{\psi}_k \right] \hat{\psi}_k + \left[ (-1)^k \frac{\hbar}{2} \Delta(\mathbf{r}) \hat{\psi}_k^\dagger \hat{\psi}_k + \frac{\hbar}{2} \Omega \left( \hat{\psi}_k^\dagger \hat{\psi}_m + \hat{\psi}_m^\dagger \hat{\psi}_k \right) \right] \quad (28.119)$$

From the Heisenberg equations of motion for the field operators of the matter wave and the light, we obtain [751]<sub>DOI</sub>,

$$\begin{aligned} i\dot{\hat{\psi}}_1 &= -\frac{1}{\hbar} [\hat{H}, \hat{\psi}_1] = \frac{\delta \hat{H}}{\hbar \delta \hat{\psi}_1^\dagger} = \left( \frac{-\hbar^2 \nabla^2}{2m} + u_{11} \hat{\psi}_1^\dagger \hat{\psi}_1 - \frac{\hbar}{2} \Delta(\mathbf{r}) \right) \hat{\psi}_1 + \frac{\hbar}{2} \Omega \hat{\psi}_2 \quad (28.120) \\ i\dot{\hat{\psi}}_2 &= -\frac{1}{\hbar} [\hat{H}, \hat{\psi}_2] = \frac{\delta \hat{H}}{\hbar \delta \hat{\psi}_2^\dagger} = \left( \frac{-\hbar^2 \nabla^2}{2m} + u_{22} \hat{\psi}_2^\dagger \hat{\psi}_2 + \frac{\hbar}{2} \Delta(\mathbf{r}) \right) \hat{\psi}_2 + \frac{\hbar}{2} \Omega \hat{\psi}_1 . \end{aligned}$$

The adiabatic potentials follow from a point-wise diagonalization of the Hamiltonian, assuming that the atomic movement evolves in sufficiently small steps.

### 28.4.3.2 One-dimensional case

The reduction of the dimensionality of the Gross-Pitaevskii equation is shown in Sec. ?? . Applying this to our case, we consider a one-dimensional potential  $V(\mathbf{r}) = V(z)$  and assume condensates being radially homogeneous within the radial diameter  $r_h$ . In this case, we can neglect the radial kinetic energy. As normalization then requires,

$$\int_{-r_h}^{r_h} \int_{-r_h}^{r_h} \int_{-\infty}^{\infty} |\hat{\psi}(\mathbf{r})|^2 d^3r = (2r_h)^2 \int_{-\infty}^{\infty} |\hat{\psi}(z)|^2 dz = 1 , \quad (28.121)$$

replacing  $\hat{\psi}(\mathbf{r}) = \frac{\hat{\phi}(z)}{2r_h}$  and  $g_{kk} = \frac{u_{kk}}{(2r_h)^2}$ , the Gross-Pitaevskii equation and the normalization condition adopt a particularly simple form,

$$i\hbar \frac{\partial}{\partial t} \hat{\phi}(z) = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V_{trap}(z) + N g_{1D} |\hat{\phi}(z)|^2 \right) \hat{\phi}(z) . \quad (28.122)$$

<sup>17</sup>We are neglecting the possibility, that the coupling force may, in principle, be inhomogeneous, if the orientation of the magnetic field is not uniform.

The coupled equations are now,

$$\begin{aligned} i\dot{\hat{\phi}}_1 &= \left( \frac{-\partial_z^2}{2m} + g_{11}\hat{\phi}_1^\dagger\hat{\phi}_1 - \frac{m}{4}\omega_z^2 z^2 - \frac{1}{2}\Delta_0 \right) \hat{\phi}_1 + \frac{1}{2}\Omega\hat{\phi}_2 \\ i\dot{\hat{\phi}}_2 &= \left( \frac{-\partial_z^2}{2m} + g_{22}\hat{\phi}_2^\dagger\hat{\phi}_2 + \frac{m}{4}\omega_z^2 z^2 + \frac{1}{2}\Delta_0 \right) \hat{\phi}_2 + \frac{1}{2}\Omega\hat{\phi}_1 . \end{aligned} \quad (28.123)$$

with,

$$\int_{-\infty}^{\infty} |\hat{\phi}_1(z)|^2 + |\hat{\phi}_2(z)|^2 dz = 1 . \quad (28.124)$$

This set of equations can be solved numerically by first identifying the ground state using the 'steepest descent' method and then propagating it in real time while slowly varying  $\Delta(\mathbf{r}, t)$  or  $\Omega(t)$ .

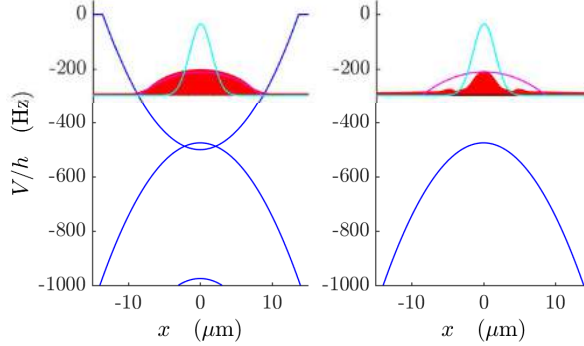


Figure 28.21: (code) Two coupled condensates.

### 28.4.3.3 Damping

A heuristic way of introducing damping could be as follows: We write down the condensate velocity field as,

$$m\mathbf{v}(\mathbf{r}, t) = \hbar \frac{\hat{\phi}^*(\mathbf{r}, t)\nabla\hat{\phi}(\mathbf{r}, t) - \nabla\hat{\phi}^*(\mathbf{r}, t)\hat{\phi}(\mathbf{r}, t)}{2m(\mathbf{r}, t)} , \quad (28.125)$$

and subject it to a friction force,

$$E_{fr} = -\gamma r v . \quad (28.126)$$

The problem with the coupled GPE approach is that in the absence of damping any even small modification of the coupling triggers collective oscillations, so that the ground state is not found. A numerical method to minimize the total energy cannot be used, because the minimum is the untrapped state, so that all atoms are lost. It seems that a master equation approach is necessary to introduce damping. An alternative (but cheap) way is the following. The coupled GPEs were written in the dressed states basis. Thus, if the Rabi frequency is strong enough to completely

decouple the dressed states, the dressed states represent good quantum numbers, and the GPEs are appropriately written in a diagonal basis, i.e. the GPEs decouple on adiabatic potentials<sup>18</sup>,

$$V_{ad,k}(z) = -(-1)^k \frac{1}{2} \sqrt{\hbar^2 \Omega^2 + [\mu_B g_F B(z) - \hbar \omega]^2}, \quad (28.127)$$

and we obtain,

$$i \dot{\hat{\phi}}_k = \left( \frac{-\partial_z^2}{2m} + V_{ad,k}(z) + g_{kk} \hat{\phi}_k^\dagger \hat{\phi}_k \right) \hat{\phi}_k. \quad (28.128)$$

#### 28.4.3.4 Ex: Multiple BECs coupled by radiation via GPEs

Programs on multiple BECs coupled by radiation via GPEs.

## 28.5 Interaction between condensates and optical cavities

In 28.4.1 we have set up the many-body Hamiltonian (28.103) describing the interaction of a matter wave (treated in mean-field approximation) with an incident light field. We emphasized the role of photonic recoil in (28.128). In the following sections we aim at applying this theory to the particular case of atoms interacting with two counterpropagating modes of an optical ring cavity. The system has already been studied in Chp. 22.6.1 in the context of CARL, where the atomic motion, as well as the light fields, have mostly been treated classically.

CARL is based on a coherent redistribution of photons between the two counterpropagating modes of a moving standing light wave mediated by atoms which are located in the mode volume. Cooperative Compton scattering induces a collective atomic recoil and a self-bunching of the atoms, which results in an exponential gain for the optical mode receiving the scattered photons. The recent observation of the MWSR [352] in a BEC raises the question about an ultra-cold version of CARL [499, 333]. In MWSR the long coherence time of a BEC establishes a strong correlation between subsequent elastic Rayleigh scattering events mediated by very stable quasi-particle excitations. The feedback of these excitations on the laser creates an *exponential* gain for the optical mode receiving the scattered photons [353, 157, 91, 424, 499, 498, 412, 354, 353].

We have discussed the classical CARL earlier in the superradiant as well as the good-cavity regime. We have also generalized the problem to the case of quantized atomic motion (see Sec. ??) and to quantized radiation fields (see Sec. ??). The internal states were always adiabatically eliminated. In the following, we will fully quantize the bosonic atomic particle field.

The advantages of this second quantization is that interatomic interactions, quantum fluctuations, and decoherence of the matter wave can be taken into account. Various proposals have been made focusing on either one of the above three aspects. Fundamental aspects of the BEC-in-a-cavity-system lead into two directions: 1. quantum synchronization and 2. quantum correlations.

<sup>18</sup>Gravitation can be included by  $V_{ad,k}(z) \rightarrow V_{ad,k}(z) + mgz$ .

The system under consideration is a BEC of two-level atoms with transition resonance frequency  $\omega_0$  trapped in an external magnetic trap, located inside the mode volume of a ring cavity and interacting with its light modes. The atomic field operators obey the commutation relations,

$$\begin{aligned} [\hat{\psi}_k(\mathbf{r}), \hat{\psi}_m^\dagger(\mathbf{r}')] &= \delta_{km} \delta^{(3)}(\mathbf{r}, \mathbf{r}') \\ [\hat{\psi}_k(\mathbf{r}), \hat{\psi}_m(\mathbf{r}')] &= 0 = [\hat{\psi}_k^\dagger(\mathbf{r}), \hat{\psi}_m^\dagger(\mathbf{r}')] , \end{aligned} \quad (28.129)$$

where  $k, m = 1, 2$  label the internal state of the atoms. In general, the light field consists of only *two* counterpropagating monochromatic modes with Rabi frequencies  $2g\hat{a}_\pm^\dagger\hat{a}_\pm$ . Choosing the coordinate system properly, we can set the wavevectors of the modes as  $\mathbf{k}_+ \cdot \hat{\mathbf{e}}_r = k\hat{z} = -\mathbf{k}_- \cdot \hat{\mathbf{e}}_r$ . The second-quantized Hamiltonian is a generalization of (22.4),

$$\mathcal{H} = \mathcal{H}_{atom} + \mathcal{H}_{atom-atom} + \mathcal{H}_{atom-cav} + \hat{H}_{cav} + \hat{H}_{laser-cav} , \quad (28.130)$$

where,

$$\begin{aligned} \mathcal{H}_{atom} &= \int d^3r \hat{\psi}_1^\dagger(\mathbf{r}) \left( \frac{\hat{p}^2}{2m} + V_1(\mathbf{r}) \right) \hat{\psi}_1(\mathbf{r}) \\ &\quad + \int d^3r \hat{\psi}_2^\dagger(\mathbf{r}) \left( \frac{\hat{p}^2}{2m} + V_2(\mathbf{r}) - \Delta_a \right) \hat{\psi}_2(\mathbf{r}) \\ \mathcal{H}_{atom-atom} &= \sum_{i=1,2} \int d^3r \hat{\psi}_i^\dagger(\mathbf{r}) \hat{\psi}_i^\dagger(\mathbf{r}) \frac{u_{ii}}{2} \hat{\psi}_i(\mathbf{r}) \hat{\psi}_i(\mathbf{r}) \\ &\quad + \int d^3r \hat{\psi}_1^\dagger(\mathbf{r}) \hat{\psi}_2^\dagger(\mathbf{r}) \frac{u_{12}}{2} \hat{\psi}_2(\mathbf{r}) \hat{\psi}_1(\mathbf{r}) , \\ \mathcal{H}_{atom-cav} &= \sum_{\pm} g\hat{a}_{\pm} \int d^3r \hat{\psi}_2^\dagger(\mathbf{r}) e^{\pm ikz} \hat{\psi}_1(\mathbf{r}) + h.c. \\ \hat{H}_{cav} &= - \sum_{\pm} \Delta_c \hat{a}_{\pm}^\dagger \hat{a}_{\pm} \\ \hat{H}_{laser-cav} &= - \sum_{\pm} \eta_{\pm} (\hat{a}_{\pm} - \hat{a}_{\pm}^\dagger) \end{aligned} \quad (28.131)$$

with  $u_{ij} \equiv 4\pi\hbar^2 a_{s,ij}/m$ .

Various approximations can be made depending on the subject of interest. For example, if only one cavity mode,  $\hat{a}_+$ , is strongly pumped, such that the field becomes intense, we may remove the term  $\hat{H}_{laser-cav}$  and describe the field mode classically by a Rabi frequency  $\Omega$ . The interaction between the pump mode and the cavity is then,  $\hat{H}_{atom-pump} = \frac{\hbar\Omega}{2} e^{-i\omega_2 t} \int d^3r \hat{\psi}_2^\dagger(\mathbf{r}) e^{ik\hat{z}} \hat{\psi}_1(\mathbf{r}) + h.c.$

A talk on this subject is available at [\(watch talk\)](#).

## 28.5.1 Ideal gas Hamiltonian after adiabatic elimination

Assuming the light fields to be tuned far from resonance we disregard spontaneous emission, as explained in Sec. 22.1.2, and adiabatically eliminate the internal states, as shown in Sec. 22.1.3 [558, 143]. On the other hand, we treat the light field and the atomic motion in second quantization. The canonical way to describe a BEC interacting with *two* optical modes  $\hat{a}_{\pm}$  is to second-quantize the single-particle Hamiltonian

(22.26),

$$\mathcal{H} \simeq \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left( \frac{\hat{\mathbf{p}}^2}{2m} + V_{\text{trap}}(\mathbf{r}) + \frac{u}{2} \hat{N}(\mathbf{r}) \right) \hat{\psi}(\mathbf{r}) + (\hat{N}U_0 - \Delta_c) \sum_{\pm} \hat{a}_{\pm}^\dagger \hat{a}_{\pm} + U_0 \hat{a}_+^\dagger \hat{a}_- \int d^3r \hat{\psi}^\dagger(\mathbf{r}) e^{-2ikz} \hat{\psi}(\mathbf{r}) + h.c. - i \sum_{\pm} \eta_{\pm} (\hat{a}_{\pm} - \hat{a}_{\pm}^\dagger) , \quad (28.132)$$

where  $\hat{\psi}(\mathbf{r})$  is now the ground-state wave function of the matter wave,  $u = 4\pi\hbar^2 a_s/m$  in the *mean field approximation* and,

$$U_0 = \frac{g^2}{\Delta_a} , \quad (28.133)$$

when the mode to mode coupling strength. This adiabatically approximated Hamiltonian looks very similar to (22.26).

## 28.5.2 Expansion into momentum states

It is useful to convert the Hamiltonian to momentum space via a plane wave expansion of the BEC according to (26.70),

$$\hat{\psi}(\mathbf{r}) = \sqrt{\frac{V}{(2\pi)^3}} \int \hat{c}_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} d^3q \quad \text{with} \quad [\hat{a}_{\mathbf{q}}, \hat{a}_{\mathbf{q}'}] = \delta_{\mathbf{q},\mathbf{q}'} . \quad (28.134)$$

The conversion of that Hamiltonian part  $\mathcal{H}_{\text{bec}}$  to momentum space has been demonstrated in (26.78),

$$\mathcal{H}_{\text{bec}} = \sum_{\mathbf{q}} \frac{\mathbf{q}}{2m} \hat{c}_{\mathbf{q}}^\dagger \hat{c}_{\mathbf{q}} + \sum_{\mathbf{q},\mathbf{q}'} \hat{c}_{\mathbf{q}}^\dagger V_{\mathbf{q}',\mathbf{q}} \hat{c}_{\mathbf{q}} + \frac{u}{2} \sum_{\mathbf{q},\mathbf{q}',\mathbf{q}''} \hat{c}_{\mathbf{q}}^\dagger \hat{c}_{\mathbf{q}'}^\dagger \hat{c}_{\mathbf{q}''} \hat{c}_{\mathbf{q}} + \mathbf{q}' - \mathbf{q}'' . \quad (28.135)$$

The light field part  $\hat{H}_{\text{cav}}$  remains unchanged and the atom-light interaction becomes using (28.3),

$$\begin{aligned} \mathcal{H}_{\text{bec-cav}} &= U_0 \int \hat{\psi}^\dagger(\mathbf{r}) \hat{a}_+^\dagger \hat{a}_- e^{-i(\mathbf{k}_+ - \mathbf{k}_-) \cdot \mathbf{r}} \hat{\psi}(\mathbf{r}) d^3r + h.c. \\ &= i\hbar U_0 \hat{a}_+^\dagger \hat{a}_- V \int \int \hat{c}^\dagger(\mathbf{q}') \hat{c}(\mathbf{q}) \delta^3(\mathbf{q} - \mathbf{q}' - 2k\hat{\mathbf{e}}_z) d^3q d^3q' = U_0 \hat{a}_+^\dagger \hat{a}_- \sum_{\mathbf{q}} \hat{c}_{\mathbf{q}-2\mathbf{k}}^\dagger \hat{c}_{\mathbf{q}} . \end{aligned} \quad (28.136)$$

All in all,

$$\mathcal{H} = \sum_{\mathbf{q}} \frac{\mathbf{q}^2}{2m} \hat{c}_{\mathbf{q}}^\dagger \hat{c}_{\mathbf{q}} + \sum_{\mathbf{q},\mathbf{q}'} \hat{c}_{\mathbf{q}}^\dagger V_{\mathbf{q}',\mathbf{q}} \hat{c}_{\mathbf{q}} + \frac{u}{2} \sum_{\mathbf{q},\mathbf{q}',\mathbf{q}''} \hat{c}_{\mathbf{q}}^\dagger \hat{c}_{\mathbf{q}'}^\dagger \hat{c}_{\mathbf{q}''} \hat{c}_{\mathbf{q}+\mathbf{q}'-\mathbf{q}''} + (\hat{N}U_0 - \Delta_c) \sum_{\pm} \hat{a}_{\pm}^\dagger \hat{a}_{\pm} + U_0 \hat{a}_+^\dagger \hat{a}_- \sum_{\mathbf{q}} \hat{c}_{\mathbf{q}-2\mathbf{k}}^\dagger \hat{c}_{\mathbf{q}} - i \sum_{\pm} \eta_{\pm} (\hat{a}_{\pm} - \hat{a}_{\pm}^\dagger) . \quad (28.137)$$



The BEC-CARL equations of motion are readily obtained from the Heisenberg equations,

$$\begin{aligned} i \frac{d\hat{c}_{\mathbf{p}}}{dt} &= [\hat{c}_{\mathbf{p}}, \mathcal{H}] = \frac{q^2}{2m} \hat{c}_{\mathbf{p}} + \sum_{\mathbf{q}} V_{\mathbf{p},\mathbf{q}} \hat{c}_{\mathbf{q}} + u \sum_{\mathbf{q},\mathbf{q}'} \hat{c}_{\mathbf{q}}^\dagger \hat{c}_{\mathbf{q}'} \hat{c}_{\mathbf{q}-\mathbf{q}'+\mathbf{p}} + U_0 \hat{a}_+^\dagger \hat{a}_- \hat{c}_{\mathbf{p}+2\mathbf{k}} + h.c. \\ i \frac{d\hat{a}_\pm}{dt} &= [\hat{a}_\pm, \mathcal{H}] = (\hat{N}U_0 - \Delta_c) \hat{a}_\pm + U_0 \hat{a}_\mp \sum_{\mathbf{q}} \hat{c}_{\mathbf{q}+2\mathbf{k}}^\dagger \hat{c}_{\mathbf{q}} + \eta_{\eta_\pm} . \end{aligned} \quad (28.138)$$

### 28.5.2.1 Discretization of the momentum space

Assuming the BEC to be initially at rest with 0 temperature, its momentum state can be written as  $\hat{c}_0$ . And if the dynamics only involves the  $z$ -axis, then all momentum states are separated by multiples of  $2\hbar k$ , such that we may replace the labeling by integer numbers:  $\hat{c}_{\mathbf{q}} \rightarrow \hat{c}_n$ . We get,

$$\begin{aligned} \mathcal{H} &= \sum_n \frac{n^2 q^2}{2m} \hat{c}_n^\dagger \hat{c}_n + \sum_{n,n'} \hat{c}_n^\dagger V_{n',n} \hat{c}_n + \frac{u}{2} \sum_{n,n',n''} \hat{c}_n^\dagger \hat{c}_{n'} \hat{c}_{n''} \hat{c}_{n+n'-n''} \\ &+ \sum_{\pm} \left( \hat{N}U_0 - \Delta_c \right) \hat{a}_\pm^\dagger \hat{a}_\pm + U_0 \hat{a}_+^\dagger \hat{a}_- \sum_n \hat{c}_{n-1}^\dagger \hat{c}_n + h.c. - \eta_{\eta_\pm} (\hat{a}_\pm - \hat{a}_\pm^\dagger) . \end{aligned} \quad (28.139)$$

Neglecting the external trapping potential and collisions the Heisenberg equations for the field and the atomic motion now read,

$$\begin{aligned} \frac{d\hat{c}_n}{dt} &= -i[\hat{c}_n, \mathcal{H}] = -i \frac{n^2 k^2}{2m} \hat{c}_n + U_0 \hat{a}_+^\dagger \hat{a}_- \hat{c}_{n+1} + h.c. \\ \frac{d\hat{a}_\pm}{dt} &= -i[\hat{a}_\pm, \mathcal{H}] = (\hat{N}U_0 - \Delta_c) \hat{a}_\pm + U_0 \hat{a}_\mp \sum_n \hat{c}_{n\mp 1}^\dagger \hat{c}_n + \eta_{\eta_\pm} . \end{aligned} \quad (28.140)$$

These equations look identical to those found in (22.112).

## 28.5.3 BECs in two internal states coupled by a cavity

A lossy cavity can act as an effective *zero temperature reservoir*. One possible implementation [364] realizes a three-level cycling scheme, with two BECs in two ground states  $|g_1\rangle$  and  $|g_2\rangle$  coherently coupled by a two-photon transition (Raman-lasers or microwave-radiofrequency combination). The ground states are additionally coupled by an irreversible Raman transition via an intermediate spontaneously decaying level  $|e\rangle$ . One transition is not driven but stimulated by a ring cavity mode  $\hat{a}$ .

The Hamiltonian consists of three parts, the BEC energy  $\mathcal{H}_{bec}$ , the interaction energy with the coherent coupling assumed to be classical  $\mathcal{H}_{cpl}$  and the interaction with the mode of a ring cavity  $\mathcal{H}_{cav}$  treated quantum mechanically ( $\hbar = 1$ ),

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_{bec} + \mathcal{H}_{cpl} + \mathcal{H}_{cav} \\ &= \int d^3r \hat{\psi}_1^\dagger \left( \frac{-\nabla^2}{2m} + V + \frac{u_{11}}{2} \hat{\psi}_1^\dagger \hat{\psi}_1 + \frac{u_{12}}{2} \hat{\psi}_2^\dagger \hat{\psi}_2 \right) \hat{\psi}_1 + \\ &+ \int d^3r \hat{\psi}_2^\dagger \left( \frac{-\nabla^2}{2m} + V + \frac{u_{12}}{2} \hat{\psi}_1^\dagger \hat{\psi}_1 + \frac{u_{22}}{2} \hat{\psi}_2^\dagger \hat{\psi}_2 \right) \hat{\psi}_2 + \\ &+ \int d^3r \left( -\Delta_{mw} \hat{\psi}_1^\dagger \hat{\psi}_1 + \frac{\Omega_{mw}}{2} \hat{\psi}_1^\dagger \hat{\psi}_2 + h.c. \right) + \int d^3r \left( g_{cv} \hat{a} \hat{\psi}_1^\dagger \hat{\psi}_2 + h.c. \right) - \Delta_{cv} \hat{a}^\dagger \hat{a} . \end{aligned} \quad (28.141)$$

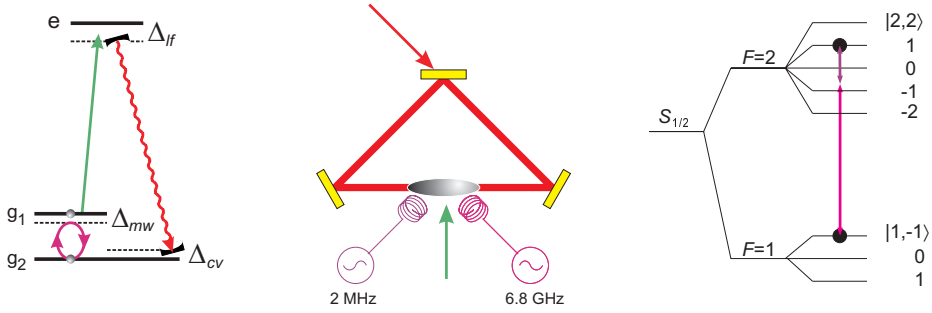


Figure 28.22: (code) (a) Level scheme with a microwave-driven hyperfine structure, a laser-driven optical transition, and a cavity-enhanced Raman deexcitation. (b) Ring cavity used for the experiment. (c) Scheme for coupling the Zeeman states  $|2, 1\rangle$  and  $|1, -1\rangle$  with a two-photon transition in a magnetic trap.

The BEC energy consists of the two energies (kinetic, potential, self) of the individual BECs and the cross-species interaction proportional to  $u_{kl} = 4\pi\hbar^2 a_{kl}/m$ . The interaction energy with the classical microwave frequency (mostly we will assume  $\Delta_{mw} = 0$ ) leads to Rabi flopping with frequency  $\Omega_{mw}$ . Finally, the incident light field is treated classically with a Rabi frequency  $\Omega_{lf}$  and a detuning  $\Delta_{lf}$ , while the cavity field is treated quantum mechanically with a coupling constant  $\Omega_{cv}$  and a detuning  $\Delta_{cv}$ . The irreversible coupling leads to an energy contribution where  $g_{cv} \equiv \Omega_{lf}\Omega_{cv}/2\Delta_{lf}$  is the two-photon Rabi-frequency if the auxiliary state is adiabatically eliminated. From the Heisenberg equations of motion for the matter wave and the optical field operators we obtain,

$$\begin{aligned}
 \dot{\hat{\psi}}_1 &= i[H, \hat{\psi}_1] = -i \frac{\delta H}{\delta \hat{\psi}_1^\dagger} & (28.142) \\
 &= -i \left( \frac{-\nabla^2}{2m} + V + u_{11}|\hat{\psi}_1|^2 + u_{12}|\hat{\psi}_2|^2 \right) \hat{\psi}_1 - i \left( \frac{\Omega_{mw}}{2} + g_{cv}\hat{a} \right) \hat{\psi}_2 - i\Delta_{mw}\hat{\psi}_1, \\
 \dot{\hat{\psi}}_2 &= i[\hat{H}, \hat{\psi}_2] = -i \frac{\delta H}{\delta \hat{\psi}_2^\dagger} \\
 &= -i \left( \frac{-\nabla^2}{2m} + V + u_{12}|\hat{\psi}_1|^2 + u_{22}|\hat{\psi}_2|^2 \right) \hat{\psi}_2 - i \left( \frac{\Omega_{mw}}{2} + g_{cv}\hat{a}^\dagger \right) \hat{\psi}_1, \\
 \dot{\hat{a}} &= i[\hat{H}, \hat{a}] - \frac{\kappa}{2}\hat{a} = -i \frac{\delta H}{\delta \hat{a}^\dagger} - \frac{\kappa}{2}\hat{a} \\
 &= -i \int d^3r g_{cv}\hat{\psi}_1\hat{\psi}_2^\dagger - \left( i\Delta_{cv} + \frac{\kappa}{2} \right) \hat{a}.
 \end{aligned}$$

**Example 123 (Single atoms in two states interacting with a cavity):** As a first example, we start from the matter wave Hamiltonian (28.141) for two coupled BECs and neglect the center-of-mass motion (and consequence the condensate part, i.e. self-interaction, kinetic energy and the external potential).

Furthermore, we assume  $\hat{\psi}_i(\mathbf{r}) = \hat{c}_i \delta^3(\mathbf{r})$ ,

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_{bec} + \mathcal{H}_{clp} + \mathcal{H}_{cav} \\ &= -\Delta_{mw} \hat{c}_1^\dagger \hat{c}_1 + \frac{\Omega_{mw}}{2} \hat{c}_1^\dagger \hat{c}_2 + g_{cv} \hat{a} \hat{c}_1^\dagger \hat{c}_2 + h.c. - \Delta_{cv} \hat{a}^\dagger \hat{a} . \end{aligned} \quad (28.143)$$

Consequently, the Heisenberg equations of motion are simply,

$$\begin{aligned} \dot{\hat{c}}_1 &= -i \left( \frac{\Omega_{mw}}{2} + g_{cv} \hat{a} \right) \hat{c}_2 - i \Delta_{mw} \hat{c}_1 \\ \dot{\hat{c}}_2 &= -i \left( \frac{\Omega_{mw}}{2} + g_{cv} \hat{a}^\dagger \right) \hat{c}_1 \\ \dot{\hat{a}} &= -i g_{cv} \hat{c}_1 \hat{c}_2^\dagger - (i \Delta_{cv} + \frac{\kappa}{2}) \hat{a} . \end{aligned} \quad (28.144)$$

Obviously, since the matter wave degree of freedom is ignored, the dynamics only concerns the Bloch vector. Simulations of these equations are exhibited in Fig. 28.23 and in movies that can be watched under ([watch movie](#)) and ([watch movie](#)).

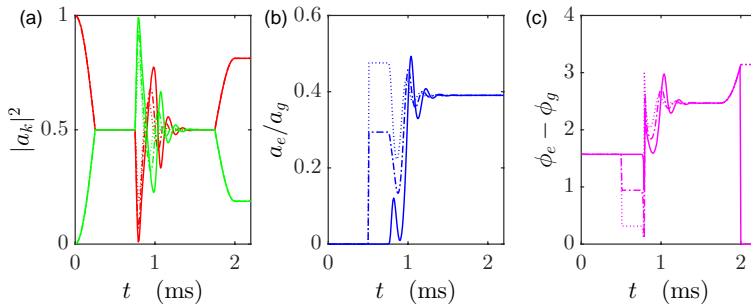


Figure 28.23: (code) Bloch vector phase stabilization in the cavity. (a) Populations and (b) coherences.

**Example 124 (Interpretation of the ultracold fusion via analogy with two-level system):** The chemical potential of the BECs in both states shifts the energy levels up depending on the inversion,  $\mu_2 - \mu_1 \propto N_2 - N_1$ . If the inversion oscillates the spontaneous Raman cycle periodically meets resonance, and takes place. Note that, since atomic motion is not considered, the energy gap due to the finite cavity detuning can only be bridged in resonance,  $\mu_2 - \mu_1 = \kappa$ . Oscillation simulates Doppler shift of thermal motion in Doppler cooling. Raman scattering takes the role of spontaneous emission in the cooling process. The only role of the cavity is to introduce irreversibility. Raman scattering is only supported in one direction: However, it is not relevant to have a ring cavity.

## 28.5.4 Exercises

### 28.5.4.1 Ex: BEC damping in cavities

Programs on BEC damping in cavities.

**28.5.4.2 Ex: Second-quantized CARL equations**

Calculate the commutators  $[\hat{\psi}_j(\mathbf{r}), \mathcal{H}]$  and  $[\hat{a}_\pm, \mathcal{H}]$ , where  $\mathcal{H}$  is the Hamiltonian (28.131) and  $\hat{\psi}_1$  and  $\hat{\psi}_2$  the ground and excited state wave functions, respectively.

**28.5.4.3 Ex: Second-quantized adiabatically approximated CARL Hamiltonian**

- Derive the adiabatically approximated CARL Hamiltonian in second quantization.
- Derive the CARL equations of motion from the adiabatically approximated Hamiltonian in second quantization.
- Show that the derived Hamiltonian simplifies to (22.26) in the single atom limit.

**28.5.4.4 Ex: BEC-CARL equations from the adiabatically approximated CARL Hamiltonian**

Derive the BEC-CARL equations from the adiabatically approximated CARL Hamiltonian (28.134).

**28.5.4.5 Ex: Origin of quantum correlations**

The BEC-CARL Hamiltonian has been shown to generate quantum correlations between optical and matter wave modes [499, 550]. Discuss whether they are a many-body effect (bosonic stimulation) or just due to coherences between motional states of single atoms.

**28.5.4.6 Ex: Ultracold fusion**

Derive from Eqs. (28.144) using the definitions (??) and (??) the Eqs. (??).

**28.6 Further reading**

H.D. Politzer, *Light incident on a Bose-condensed gas* [DOI]

A. Görlitz et al., *Enhancement and Suppression of Spontaneous Emission and Light Scattering by Quantum Degeneracy* [DOI]

P.C. Bons et al., *Quantum Enhancement of the Index of Refraction in a Bose-Einstein Condensate* [DOI]

O. Zobay et al., *Dynamics of matter-wave and optical fields in superradiant scattering from Bose-Einstein condensates* [DOI]

Y. Yoshikawa et al., *Observation of Superradiant Raman Scattering in a Bose-Einstein Condensate* [DOI]

Y. Yoshikawa et al., *Superradiant light scattering from thermal atomic vapors* [DOI]

M.M. Cola et al., *Theory of Collective Raman Scattering from a Bose-Einstein Condensate* [DOI]

- M.M. Cola et al., *Robust Generation of Entanglement in Bose-Einstein Condensates by Collective Atomic Recoil* [\[DOI\]](#)
- M.M. Cola et al., *A Condensate in a Lossy Cavity: Collective Atomic Recoil and Generation of Entanglement* [\[DOI\]](#)
- M.M. Cola et al., *Entanglement in a Bose-Einstein condensate by collective atomic recoil* [\[DOI\]](#)
- D.M. Stamper-Kurn et al., *Spinor Condensates and Light Scattering from Bose-Einstein Condensates* [\[DOI\]](#)
- D. Schneble et al., *The Onset of Matter-Wave Amplification in a superradiant Bose-Einstein-Condensate* [\[DOI\]](#)
- M.G. Moore et al., *Quantum optics of a Bose-Einstein condensate coupled to a quantized light field* [\[DOI\]](#)
- M.G. Moore et al., *Atomic Four-Wave Mixing Fermions versus Bosons* [\[DOI\]](#)
- M.G. Moore et al., *Optical control and entanglement of atomic Schroedinger fields* [\[DOI\]](#)
- W. Ketterle et al., *Does Matter Wave Amplification Work for Fermions* [\[DOI\]](#)
- N. Piovella et al., *Quantum fluctuations and entanglement in the collective atomic recoil laser using a Bose-condensate* [\[DOI\]](#)
- D. Jaksch et al., *Uniting Bose-Einstein condensates in optical resonators* [\[DOI\]](#)
- S. Ritter et al., *Dynamical Coupling between a Bose-Einstein Condensate and a Cavity Optical Lattice* [\[DOI\]](#)
- D. Schneble et al., *Raman amplification of matter waves* [\[DOI\]](#)
- G.A. Pratavia et al., *Trap environment effects over quantum statistics and atom-photon correlations in the collective-atomic-recoil laser* [\[DOI\]](#)
- S.A. Gardiner et al., *Cavity-assisted quasiparticle damping in a Bose-Einstein Condensate* [\[DOI\]](#)
- P. Horak et al., *Coherent Dynamics of Bose-Einstein Condensates in High-finesse Optical Cavities* [\[DOI\]](#)
- P. Horak et al., *Dissipative Dynamics of Bose Condensates in Optical Cavities* [\[DOI\]](#)
- W. Ketterle et al., *Collective Enhancement and Suppression in Bose-Einstein Condensates* [\[DOI\]](#)
- W. Ketterle et al., *Does Matter Wave Amplification Work for Fermions?* [\[DOI\]](#)
- W. Ketterle, *Comment on 'Electromagnetic Wave Dynamics in Matter-Wave Superradiant Scattering'* [\[DOI\]](#)

## Part VI

# Instrumentation of a Quantum Optics Lab



# Chapter 29

## Gaussian optics and the polarization of light

The objective of this part of the course is to introduce the student into the basics of *Gaussian optics* and *polarizations optics*. The student will learn how to transform the diameter and the divergence of a Gaussian beam using lenses and telescopes and to analyze and manipulate the polarization of a laser beam.

### 29.1 Some more basic notions

#### 29.1.1 Definition of photometric quantities

The *radiant energy*  $W$  is the total energy emitted from a source. The *radiant power*  $P$  (or radiant flux) is the total energy emitted per second. The *radiance*  $L(\Omega)$  is defined as the power radiated (emitted, reflected, transmitted or received) under an angle  $\theta$  through a surface element  $d\mathbf{A}$  into a solid angle element  $d\Omega = \sin\theta d\theta d\phi$ . It is a directional quantity indicating how much of the power will be received by an optical system looking at that surface from a specified angle of view,

$$P = \int L(\Omega) dA_n d\Omega . \quad (29.1)$$

Spectral densities are denoted by an index  $\nu$ , e.g.  $P = \int P_\nu(\nu) d\nu$ . In (29.1),  $dA_n \equiv \hat{\mathbf{n}} \cdot d\mathbf{A} = dA \cos\theta$  is the projection of the surface element onto the surface normal. The quantity,

$$I^* = \int L(\Omega) d\Omega \quad (29.2)$$

is called *radiant intensity*.

**Example 125 (*Angular distribution of thermal radiation*):** In a black-body in thermal equilibrium with its surroundings (e.g the walls of a cavity) the radiation is isotropic with a spectral energy distribution given by Planck's law. This means that at any point of the volume of the blackbody radiator an imaginary volume element radiates energy in all directions of space, such that the radiance into a specific solid angle element is,

$$L(\Omega) = \bar{u} \frac{c}{4\pi} . \quad (29.3)$$



Radiation passing under an angle  $\theta$  through a hole of size  $dA = dA_n / \cos \theta$  into a specific solid angle element  $d\Omega$  generates the radiance,

$$\frac{\partial^2 P}{\partial \Omega \partial A} = L(\Omega) \cos \theta . \tag{29.4}$$

In *any* direction we get,

$$\frac{\partial P_\nu}{\partial A} = \int_{\text{half sphere}} L_\nu(\Omega) \cos \theta d\Omega = \bar{u} \frac{c}{4\pi} \int_0^{2\pi} d\phi \int_0^{\pi/2} \cos \theta \sin \theta d\theta = \frac{c\bar{u}}{4} . \tag{29.5}$$

Summing up over all surface elements of a sphere of radius  $R$ ,

$$P = \int \frac{\partial P}{\partial A} dA = \frac{c\bar{u}}{4} R^2 \int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta = \pi R^2 c\bar{u} . \tag{29.6}$$

Accordingly, the spectral distribution is, using Planck's law,

$$P_\nu = P \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{\beta h\nu} - 1} = \frac{8\pi^2 R^2 h\nu^3}{c^2} \frac{1}{e^{\beta h\nu} - 1} . \tag{29.7}$$

A detector covers itself a finite solid angle  $d\Omega = \frac{dA' \cos \theta'}{r^2}$ . The radiant flux for  $r^2 \gg dA, dA'$  can then be expressed as,

$$d\Phi = L(\Omega) dA \cos \theta d\Omega = L(\Omega) dA \cos \theta \frac{dA' \cos \theta'}{r^2} \tag{29.8}$$

that is 
$$\Phi = \int_A \int_{A'} \frac{L(\Omega)}{r^2} \cos \theta \cos \theta' dA dA' .$$

Note that for isotropic sources (29.8) is symmetric upon interchanging emitter and detector with regard to  $\theta$  and  $\theta'$  or  $dA$  and  $dA'$ . Furthermore, the formula demonstrates that the radiant flux emitted into the unit solid angle is proportional to  $\cos \theta$  (Lambert's law). An example for such a source is a hole with the area  $dA$  in a blackbody radiation cavity (see Fig. 29.1). Solve Excs. 29.1.2.1 and 29.1.2.2.

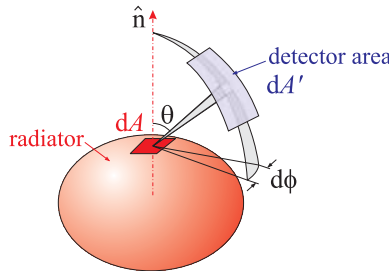


Figure 29.1: Illustration of the radiance.

Note that it is impossible to increase the radiance of a source by any sophisticated imaging optics [187]. This means that the image  $dA^*$  of a radiation source  $dA$  never has a larger radiance than the source itself. It is true that the flux density can be increased by focussing the radiation. The solid angle, however, into which radiation

from the image  $dA^*$  is emitted is also increased by the same factor. Therefore, the radiance does not increase. In fact, because of inevitable reflection, scattering, and absorption losses of the imaging optics, the radiance of the image  $dA^*$  is, in practice, always less than that of the source. A strictly parallel light beam would be emitted into the solid angle  $d\Omega = 0$ . With a finite radiant power this would imply an infinite radiance  $L$ , which is impossible. This illustrates that such a light beam cannot be realized. The radiation source for a strictly parallel beam anyway has to be a point source in the focal plane of a lens. Such a point source with zero surface cannot emit any power.

**Example 126 (Radiance of the sun):** An area  $A = 1 \text{ m}^2$  of the Earth's surface receives at normal incidence from the sun about  $P/A = 1.35 \text{ kW/m}^2$  of intensity. Since the sun covers an angle of  $\theta = 0.53^\circ$  seen from the Earth, we can estimate the sun's radiance as,

$$L = \frac{P}{A\Omega} = \frac{P}{A \int_0^{2\pi} \int_0^\theta \sin\theta d\theta d\phi} \simeq \frac{P}{A\pi\theta^2} \approx 2 \cdot 10^4 \text{ kW m}^{-2} \text{ ster}^{-1} .$$

The total power received by the Earth is  $\frac{P}{A}\pi R_{Earth}^2$ . The total power emitted by the sun is  $\frac{P}{A}4\pi d_{sun-Earth}^2$ .

**Example 127 (Radiance of a HeNe laser):** We consider a HeNe laser emitting  $P = 1 \text{ mW}$  of power from a  $w_0 = 1 \text{ mm}$  beam waist into an angle of  $2\theta = 0.067^\circ$ . With a typical emission bandwidth of  $\Delta\nu = 1 \text{ MHz}$  the spectral radiance is,

$$L_\nu = \frac{P_\nu}{A\Omega} \simeq \frac{P}{\pi w_0^2 \pi\theta^2 \Delta\nu} \approx 1 \text{ kW s m}^{-2} \text{ ster}^{-1} .$$

For comparison, the sun's radiance at its surface ( $T = 6000 \text{ K}$ ) at the same wavelength as the HeNe laser is,

$$L_\nu = \frac{L u_\nu}{\bar{u}} \approx 5 \text{ nW s m}^{-2} \text{ ster}^{-1} .$$

## 29.1.2 Exercises

### 29.1.2.1 Ex: Emission of an argon laser

The angular divergence of the output from a  $P = 1 \text{ W}$  argon laser is assumed to be  $\alpha = 4 \cdot 10^{-3} \text{ rad}$ .

a. Calculate the radiance  $L$  and the radiant intensity  $I_1$  of the laser beam and the irradiance  $I$  (intensity) at a surface  $1 \text{ m}$  away from the output mirror, when the laser beam diameter at the mirror is  $2w_s = 2 \text{ mm}$ .

b. What is the spectral power density  $u(\nu)$  if the laser bandwidth is  $1 \text{ MHz}$ ?

### 29.1.2.2 Ex: Photosynthetically active radiation

The photon flux density and the photosynthetically active radiation (PAR) are defined as,

$$\eta_{photon} \equiv \frac{\int_{\lambda_1}^{\lambda_2} u(\lambda, T) \frac{\lambda}{hcN_A} d\lambda}{\int_{\lambda_1}^{\lambda_2} u_{Pl}(\lambda, T) d\lambda} \quad \text{and} \quad \eta_{PAR} = \frac{\int_{\lambda_1}^{\lambda_2} u(\lambda, T) d\lambda}{\int_0^\infty u(\lambda, T) d\lambda} ,$$

where  $\lambda_1 = 400 \text{ nm}$  and  $\lambda_2 = 700 \text{ nm}$  delimit the range, where photosynthesis takes place. Calculate both quantities for a blackbody at  $T = 5800 \text{ K}$  temperature. Plot them as a function of temperature in the range  $T = 300..6000 \text{ K}$ .

## 29.2 Introduction to Gaussian optics

### 29.2.1 Wave equation and beam parameters

At first sight, one might think that the propagation of laser light is well described by the laws of geometrical optics. On closer inspection it turns out, however, that laser beams behave in many respects more like plane waves with their energy is concentrated near an optical axis. The electro-magnetic fields satisfy the *wave equation*,

$$k^2 u + \nabla^2 u = 0 . \quad (29.9)$$

For waves propagating in  $z$  direction,  $u = \psi(x, y, z)e^{-ikz}$ , one obtains a Schrödinger-like equation [402],

$$2ik \frac{\partial \psi}{\partial z} - \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi}{\partial y^2} = 0 , \quad (29.10)$$

where  $\partial^2 \psi / \partial z^2$  has been neglected.

To describe a *Gaussian beam*, we choose an exponential ansatz and introduce two parameters, which can vary along the propagation axis  $z$ :  $P(z)$  is a complex phase shift and  $q(z)$  a complex parameter, whose imaginary part describes the diameter of the beam. The ansatz,

$$\psi = e^{-i[P(z) + k(x^2 + y^2)/2q(z)]} \quad (29.11)$$

leads to <sup>1</sup>,

$$0 = (q' - 1) \frac{ik(x^2 + y^2)}{q^2} - 2iP' + \frac{2}{q} . \quad (29.12)$$

In order for Eq. (29.12) to hold for all  $x$  and  $y$ , we need  $q' = 1$  and  $P' = \frac{-i}{q}$ . Integrating  $q'$ , we find

$$q = q_0 + z . \quad (29.13)$$

It is useful to introduce real beam parameters,

$$\frac{1}{q} \equiv \frac{1}{R} - i \frac{\lambda}{\pi w^2} . \quad (29.14)$$

Inserting these into Eq. (29.10),

$$\psi = e^{-iP - i \frac{k(x^2 + y^2)}{2R} - \frac{(x^2 + y^2)}{w^2}} , \quad (29.15)$$

it becomes clear that  $R(z)$  is the radius of curvature and  $w(z)$  the beam diameter. Evaluating  $q_0$  at the position of the focus (waist of the beam), where  $R = \infty$ , we obtain from (29.13) and (29.14)

$$w^2(z) = w_0^2 \left[ 1 + \left( \frac{\lambda z}{\pi w_0^2} \right)^2 \right] \quad \text{and} \quad R(z) = z \left[ 1 + \left( \frac{\pi w_0^2}{\lambda z} \right)^2 \right] . \quad (29.16)$$

<sup>1</sup>See script on *Electrodynamics* (2020), Sec. 7.4.2..

Normalizing the intensity to the total power, we may write the radial intensity distributions as,

$$I_z(x, y) = \frac{2P}{\pi w(z)^2} e^{-2(x^2+y^2)/w(z)^2} . \tag{29.17}$$

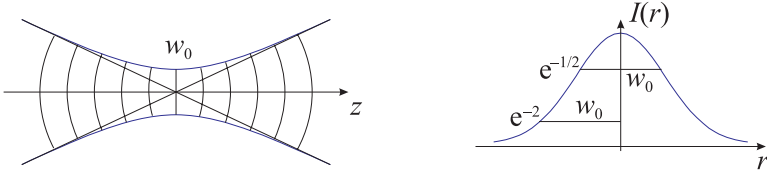


Figure 29.2: (Left) Propagation of the beam along the optical axis. (Right) Cross section of a Gaussian laser beam.

### 29.2.2 Transfer matrices

For the practical work with Gauss beams it is helpful to introduce transfer matrices, which describe the transformation of a Gauss beam through optical components along the optical axis. The matrix

$$\mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{29.18}$$

transforms the beam parameter  $q$  in the following way:

$$q(z) = \frac{aq(0) + b}{cq(0) + d} . \tag{29.19}$$

Transfer matrices allow to calculate, how the parameters  $R$  and  $w$  transform along the optical axis across the optical elements or in free space. The most common optical elements are lenses, crystals, prisms, mirrors and cavities. For example, the matrix for propagation in free space of a beam over a distance  $d$  is,

$$\mathbf{M} = \begin{pmatrix} 1 & d \\ 0 & 1 \end{pmatrix} \tag{29.20}$$

and the matrix for transformation through a thin lens with focal distance  $f$ ,

$$\mathbf{M} = \begin{pmatrix} 1 & 0 \\ -1/f & 1 \end{pmatrix} . \tag{29.21}$$

It is interesting to note that the transfer matrices are the same as those, which in classical beam optics transform the vector, whose components are the distance of the beam from the optical axis  $y$  and its divergence  $y'(z)$ :

$$\begin{pmatrix} y(z) \\ y'(z) \end{pmatrix} = \mathbf{M} \begin{pmatrix} y(0) \\ y'(0) \end{pmatrix} . \tag{29.22}$$

Fig. 29.3 shows that coupling a Gaussian beam of light into a cavity requires matching of the phase fronts. Solve the Excs. 29.2.3.1 to 29.2.3.16 [187, 402, 715].

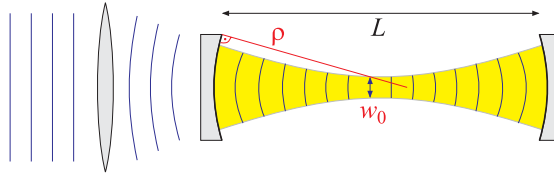


Figure 29.3: Coupling a Gaussian beam of light into cavity requires matching of the phase fronts.

### 29.2.3 Exercises

#### 29.2.3.1 Ex: Imaging through a thin lens

In classical ray optics the equations describing the focusing of a thin lens are given by,

$$\frac{1}{f} = \frac{1}{g} + \frac{1}{b} \quad \text{and} \quad \frac{b}{g} = \frac{B}{G},$$

where  $f$  is the focal distance of the lens,  $g$  the distance between the object and the lens,  $b$  the distance between the image and the lens,  $G$  the size of the object, and  $B$  the size of the image.

At what distance from an object of size  $G = 1$  mm do you have to place a thin lens with focal distance  $f = 100$  mm in order to obtain a ten times larger image? Test your result in practice.

#### 29.2.3.2 Ex: Image of a convex lens

Show that with a convex lens of focal distance  $f$  the smallest distance between object and image should be  $s = 4f$ .

#### 29.2.3.3 Ex: Telescope with ray optics

In classical optics the transfer matrix for the propagation of a beam through free space and through a thin lens are given, respectively, by

$$M_{free} = \begin{pmatrix} 1 & d \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad M_{lens} = \begin{pmatrix} 1 & 0 \\ -1/f & 1 \end{pmatrix}.$$

The transfer between a point  $z_0$  of the optical axis and a point  $z_1$  is described by

$$\begin{pmatrix} y(z_1) \\ y'(z_1) \end{pmatrix} = M_{free} \begin{pmatrix} y(z_0) \\ y'(z_0) \end{pmatrix}.$$

Here,  $y$  is the distance of a beam ray from the optical axis and  $y' = \frac{dy}{dx}$  its divergence. Use this formalism to design a 3 times magnifying telescope with two lenses have, respectively, the focal lengths  $f_1 = 100$  mm and  $f_2 = 300$  mm.

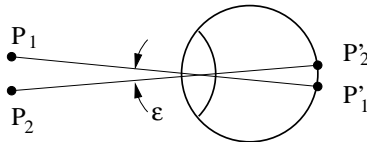
#### 29.2.3.4 Ex: Ray tracing

Simulate the trajectory of a ray of light traversing under an angle a layer of a material with a refraction index characterized by a Gaussian profile.

**29.2.3.5 Ex: The eye**

The effective distance between the cornea and the lens of the eye is 2.5 cm, and the lens is in contact with the eye. To resolve two very close points, their images on the retina must be on two non-adjacent cone cells (i.e. there must be at least one non-activated cone cell between the images). The cone cells are about  $1\ \mu\text{m}$  apart.

- What is the smallest angle  $\epsilon$  under which two points are still separately perceptible? Assume that the direct beams  $P, P'$  are not refracted.
- How close can the two points  $P_1$  and  $P_2$  be, at a distance of 20 m from the eye, so that they are still separately perceptible?

**29.2.3.6 Ex: Microscope**

A simple homemade microscope consists of two convex lenses, each one with a diffractive power of 20 dpt, fixed at the extremities of a 30 cm long tube.

- Wie groß ist die Tubuslänge dieses Mikroskops?
- Wie groß ist der Abbildungsmaßstab des Mikroskops?
- Welche Vergrößerung erreicht das Mikroskop? Gehen Sie davon aus, dass die deutliche Sehweite 25 cm beträgt.
- Wie weit muss sich der Gegenstand vor dem Objektiv befinden, damit er im Auge des Betrachters scharf abgebildet wird?

**29.2.3.7 Ex: Classical cloaking with four lenses**

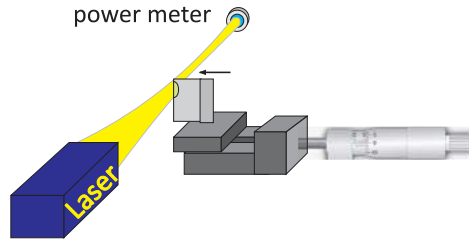
Can you design a system of four lenses (focal distances  $f_1, f_2, f_3 = f_2$ , and  $f_4 = f_1$ ) separated by three distances  $t_1 = f_1 + f_2, t_2$ , and  $t_3 = t_1$ , such that the system appears to be invisible for an observer looking through the lenses [132]?

**29.2.3.8 Ex: Diameter of a Gaussian beam**

You are blocking part of a laser beam with a razor blade mounted on a translation stage allowing you to vary the horizontal position. At the same time, you observe the transmitted power  $P$ . You observe that, for varying the power between 16% and 84%, you need to vary the translation by  $140\ \mu\text{m}$ . What is the diameter of the Gaussian beam?

**29.2.3.9 Ex: Diffraction of a Gaussian beam at a slit**

- Determine the power loss suffered by a Gaussian beam passing through a one-dimensional slit, assuming that the beam hits the slit in its center.
- Calculate the diffraction pattern produced by the slit.
- A laser beam ( $\lambda = 633\ \text{nm}$ ) loses 50% of its power after being passed through a



slit. At a distance of  $L = 1$  m behind the slit appear diffraction patterns exhibiting first minima at  $\Delta x = 1$  mm to both sides of the central peak. Determine the diameter of the Gaussian beam.

### 29.2.3.10 Ex: Diffraction of a Gaussian beam at a pinhole

- Determine the power loss suffered by a Gaussian beam passing through the center of a pinhole of radius  $R$ .
- A laser beam ( $\lambda = 633$  nm) loses 50% of its power after being passed through a slit. At a distance of  $L = 1$  m behind the slit appear diffraction patterns exhibiting a first minimum at a distance  $\Delta b = 1$  mm from the optical axis. Determine the diameter of the Gaussian beam. Help: The first ring of destructive interference occurs under an angle of  $\sin \theta = 1.22 \frac{\lambda}{2R}$ .

### 29.2.3.11 Ex: Focusing a HeNe laser

The output beam from an HeNe laser with a confocal resonator ( $\rho = L = 30$  cm) is focused by a lens of  $f = 30$  cm, 50 cm away from the output mirror. Calculate the location of the focus, the Rayleigh length, and the beam waist in the focal plane.

### 29.2.3.12 Ex: Spatial filtering

A nearly parallel Gaussian beam with  $\lambda = 500$  nm is expanded by a telescope with two lenses of focal lengths  $f_1 = 1$  cm and  $f_2 = 10$  cm, illustrated in the figure. The spot size at the entrance lens is  $w = 1$  mm.

- Why does an aperture in the focal plane improve the quality of the wave fronts in the expanded beam by eliminating perturbations due to diffraction effects by dust and other imperfections on the lens surfaces?
- What is the diameter of this aperture, if 95% of the intensity is transmitted?

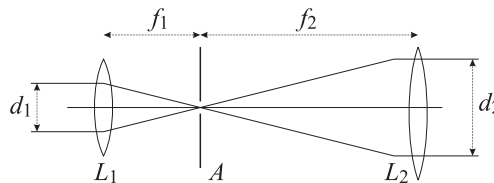
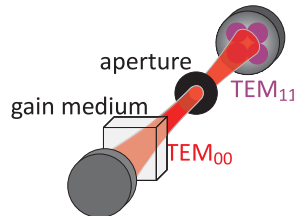


Figure 29.4: Beam-expanding telescope with an aperture in the focal plane.

### 29.2.3.13 Ex: Transverse mode selection in an Ar laser

An argon laser oscillating at  $\lambda = 488 \text{ nm}$  with resonator length  $d = 100 \text{ cm}$  and two mirrors with radius  $R_1 = \infty$  and  $R_2 = 400 \text{ cm}$  has an intracavity circular aperture close to the spherical mirror to prevent oscillation on transversal modes. Estimate the maximum diameter of the aperture that introduces losses  $\gamma_{diff} < 1\%$  for the  $\text{TEM}_{00}$  mode, but prevents oscillation of higher transverse modes, which without the aperture have a net gain of 10%.



### 29.2.3.14 Ex: Anamorphic prism

A prism can be used for expansion of a laser beam if the incident beam is nearly parallel to the prism surface. Calculate the angle of incidence  $\alpha$  for which a laser beam transmitted through a rectangular glass prism with an  $\varepsilon = 45^\circ$  base angle is expanded tenfold.

### 29.2.3.15 Ex: Anamorphic prism pair

An *anamorphic prism* pair is a setup consisting of two prisms through which a laser beam is passed under specific angles. The angles can be chosen such as to change the beam diameter only in the  $p$ -plane.

- Calculate, for a single prism with refractive index  $n = 1.5$ , the beam expansion for an incidence angle of  $\theta_1 = 57^\circ$  and an exit angle of  $0^\circ$ . How large must the base angle  $\beta$  of the prism be for this to be possible?
- How must the second prism be aligned in order for the beam transmitted to this second prism to remain parallel to the incident beam? Note, that an anamorphic

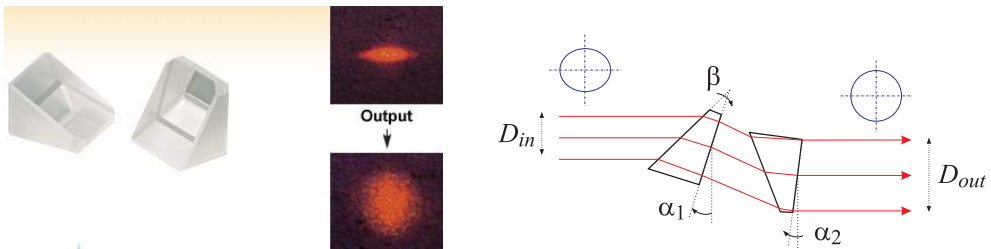


Figure 29.5: (Left) Anamorphic prisms (Thorlabs, PS870). (Right) Geometry of the beam transformation. The entrance side of a prism is often chosen close to the Brewster angle, while the exit side treated carries an anti-reflexion coating.

prism pair does not allow to correct for astigmatism. This requires cylindrical lenses.



**29.2.3.16 Ex: Beam steering with two wedged substrates**

The wavevector of a laser beam is generally aligned with one or more adjustable reflective mirrors. Alternatively, one may use a pair of rotatable transmissive wedged substrates. Calculate the wave vector of a laser beam after its transmission through two  $\epsilon = 3^\circ$  wedged, 2 mm thick, AR-coated substrates with the refractive index  $n_{rfr} = 1.5134$  at 689 nm, each one rotated by  $\theta_{1,2}$  from some normal position.

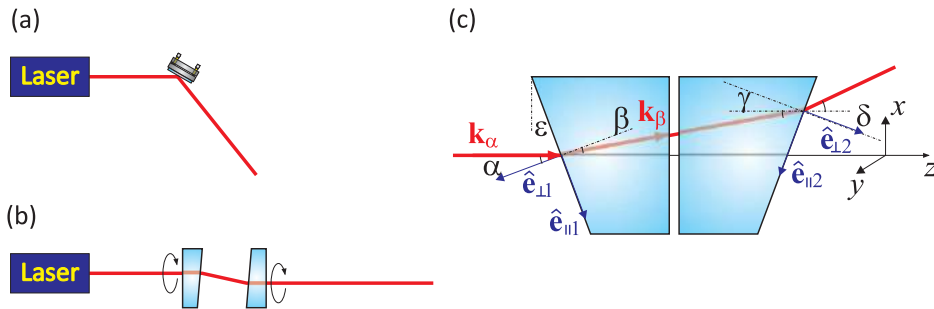


Figure 29.6: Beam steering with two rotatable wedged substrates (see Thorlabs, PS810).

**29.2.4 Experiment: Measuring the diameter of a Gaussian laser beam**

Most laser beams exhibit a Gaussian shape transverse intensity distribution, as we will study in this experiment.

1. Measure the phase profile of a helium-neon laser. To this end fix a razor blade on a translation stage and move it sideways into the beam. From the power of the partially blocked beam  $\int_F I(x, y) dx dy$ , where  $F$  is the cross section of the unblocked part of the beam,  $w(z)$  can be determined (see Excs. 29.2.3.8 to 29.2.3.10).

**29.2.5 Experiment: Measuring the parameters of a Gaussian laser beam**

Once a Gaussian beam has been characterized at a given position  $z$ , the transfer matrix formalism allows us to calculate its shape at any position along the optical axis. In this experiment, we will study the propagation of a Gaussian beam through free space [see Eqs. (29.16)] and its transformation through a thin lens with focal distance  $f$ . For the latter one, we obtain directly after the lens,

$$\frac{1}{R(z \searrow 0)} = \frac{1}{R(z \nearrow 0)} - \frac{1}{f}. \quad (29.23)$$

1. Focus the beam with a lens. Measure the beam diameter at 3 different locations. Compare with the prediction of Gaussian optics.
2. Set up a 1:3 telescope and verify that the outgoing beam is collimated.

### 29.2.6 Experiment: Spatial filtering with a pinhole

Laser light emitted from diode lasers is often astigmatic and has an irregular beam profile. The beam profile can be purified by passing it through an optical fiber or a pinhole, however, at the price of losing power.

1. Focus the beam of a HeNe laser with a lens of  $f = 100$  mm focal distance onto a pinhole. Observe the interference fringes and, from their distance from the optical axis, infer the diameter of the pinhole.
2. Remove the higher-order diffraction rings with an iris and compare the beam profile with that of a Gaussian beam. What are the divergence and the waist of the spatially filtered beam (see Exc. 29.2.3.10)?

## 29.3 Introduction to polarization optics

A laser usually has a well-defined polarization, e.g., linear or circular. The polarizations can be transformed into one another through a *quarter waveplate* ( $\lambda/4$ ) or a *half waveplate* ( $\lambda/2$ ) by a Fresnel rhomb or other birefringent elements. Superpositions of polarizations can be separated by a *polarizing beam splitter*.

Waveplates consist of thin sheets of *birefringent crystals*, which are transparent material characterized by anisotropic refraction indices. Cut in a particular way, a birefringent crystal can exhibit a polarization-dependent refraction index, allowing to control the retardation of a light beam as a function of its polarization. The thickness of a waveplate determines the retardation of one polarization axis with respect to the other.



Figure 29.7: (Left) Transmission through a birefringent crystal. (Right)  $\lambda/2$ -waveplate mounted in a rotation stage.

In practice, the degree of freedom of polarization is often used for separating counterpropagating light fields, e.g. in ring lasers, by means of elements called *optical diode* or *optical isolator*, which consist of a Faraday rotator and  $\lambda/2$  waveplate. Another practical example is the use of  $\lambda/4$  in double passage. An incoming beam can be separated from a returning beam by using a  $\lambda/4$  waveplate and a polarizing beam splitter.

### 29.3.1 Jones matrices

The term *polarization* is defined in relation to a fixed coordinate system, while the term *helicity* denotes the direction of rotation of the polarization vector with respect to the direction of propagation of the light beam. The polarization of a beam propagating in  $z$ -direction can easily be expressed by a vector of complex amplitude,

$$\mathbf{E}(\mathbf{r}, t) = \begin{pmatrix} a \\ b \\ 0 \end{pmatrix} e^{i\mathbf{kr} - i\omega t} = \begin{pmatrix} 1 \\ e^{-i\phi} |b|/|a| \\ 0 \end{pmatrix} |a| e^{i\mathbf{kr} - i\omega t} . \quad (29.24)$$

The angle  $\phi = \arctan \frac{\text{Im } ab^*}{\text{Re } ab^*}$  determines the polarization of the light beam. A polarization is linear when  $\phi = 0$  and circular when  $\phi = \pi/2$ .  $|b|/|a|$  is, hence, the degree of ellipticity. A polarization rotator for linearly polarized light (e.g., a sugar solution) is described by the following *Jones matrix* (we will restrict to the  $x$ - $y$ -plane)

$$M_{\text{rotator}}(\phi) = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} , \quad (29.25)$$

where  $\phi$  is the rotation angle. For the Faraday rotator the sign of the rotation angle depends on the propagation direction of the laser beam. A *polarizer* projects the polarization onto a specific axis. In the case of the  $x$ -axis Jones matrix is,

$$M_{\text{polarizer}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} . \quad (29.26)$$

If the rotation angle is  $\phi$ ,

$$M_{\text{polarizer}}(\phi) = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix}^{-1} . \quad (29.27)$$

Other components, such as electro-optical modulators or phase plates are birefringent crystals, which act only on one of the two optical axes. If only the  $y$  axis is optically active, the Jones' matrix is,

$$M_{\theta\text{-waveplate}} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix} . \quad (29.28)$$

For  $\theta = 2\pi/n$  we obtain a  $\lambda/n$ -waveplate. When we rotate the waveplate and therefore the optically inactive axis to an angle  $\phi$ , the Jones matrices are,

$$\begin{aligned} M_{\theta\text{-waveplate}}(\phi) &= \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix}^{-1} \\ &= \begin{pmatrix} \cos^2 \phi + e^{i\theta} \sin^2 \phi & -\sin \phi \cos \phi + e^{i\theta} \sin \phi \cos \phi \\ -\sin \phi \cos \phi + e^{i\theta} \sin \phi \cos \phi & \sin^2 \phi + e^{i\theta} \cos^2 \phi \end{pmatrix} . \end{aligned} \quad (29.29)$$

In most cases, we use quarter waveplates  $\lambda/4$ ,

$$M_{\lambda/4}(\phi) = \begin{pmatrix} \cos^2 \phi + i \sin^2 \phi & (-1 + i) \sin \phi \cos \phi \\ (-1 + i) \sin \phi \cos \phi & \sin^2 \phi + i \cos^2 \phi \end{pmatrix} \quad (29.30)$$

and half waveplates  $\lambda/2$ ,

$$M_{\lambda/2}(\phi) = \begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ -\sin 2\phi & -\cos 2\phi \end{pmatrix}. \quad (29.31)$$

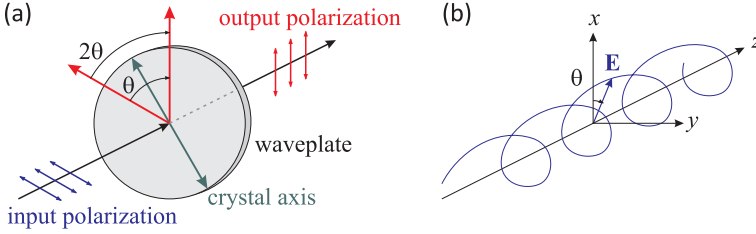


Figure 29.8: (a) Rotation of the polarization by a birefringent waveplate. (b) Illustration of a circularly polarized light wave.

Combinations of  $\lambda/2$  waveplates and *Faraday rotators* are used as *optical isolator*, also called *optical diode*.

### 29.3.2 Fresnel formulae

Reflection and transmission of a beam of light at a surface depend on the polarization of the light and the angle of incidence. They are described by the *Fresnel formula*:

$$\begin{aligned} \left(\frac{I_{0t}}{I_{0i}}\right)_s &= T_s = \left(\frac{2 \sin \theta_t \cos \theta_i}{\sin(\theta_i + \theta_t)}\right)^2 \\ \left(\frac{I_{0r}}{I_{0i}}\right)_s &= R_s = \left(\frac{-\sin(\theta_i - \theta_t)}{\sin(\theta_i + \theta_t)}\right)^2 \\ \left(\frac{I_{0t}}{I_{0i}}\right)_p &= T_p = \left(\frac{2 \sin \theta_t \cos \theta_i}{\sin(\theta_i + \theta_t) \cos(\theta_i - \theta_t)}\right)^2 \\ \left(\frac{I_{0r}}{I_{0i}}\right)_p &= R_p = \left(\frac{\tan(\theta_i - \theta_t)}{\tan(\theta_i + \theta_t)}\right)^2. \end{aligned} \quad (29.32)$$

The angles of incidence and transmission are related by Snell's law:  $n_1 \sin \theta_i = n_2 \sin \theta_t$ .

The *Brewster angle*  $\theta_{i,B}$  is reached, when  $\theta_{i,B} + \theta_t = 90^\circ$ , i.e., when following Snell's law,

$$n_1 \sin \theta_{i,B} = n_2 \sin(90^\circ - \theta_{i,B}) = n_2 \cos \theta_{i,B}. \quad (29.33)$$

Hence, the Brewster angle is given by,

$$\tan \theta_{i,B} = \frac{n_2}{n_1}. \quad (29.34)$$

Resolve the exercises 29.3.3.1 to 29.3.3.5.

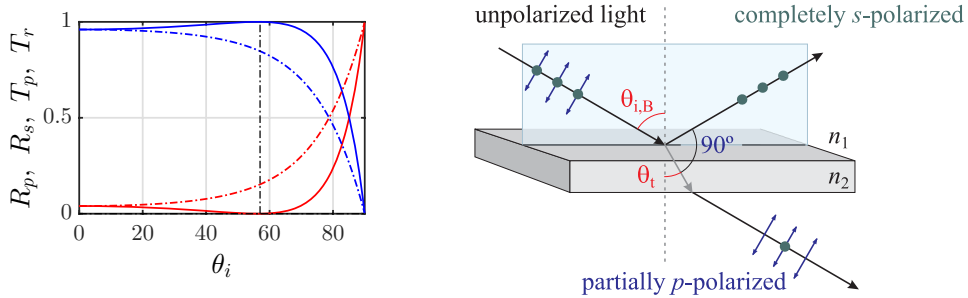


Figure 29.9: (code) (Left) Fresnel formulae showing the angular dependence of  $t_s$  (red solid),  $r_s$  (green dash-dotted),  $t_p$  (blue dashed), and  $r_p$  (cyan dotted) for reflection from and transmission through a piece of glass-air interface. (Right) Interfaces between optical media with different reflection indices can act like polarizers: Light reflected from a glass surface under the Brewster angle is completely  $s$ -polarized, while the transmitted light is partially  $p$ -polarized. The notation  $s$  comes from *senkrecht*, i.e. perpendicular to the plane spanned by the incident and reflected light beams, while  $p$  means *parallel* to this plane.

### 29.3.3 Exercises

#### 29.3.3.1 Ex: Light power control using polarization optics

The power of a laser beam can be regulated by a combination of a half-wave plate and a polarizing beam splitter. By how many degrees do you have to rotate the waveplate in order to reduce the light power by a factor of 2? Use the Jones matrices to justify your response. **Advice:** Look up the Jones matrices (29.31) and (29.26). Test your result in practice.

#### 29.3.3.2 Ex: Jones matrices

Consider a linearly polarized laser beam passing twice through a  $\lambda/4$ , first in direction of the optical axis, the second time in opposite direction. Calculate the final polarization.

#### 29.3.3.3 Ex: Intensity transmitted through a polarizer

Unpolarized light of intensity  $I_0$  is transmitted through a polarizer with thickness  $d = 1$  mm. Calculate the transmitted intensity when the absorption coefficients for the two polarizations are  $\alpha_{\parallel} = 100 \text{ cm}^{-1}$  and  $\alpha_{\perp} = 5 \text{ cm}^{-1}$ .

#### 29.3.3.4 Ex: Thickness of a half-waveplate

A birefringent quartz crystal is characterized by different refractive indices of the ordinary beam  $n_o = 1.544$  and the extraordinary beam  $n_e = 1.553$ . Calculate the necessary thickness of a quartz waveplate to be used as a  $\lambda/2$  retarder at 633 nm. Choose an appropriate waveplate from the Thorlabs catalogue. How thick would a calcite waveplate ( $n_o = 1.658$ ,  $n_e = 1.486$ )?

**29.3.3.5 Ex: Faraday isolator**

A Faraday rotator is a device exploiting the Faraday effect to rotate the polarization of a light beam according to the Jones matrix,

$$M_{Faraday}(\phi) = \begin{pmatrix} \cos \phi & -\mathbf{k} \cdot \hat{\mathbf{e}}_z \sin \phi \\ \mathbf{k} \cdot \hat{\mathbf{e}}_z \sin \phi & \cos \phi \end{pmatrix}, \quad (29.35)$$

where  $\mathbf{k}$  is the wavevector of the light beam. An optical diode is composed by a  $\phi = 45^\circ$  Faraday rotor sandwiched between two polarizers rotated by  $\phi = 45^\circ$  with respect to each other.

- How is the polarization of a light beam changed after a double passage (back and forth) through a Faraday rotator?
- Calculate what happens to a light beam upon a single passage through a Faraday rotator in either direction  $\mathbf{k}$  and  $-\mathbf{k}$ ?

**29.3.4 Experiment: Polarization of a helium-neon laser**

We will now analyze and manipulate the polarization of a laser beam in practice.

- Pass the beam of a helium-neon laser through a polarizer and a quarter- resp. half-waveplate. Analyze the polarization using a rotatable second polarizer for various rotation angles of the waveplate. Sketch the transmitted intensity as a function of the rotation angle of the beamsplitter in a polar diagram. How good can you achieve linear and circular polarization?
- Characterize the polarization of a helium-neon laser by sketching the transmitted intensity through a polarizing beamsplitter as a function of the rotation angle of the beamsplitter in a polar diagram. Now couple the laser beam to a Fabry-Pérot interferometer. What do you observe? Place a quarter-waveplate at the output of the helium-neon laser and characterize again the polarization. What do you observe at the Fabry-Pérot interferometer?
- Use a quarter-waveplate to separate a beam of light from a counterpropagating beam according to Fig. 29.10.

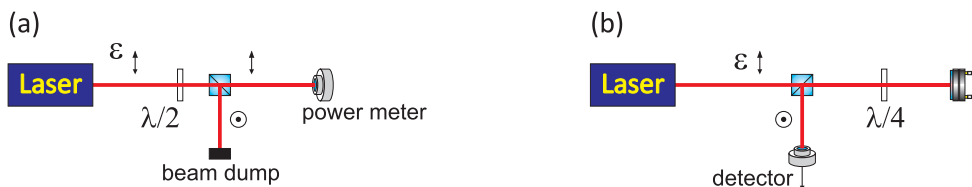


Figure 29.10: (a) Power control of a light beam and (b) separation of counterpropagating beams through polarization optics.

- Characterize an optical insulator. Optimize its extinction.

### 29.3.5 Experiment: Measuring the Brewster angle

Any interface between two transparent materials with different refraction indices reflects a part of incident light depending on the polarization and the angle of incidence, as predicted by Fresnel's formulae (29.32).

1. Measure the transmission by a glass plate as a function of the angle of incidence for two orthogonal polarizations and determine the Brewster angle.
2. Mirrors can change the polarization of a light beam and, for example, transform a linear polarization into elliptical. Determine the degree of ellipticity for a given mirror.
3. How does a mirror transform the polarization and the helicity of a reflected laser beam?

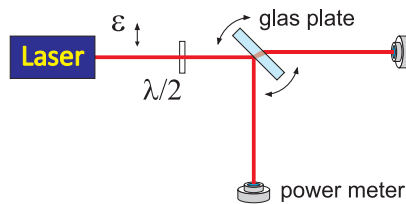


Figure 29.11: Measuring the Brewster angle by varying the tilt of a glass plate.

### 29.3.6 Experiment: Pockels cell

*Pockels cells* are birefringent crystals allowing to manipulate the polarization of a laser beam by application of a voltage.

1. Prepare a laser beam by passing it through a polarizer followed by a half-waveplate and a second polarizer. Observe the intensity transmitted and reflected through the last polarizer as a function of the rotation angle of the half-waveplate.
2. Use the EOM as a Pockels cell by placing it between the half-waveplate and the second polarizer. Supply a voltage between 0 V and 350 V to the EOM. Measure the intensity of reflected and transmitted light as a function of the supplied voltage and prepare a diagram. What do you observe when you rotate either the half-waveplate or the EOM?

## 29.4 Laguerre-Gaussian light modes

Light beams not only possess polarization, but can also have orbital angular momentum. This property of light can impressively be demonstrated at the so-called *Laguerre-Gaussian modes*.

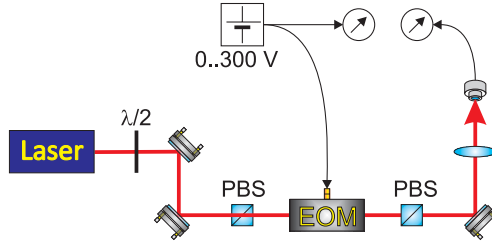


Figure 29.12: Scheme for using an EOM as a Pockels cell.

These modes can be produced by means of masks resembling *Fresnel zone plate*. Fresnel zone plates are masks consisting of concentric sequences of bright (transmitting) and dark (absorbing) rings. The diameters of the rings are selected in such a way that the diameters of the rings defined by the bright rings interfere constructively at a certain distance  $f_1$  on the optical axis and form a 'focus' there. For this purpose, the distance  $d_n$  of the  $n^{\text{th}}$  ring must satisfy the condition,

$$d_n = \sqrt{(f_1 + n\lambda)^2 - f_1^2} \simeq \sqrt{2f_1n\lambda} . \tag{29.36}$$

For a given zone plate there are other focuses at smaller distances,

$$f_k = \frac{d_n^2 - k^2n^2\lambda^2}{2kn\lambda} \simeq \frac{d_n^2}{2kn\lambda} = \frac{f_1}{k} . \tag{29.37}$$

In order to separate the beams diffracted by the zone plate into a given focus from those diffracted into other focuses or not being diffracted at all, we pass the beam through an iris diaphragm localized at the desired focus and recollimate the beam by means of a lens, as shown in Fig. 29.13.

The phase profile of the beam can be viewed interferometrically (see Fig. 29.13) by overlapping a plane wave laser beam. With a *neutral density filter* the intensities of the overlapping beams can be adjusted to maximize the contrast.

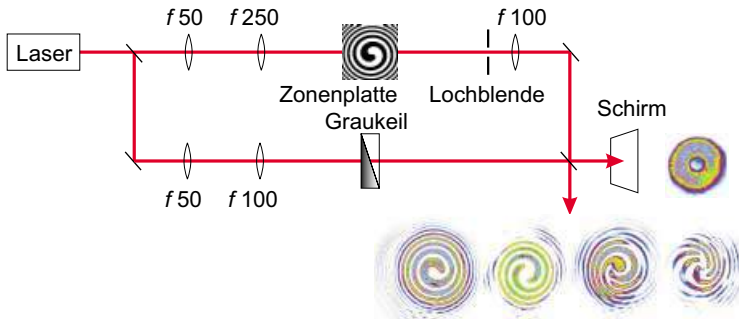


Figure 29.13: Creation of Laguerre-Gaussian modes.

Now, for realizing Laguerre-Gaussian light modes, we use Fresnel zone plates with spiral patterns, instead of concentric rings. In contrast to the Gaussian mode, the Laguerre-Gauß modes exhibit an intensity minimum on the optical axis (doonat mode). Their phase profiles can be viewed by interferometry [12].



### 29.4.1 *Experiment: Generating a Laguerre-Gaussian mode*

In this experiment, we will...

1. Construct the interferometer sketched in Fig. 29.13 using adequate Fresnel zone plates. What do you observe in the diffracted beam and in the interferogram, when instead of filtering the principal focus  $f_1$  you filter a higher order focus?
2. Pass a Laguerre-Gauß laser beam through a  $\lambda/2$  waveplate. How does the angular orbital momentum change when you change the rotation? What happens upon reflection from a mirror?
3. Slightly misalign the mode-matching between the Laguerre-Gauß beam and the Gaussian reference beam until you observe multiple fringes. What do you observe?

## 29.5 Further reading

M. Born, *Principles of Optics* [ISBN]

H. Kogelnik et al., *Laser Beams and Resonators* [DOI]

W. Demtröder, *Atoms, Molecules and Photons: An Introduction to Atomic, Molecular, and Quantum Physics* [ISBN]

J. Weiner et al., *Light-matter interaction, Fundamentals and applications* [DOI]

G.A. Fowles, *Introduction to Modern Optics* [ISBN]

J.S. Choi et al., *Paraxial ray optics cloaking* [DOI]

### 29.5.1 on Laguerre-Gauss modes

L. Allen et al., *Orbital Angular Momentum of Light and the Transformation of Laguerre-Gaussian Laser Modes* [DOI]

# Chapter 30

## Electronics and radiofrequency

For the control and regulation of important quantum optical devices, such as EOMs, AOMs, laser diodes, photodiodes, piezos etc., *electronic circuits* are necessary. The aim of this chapter is to provide practical know-how in the basics of electronics.

### 30.1 Introduction to electronic circuits

#### 30.1.1 Passive electronic components

Electronic components which are characterized by a fixed impedance are called *passive*. The most common devices are resistors, capacitors, and inductances. For their handling, it is useful to be able to identify their impedance from their labeling.

The values of the resistances of resistors are generally codified by colored rings. The first ring to be considered is the one closest to a terminal. In case of 4 rings, the first two rings are to be considered as digits, the third ring gives the exponent 10. With five rings, the first three are digits and the fourth gives the exponent of 10. The last ring, in both cases specifies the tolerance of the value of the resistance.

There are various types of capacitors depending on the employed materials for the dielectric medium (paper, ceramics, polyester, electrolyte made of aluminum and electrolyte made of tantalum). Electrolyte capacitors have a defined polarity, and an reversion of their voltage supply can result in their explosion. The value of the capacitance is generally written on their body, as well as their maximum allowed operating voltage. Also the polarity of electrolyte capacitors is always indicated (although there can be some confusion with regard to the physical and technical direction of the current flow). Ceramic and polyester capacitors can have their values either written in letters or color coded. The color code sequence is similar to that of resistors, with the first two digits devoted to the digits, the third to the multiplier exponent, the fourth to the tolerance, and the fifth for the maximum voltage. In case of printed numbers, the first two numbers represent the first two digits, and the third one represents the numbers of 0 before the decimal point. In all cases (colors or digits), the value is given in picoFarads. With more modern serigraphic techniques, some capacitors have their values printed directly in Farads (micro, nano and pico). In these cases, the letter denoting the unit also serves to mark the decimal point. For example, 2n2 means 2.2 nF.

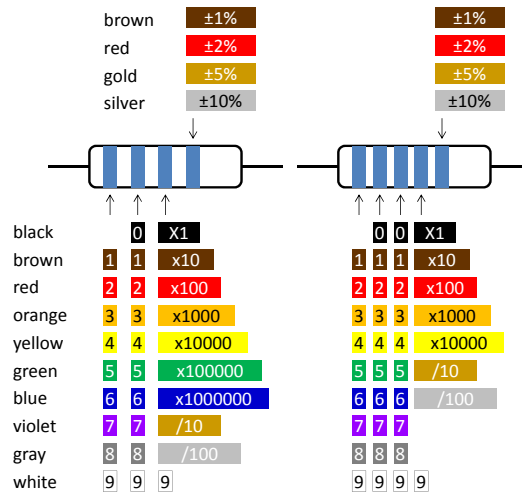


Figure 30.1: Color code for resistors with 4 and 5 rings.

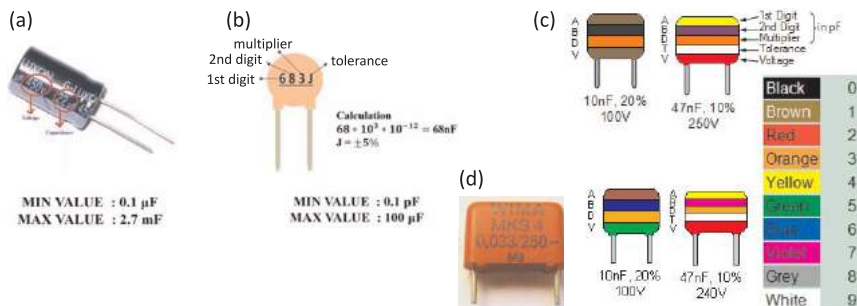


Figure 30.2: (Left) Electrolyte aluminum capacitors. (Center) Polyester capacitor and color code. (Right) Ceramic capacitor.

### 30.1.2 Active electronic components and the $pn$ -junction

Diodes, transistors, photodiodes, operational amplifiers are called *active components*, because their current-to-voltage curve is non-linear, their response  $I = I(U)$  cannot be described by a single constant value, but depends on the applied voltage.

During this course we will work a lot with *operational amplifiers* (OpAmp), which are integrated circuits designed to amplify input signals with characteristics that are entirely determined by external components. This feature makes them easy to use and extremely versatile.

OpAmps are generally found encapsulated in DIL type housings (dual in line), which means that they have two lines of 4 pins. The sequence of pins is numerated in counter-clockwise orientation, and they have a mark on the side of pin 1. It is always recommend to obtain the datasheet of the OpAmp since, despite a usual pin compatibility ensured by the various OpAmp manufacturers, deviations are frequent.

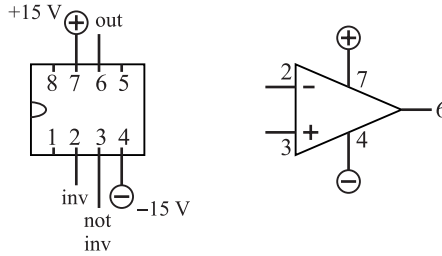


Figure 30.3: (Left) Schematic symbol of an OpAmp; (Right) Pin layout of a standard OpAmp.

### 30.1.3 Electronic circuits

Amplification or control circuits are nowadays mostly realized with *operational amplifiers (OpAmp)*. The advantage of an OpAmp compared to circuits based on transistors is, that their properties are almost independent of their internal structure. Hence, their properties can be personalized via an external feedback realized with external components. The input of an OpAmp does not require current. OpAmps amplify the voltage difference between the non-inverting input (+) and the inverting (-). For most practical matters we can assume, that the OpAmp has infinite amplification and negligible input impedance.

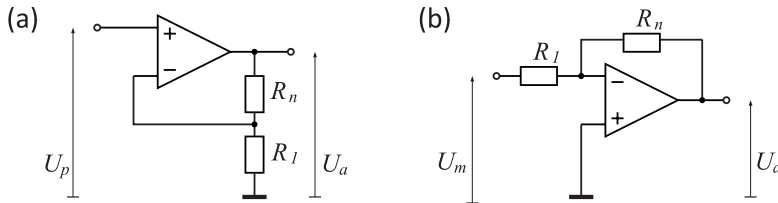


Figure 30.4: (Left) Principle scheme of a standard OpAmp. (Center) Non-inverting amplifier. (Right) Inverting amplifier.

OpAmps can be used as *inverting amplifiers* or *non-inverting amplifiers*. Using *Kirchhoff's rules* for the *loops* and *nodes* of the circuit, we find for a non-inverting amplifier,

$$\frac{U_e}{R_1} = -\frac{U_a}{R_1 + R_n} \quad , \quad G = 1 + \frac{R_n}{R_1} \quad (30.1)$$

This becomes clear noting that, since no voltage is dropped between the inputs (+) and (-), the input voltage must be equal to the voltage drop at  $R_1$ . And since the non-inverting input does not deliver current, the currents traversing the resistances  $R_n$  and  $R_1$  must be equal. For the inverting amplifier, we find,

$$\frac{U_a}{R_n} = -\frac{U_e}{R_1} \quad , \quad G = -\frac{R_n}{R_1} \quad (30.2)$$

This becomes clear noting that, since the input (-) does not drag current, the currents traversing the resistances  $R_n$  and  $R_1$  must cancel each other.

Changing the resistances  $R$  to inductances  $L$  or capacitances  $C$ , it becomes possible to influence the frequency response of the amplifying circuit. The impedance are,

$$Z_L = iL\omega \quad , \quad Z_C = \frac{1}{iC\omega} . \quad (30.3)$$

For the calculation of the amplification with complex impedances, we just take the absolute value of the gain  $G$ .

### 30.1.4 The thermoelectric effect

#### 30.1.4.1 Seebeck effect

The Seebeck effect is a classic example of an electromotive force (EMF) and leads to measurable currents or voltages in the same way as any other EMF. The local current density is given by,

$$\mathbf{J} = \sigma(-\nabla V + \mathbf{E}_{emf}) , \quad (30.4)$$

where  $V$  is the local voltage, and  $\sigma$  is the local conductivity. In general, the Seebeck effect is described locally by the creation of an electromotive field,

$$\mathbf{E}_{emf} = -S\nabla T , \quad (30.5)$$

where  $S$  is the Seebeck coefficient (also known as thermopower), a property of the local material, and  $\nabla T$  is the temperature gradient.

The Seebeck coefficients generally vary as function of temperature and depend strongly on the composition of the conductor. For ordinary materials at room temperature, the Seebeck coefficient may range in value from  $-100 \mu\text{V}/\text{K}$  to  $+1000 \mu\text{V}/\text{K}$ .

If the system reaches a steady state, where  $\mathbf{J} = 0$ , then the voltage gradient is given simply by the emf:

$$-V = S\Delta T . \quad (30.6)$$

This simple relationship, which does not depend on conductivity, is used in the thermocouple to measure a temperature difference; an absolute temperature may be found by performing the voltage measurement at a known reference temperature. A metal of unknown composition can be classified by its thermoelectric effect if a metallic probe of known composition is kept at a constant temperature and held in contact with the unknown sample that is locally heated to the probe temperature. It is used commercially to identify metal alloys. Thermocouples in series form a *thermopile*. Thermoelectric generators are used for creating power from heat differentials.

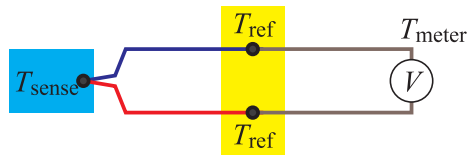


Figure 30.5:

30.1.4.2 Peltier effect

When an electric current is passed through a circuit of a thermocouple, heat is evolved at one junction and absorbed at the other junction. This is known as Peltier Effect and is named after a physicist. The Peltier effect is the presence of heating or cooling at an electrified junction of two different conductors. When a current is made to flow through a junction between two conductors, A and B, heat may be generated or removed at the junction. The Peltier heat generated at the junction per unit time is,

$$\dot{Q} = (\Pi_A - \Pi_B)I , \tag{30.7}$$

where  $\Pi_A$  and  $\Pi_B$  are the Peltier coefficients of conductors A and B, and  $I$  is the electric current (from A to B). The total heat generated is not determined by the Peltier effect alone, as it may also be influenced by Joule heating and thermal-gradient effects (see below).

The Peltier coefficients represent how much heat is carried per unit charge. Since charge current must be continuous across a junction, the associated heat flow will develop a discontinuity if  $\Pi_A$  and  $\Pi_B$  are different. The Peltier effect can be considered as the back-action counterpart to the Seebeck effect (analogous to the back-EMF in magnetic induction): if a simple thermoelectric circuit is closed, then the Seebeck effect will drive a current, which in turn (by the Peltier effect) will always transfer heat from the hot to the cold junction. The close relationship between Peltier and Seebeck effects can be seen in the direct connection between their coefficients [344, 686]:

$$\Pi = TS . \tag{30.8}$$

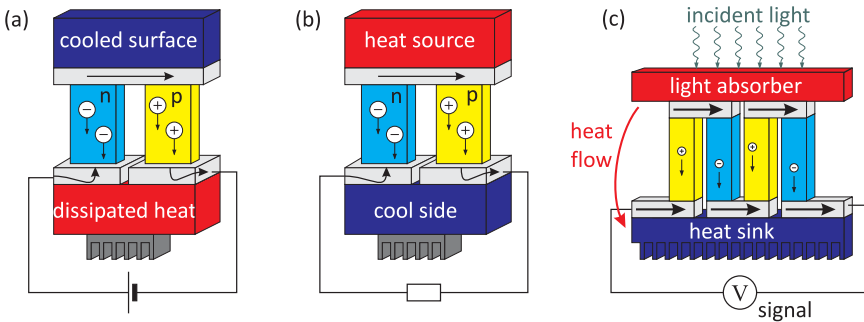
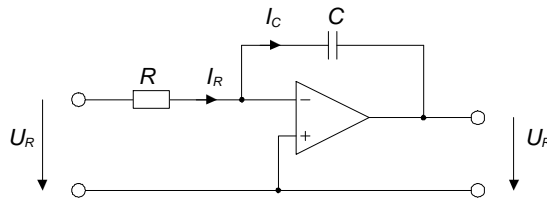


Figure 30.6: (a) Peltier cooler, (b) voltage generator or heat sensor, and (c) heat or radiation sensor with thermocouples connected in parallel.

30.1.5 Exercises

30.1.5.1 Ex: Integrator with operational amplifier

Based on the two golden rules for operational amplifiers, (1)  $I_+ = I_- = 0$  A and (2)  $U_+ = U_-$ , show that the output voltage  $U_a$  at the integrated circuit shown in the figure is:  $U_a = \frac{1}{RC} \int U_e dt$ .



### 30.1.5.2 Ex: Low-pass filter using an OpAmp

Using an inverting operational amplifier design a simple low-pass filter with a constant amplification of 10 at low frequencies and diminishing gain above 10 kHz. Calculate the Bode diagram (i.e. the frequency-dependent gain and phase-shift of your circuit. What is the gain reduction per octave?

### 30.1.6 Experiment: Amplifiers and active filters

Here, we will learn how to use OpAmps: We will start mounting a 10-fold inverting amplifier on a breadboard and then modify the external passive components, such as to build a low-pass filter.

1. Assemble on a breadboard a simple inverting amplifier using an OpAmp. Use 10 k $\Omega$  resistors at the input aim for an amplification factor of 10.
2. Test the circuit with a frequency generator and an oscilloscope.
3. Modify the circuit such as to obtain a low-pass filter with  $f_g = 50$  kHz bandwidth and test the circuit again.

### 30.1.7 Experiment: Peltier element and thermistor

Here, we will learn how to use a Peltier element and a thermistor. A *thermistor* is nothing else than a well-calibrated resistor with temperature-dependent resistance (see Fig. 30.8).

1. Connect a Peltier element to a 1 A current source and bring one of the two surfaces of the Peltier element into thermal contact with a heat sink. What do you observe?
2. Bring a 10k $\Omega$  thermistor in thermal contact with either of the two surfaces of the Peltier element and measure its resistance. What do you observe?
3. Can you imagine a feedback logic evaluating the measured resistance in order to control the current applied to the Peltier element such as to maintain constant the temperature of the surface not connected to the heat sink.

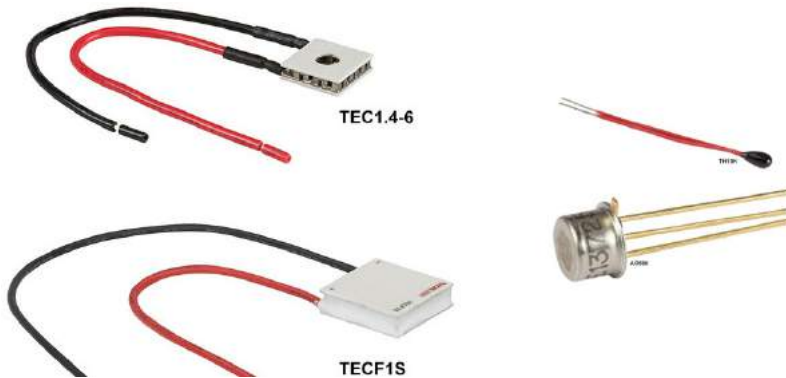


Figure 30.7: Pictures of Peltier elements, a thermistor, and an AD590 temperature transducer.

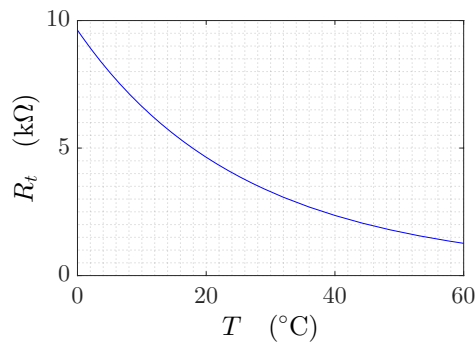


Figure 30.8: Calibration curve for a 10 kΩ thermistor from Thorlabs.

## 30.2 Detectors

### 30.2.1 Photodiodes

Most active components are many of *semiconductor* characterized by a relatively large band gap between the valence band and the conduction band. By appropriate doping of the material with donors (*p*-type) or acceptors (*n*-type) a semiconductor can be made conductive. The most basic semiconductor element, which is the *diode* consists of a junction of two types of semiconductors, as shown in Fig. 30.9.

Our first task will be to construct a *photo detector*. The central part of a photodetector is the photodiode. We have at our disposal silicon *pin*-photodiodes of the type C30822E of the company Perkin Elmer and of the type FFD100.

Photodiodes exploit an intrinsic photoeffect of semiconductor *pn*-junctions. In the transition region, free electrons of the *n*-type semiconductor and excess holes of the *p*-type semiconductor are drifting into the respective opposite semiconductor, where they recombine. The consequence is a transition zone with a charge carrier depletion, which acts as a barrier and has an intrinsic capacitance. The charge carrier imbalance



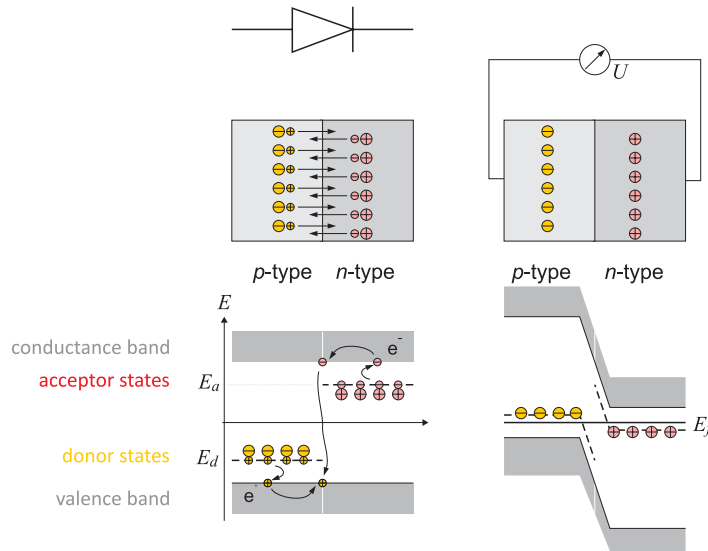


Figure 30.9: Joining a  $p$ -type and a  $n$ -type doped semiconductor (left) one observes a charge carrier redistribution across the  $pn$  transition (right).

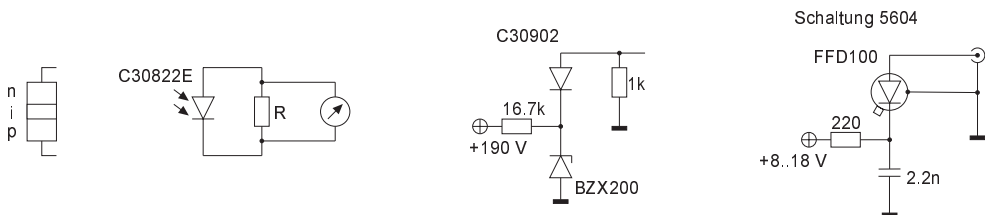


Figure 30.10: Circuit with photodiode.

gives rise to an electric field across the junction. The energy liberated during the recombination process can be dissipated via emission of light.

The reverse process is also possible: Via the intrinsic photoeffect, light irradiated into the  $pn$ -junction can lift electrons from the valence into the conduction band, thus generating pairs of charge carriers. Under the influence of the electric field across the junction, the holes flow to the edge of the  $p$  domain and the electrons flow to the  $n$  domain. This part of the current is called *drift current*. A smaller part, called the *diffusion current*, has its origin in the diffusion of the electron-hole pairs formed in the edge regions. Since these minority charge carriers have only a limited lifetime before they recombine, only the part of the current generated within a few units of the diffusion lengths near the charge carrier zone contributes. This results in an external photovoltaic voltage at the electrodes of the photodiode. If the photodiode is connected to a load, a photocurrent will flow, which is composed, as mentioned above, by the drift current of the charge carrier zone and the diffusion current from its edges.

The principal scheme of a pin diode is illustrated in Fig. 30.11(left): A weakly

doped intrinsic layer separates the  $p$  and the  $n$  conductor. This reduces the capacity of the barrier. The current at short circuit is proportional to the light power. A photodiode is always operated in blocking direction. A negative offset voltage reduces the capacity of the  $pn$ -junction.

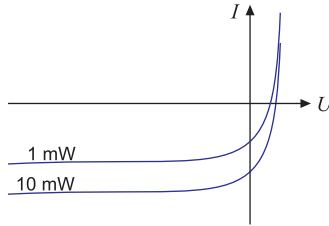


Figure 30.11: (code)  $U$ - $I$  dependence of a photodiode.

Despite all measures the  $pn$ -junction capacity remains finite. One can model the impact of the  $pn$ -junction capacity via a replacement diagram. The voltage drop is

$$\frac{U(\omega)}{U_0} = \frac{R_L \parallel \frac{1}{i\omega C}}{R_i + (R_L \parallel \frac{1}{i\omega C})} = \frac{\frac{R_i \parallel R_L}{R_i}}{1 + i\omega C(R_i \parallel R_L)} \quad (30.9)$$

For high load resistances the frequency response obviously becomes load-independent. For small loads,  $R_L < R_i$ , the band width of the photodiode is dramatically increased to  $\omega_g = 1/R_L C$ . In the same time, however, the amplification drops to  $V = R_L/R_i$ .

### 30.2.2 Exercises

#### 30.2.2.1 Ex: Photomultiplier

The anode of a photomultiplier tube is connected by a resistor of  $R = 1 \text{ k}\Omega$  to ground. The stray capacitance is  $10 \text{ pF}$ , the current amplification  $10^6$ , and the anode rise time  $1.5 \text{ ns}$ . What is the peak amplitude and the halfwidth of the anode output pulse produced by a single photoelectron? What is the dc output current produced by  $10^{-12} \text{ W}$  cw radiation at  $\lambda = 500 \text{ nm}$ , if the quantum efficiency of the cathode is  $\eta = 0.2$  and the anode resistor  $R = 10^6 \text{ }\Omega$ ? Estimate the necessary voltage amplification of a preamplifier (a) to produce  $1 \text{ V}$  pulses for single-photon counting; and (b) to read  $1 \text{ V}$  on a dc meter of the cw radiation?

#### 30.2.2.2 Ex: Optical image intensifier

A manufacturer of a two-stage optical image intensifier states that incident intensities of  $10^{-17} \text{ W}$  at  $\lambda = 500 \text{ nm}$  can still be 'seen' on the phosphor screen of the output state. Estimate the minimum intensity amplification, if the quantum efficiency of the cathodes and the conversion efficiency of the phosphor screens are both  $0.2$  and the collection efficiency of light emitted by the phosphor screens is  $0.1$ . The human eye needs at least  $20 \text{ photons/s}$  to observe a signal.

### 30.2.2.3 Ex: Photovoltaic detector

Estimate the maximum output voltage of an open photovoltaic detector at room temperature under  $10 \mu\text{W}$  irradiation when the photocurrent of the shortened output is  $50 \mu\text{A}$  and the dark current is  $50 \text{nA}$ .

### 30.2.3 Experiment: Taking the response function of a photodiode

In this part of the lab course, we will learn to solder and set up simple electronic circuits. We will also learn how to identify the connections of a photodiode and mount into a case with BNC connectors. Finally, we will characterize the photodiode for use in future applications. Initially, we will work without offset voltage, later we will apply a voltage and identify its impact <sup>1</sup>.

1. Connect an LED to a function generator and make it blink at low frequencies adjusting the offset and the amplitude of the output voltage. Shine the light onto your photodiode and monitor the signal on an oscilloscope. Explain your observations.
2. Reduce the amplitude and adjust the offset until you observe a sinusoidal signal. Increase the frequency and explain your observations. (Note that the response of LEDs is extremely fast (MHz).) Determine the bandwidth of your detector.
3. Measure the current at short circuit. Connect a  $R = 10 \text{k}\Omega$  resistive load in parallel to the photodiode output and measure the voltage drop into this load.
4. Characterize the photodetector with respect to its sensitivity ( $\text{em A/W}$ ) by varying the load.
5. How is the frequency response of the photodiode modified by the load? Measure bandwidth as a function of the load. Adjust the load until the detector (circuit including photodiode and resistor) has a bandwidth of  $10 \text{kHz}$  (which is sufficient for many applications).
6. Apply a  $10 \text{V}$  voltage in reverse direction and analyze again the sensitivity and the bandwidth of your photodetector. Note that the blinking LED can be replaced by a rotating chopper wheel.

## 30.3 Introduction to radiofrequency components

### 30.3.1 VCOs and the generation of rf-sidebands

*Voltage-controlled oscillators* (*VCO*) serve to generate variable radiofrequencies. They are the basis for most function generators. A useful particularity of VCOs is the possibility modulate the frequency and phase of an optical carrier wave by modulating the control voltage of a VCO at low frequency.

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<sup>1</sup>Datasheet for the Photodiode FFD100 see appendix Fig. 34.20, data sheet for the Photodiode C30822E see appendix Fig. 34.21.

The modulation of the carrier wave generates sidebands. This can be seen by expanding the signal which carries the phase modulation into a Fourier series,

$$Ae^{i\omega t+i\beta \sin \Omega t} = Ae^{i\omega t} \sum_{k=-\infty}^{\infty} J_k(\beta)e^{ik\Omega t} \simeq Ae^{i\omega t} + J_1(\beta)Ae^{i\omega t+i\Omega t} + J_{-1}(\beta)Ae^{i\omega t-i\Omega t} \tag{30.10}$$

when the *modulation index*  $\beta$  is small. Here,  $J_{-k}(\beta) = (-1)^k J_k(\beta)$  are the Bessel functions. This is in contrast to amplitude modulation, which is described by only two symmetric sidebands,

$$A(1 + \beta \sin \Omega t) e^{i\omega t} = Ae^{i\omega t} \left( 1 + \frac{\beta}{2i} (e^{i\Omega t} - e^{-i\Omega t}) \right) . \tag{30.11}$$

For *amplitude modulation (AM)* the beat signals between the carrier frequency and the two sidebands are in phase, i.e.,

$$\left| e^{i\omega t} + e^{i(\omega \pm \Omega)t} \right|^2 = 2 + e^{i\Omega t} + e^{-i\Omega t} . \tag{30.12}$$

For *phase modulation (PM)* the beat signal are in counter-phase, i.e.,

$$\left| e^{i\omega t} + e^{i(\omega \pm \Omega)t+i\pi/2} \right|^2 = 2 + ie^{\pm i\Omega t} - ie^{\mp i\Omega t} . \tag{30.13}$$

In the case of AM, the amplitude is blurred, but the phase at zero-crossing is well defined. In the case of PM, the amplitude in the antinode is sharp, but the phase of the zero-crossing is blurred.

It is not easy to transform AM into PM, and vice versa. In fact, the phase between carrier and sidebands can be varied, for example by adding an AC voltage,  $\sqrt{2}e^{i\omega t+3i\pi/4}$  to the signal; however, it is not easy to transform synchronized phases into opposite phases.

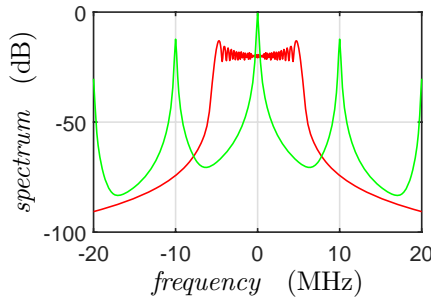


Figure 30.12: (code) Frequency spectra of a phase-modulated carrier frequency for  $\Delta\omega = 5$  MHz modulation excursion and (red)  $\omega = 100$  kHz modulation frequency ( $\beta = \frac{\Delta\omega}{\Omega} = 50$ ) and (green)  $\omega = 10$  MHz modulation frequency ( $\beta = 0.5$ ). Furthermore, a  $\gamma = 100$  kHz resolution linewidth is assumed.

As shown in Eq. (30.10), the spectrum of a signal with phase modulation (PM) consists of discrete lines, called sidebands, whose amplitudes are given by Bessel

functions,

$$S(\omega) = \sum_{k=-\infty}^{\infty} |A\mathcal{J}_k(\beta)|^2 \delta(\omega + k\Omega) . \quad (30.14)$$

In real systems, the sidebands have finite widths  $\gamma$  due to frequency noise or the finite resolution of the detectors. In the case of Lorentzian line profiles, we have,

$$S(\omega) = \sum_{k=-\infty}^{\infty} |A\mathcal{J}_k(\beta)|^2 \frac{\beta^2}{(\omega - k\Omega)^2 + \beta^2} . \quad (30.15)$$

### 30.3.2 Mixers

A *frequency mixer* is a nonlinear electrical circuit that creates new frequencies from two input signals, e.g. the sum and difference of the input frequencies. A device that has a non-linear (e.g. exponential) characteristic can act as a mixer. Passive mixers use one or more diodes and rely on their non-linear relation between voltage and current. Active mixers use an amplifying device (such as a transistor) to increase the strength of the product signal.

Mixers may be classified by their topology: An unbalanced mixer, in addition to producing a product signal, allows both input signals to pass through and appear as components in the output. A single-balanced mixer is arranged with one of its inputs applied to a balanced (differential) circuit so that either the local oscillator (LO) or signal input (RF) is suppressed at the output, but not both. A double-balanced mixer has both its inputs applied to differential circuits, so that neither of the input signals and only the product signal appears at the output. Double balanced mixers are more complex and require higher drive levels than unbalanced and single-balanced designs.

In practice, mixers are widely used to shift signals from one frequency range to another, a process known as *heterodyning*, in order to facilitate signal transmission or further signal processing. Frequency mixers are also used to modulate a carrier signal in radio transmitters, as product detectors, phase detectors, or frequency multipliers.

#### 30.3.2.1 Diode

The non-linearity (or non-Ohmic behavior) of a diode can be used to create a simple unbalanced mixer producing the original frequencies as well as their sum and their difference. The current  $I$  through an ideal diode as a function of the voltage  $U$  across it is given by an exponential function,

$$I = I_0(e^{qU/k_B T} - 1) . \quad (30.16)$$

The exponential can be expanded as  $e^x - 1 \simeq x + \frac{x^2}{2}$ . Suppose that the sum of the two input signals  $U_1 + U_2$  is applied to a diode, and that an output voltage is generated that is proportional to the current through the diode [e.g. by providing the voltage that is present across a resistor in series with the diode, as shown in Fig. 30.13(a)]. Then, disregarding the constants in the diode equation, the output voltage will have the form,

$$\begin{aligned} U_0 &= (U_1 + U_2) + \frac{1}{2}(U_1 + U_2)^2 + \dots \\ &= (U_1 + U_2) + \frac{1}{2}(U_1^2 + 2U_1U_2 + U_2^2) + \dots \end{aligned} \quad (30.17)$$

The ellipsis represents all the higher powers of the sum which we assume to be negligible for small signals.

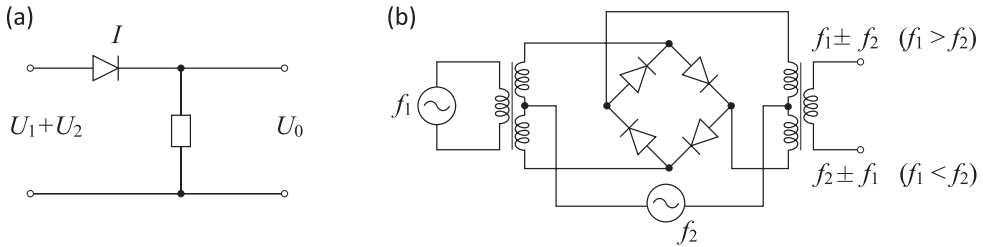


Figure 30.13: (a) Mixing two signal at a diode. (b) Schematic diagram of a double-balanced passive diode mixer (also known as a ring modulator). There is no output unless both  $f_1$  and  $f_2$  inputs are present, though  $f_2$  (but not  $f_1$ ) can be DC.

Suppose that two input sinusoids of different frequencies,  $U_1 = \sin \omega_1 t$  and  $U_2 = \sin \omega_2 t$  are fed into the diode. The signal  $U_0$  becomes:

$$U_0 = (\sin \omega_1 t + \sin \omega_2 t) + \frac{1}{2}(\sin^2 \omega_1 t + 2 \sin \omega_1 t \sin \omega_2 t + \sin^2 \omega_2 t) + \dots \quad (30.18)$$

Ignoring all terms except for the  $\sin \omega_1 t \sin \omega_2 t$  term we get,

$$U_0 = 2 \sin \omega_1 t \sin \omega_2 t + \dots = \cos(\omega_1 t - \omega_2 t) - \cos(\omega_1 t + \omega_2 t) + \dots, \quad (30.19)$$

demonstrating how new frequencies are created from the mixer.

### 30.3.2.2 Switching

Another form of mixer operates by switching, with the smaller input signal being passed inverted or non-inverted according to the phase of the local oscillator (LO). This would be typical of the normal operating mode of a packaged double balanced mixer, with the local oscillator drive considerably higher than the signal amplitude.

The aim of a switching mixer is to achieve linear operation over the signal level by means of hard switching, driven by the local oscillator. Mathematically, the switching mixer is not much different from a multiplying mixer. Instead of the LO sine wave term, we would use the signum function. In the frequency domain, the switching mixer operation leads to the usual sum and difference frequencies, but also to further terms, e.g.  $\pm 3f_{LO}$ ,  $\pm 5f_{LO}$ , etc.. The advantage of a switching mixer is that it can achieve (with the same effort) a lower noise figure and larger conversion gain. This is because the switching diodes or transistors act either like a small resistor (switch closed) or large resistor (switch open), and in both cases only a minimal noise is added. From the circuit perspective, many multiplying mixers can be used as switching mixers, just by increasing the LO amplitude.

### 30.3.2.3 Modulation and demodulation

Mixers are often used for modulation or demodulation purposes. Suppose we have on one hand a *carrier* signal,  $U_{carrier} = \cos \omega t$ , also called *local oscillator*. This may be a constant radiofrequency emitted by an antenna or a microwave. On the other hand,

we have a reference signal which we want to transport somewhere else,  $U_{ref} = \cos \Omega t$ . Used as a modulator the mixer will simply multiply,

$$U_{mod} = U_{carrier} U_{ref} = \cos \omega t \cos \Omega t = \frac{1}{2} \cos[(\omega - \Omega)t] + \frac{1}{2} \cos[\omega + \Omega)t] . \quad (30.20)$$

Thus the mixer output contains two frequencies, the sum and the difference. Supposing that  $\omega$  is a frequency in a range that can be radiated by antenna and  $\Omega$  an acoustic frequency, both frequency components  $\omega \pm \Omega \simeq \omega$  will be radiated.



Figure 30.14: Picture of a radiofrequency mixer.

On the side of the receiver, who also has access to a synthesizer generating a signal  $U_{carrier} = \cos \omega t$ , we will use the mixer as a demodulator,

$$U_{demod} = U_{carrier} U_{mod} = \cos^2 \omega t \cos \Omega t = \frac{1}{2} (\cos 2\omega t + 1) \cos \Omega t . \quad (30.21)$$

If  $\omega \gg \Omega$ , the carrier oscillation can easily be removed by a low-pass filter,

$$U_{filtered} = \frac{1}{2} \cos \Omega t \propto U_{ref} . \quad (30.22)$$

That is, we recover the original information. And this holds even when the reference signal is (slowly) varying in amplitude or frequency, such as in the case of an acoustic signal<sup>2</sup>. Resolve Exc. 30.3.3.1.

### 30.3.2.4 Filtering with a mixer

Suppose we have a signal containing many frequency components (which may vary slowly in time),  $U_{noisy}(t) = \sum_n A(\omega_n) e^{i\omega_n t}$  in complex notation, and that the signal we are interested in is an amplitude at a known particular frequency  $\omega_0$ . By demodulating,

$$U_{sig}(t) = U_{noisy}(t) e^{-i\omega_0 t} = \sum_n A(\omega_n) e^{i\omega_n t} e^{-i\omega_0 t} = \sum_n A(\omega_n) e^{i(\omega_n - \omega_0)t} , \quad (30.23)$$

and low-pass filtering the lowest frequency component, i.e.  $\omega_n - \omega_0 \simeq 0$ ,

$$U_{filtered} = A(\omega_0) . \quad (30.24)$$

This even holds for continuous noise spectra,  $U_{noisy}(t) = \int A(\omega) e^{i\omega t} d\omega$ , since,

$$U_{sig}(t) = U_{noisy}(t) e^{-i\omega_0 t} = \int_{-\infty}^{\infty} A(\omega) e^{i\omega t} e^{-i\omega_0 t} d\omega = \int_{-\infty}^{\infty} A(\omega + \omega_0) e^{i\omega t} d\omega , \quad (30.25)$$

<sup>2</sup>In complex notation,  $U_{in} = e^{i\omega t}$ ,  $U_{mod} = U_{in} e^{i\Omega t} = e^{i(\omega + \Omega)t}$ ,  $U_{demod} = U_{mod} e^{-i\omega t} = e^{i\Omega t}$ .

and low-pass filtering with a filter bandwidth  $\Delta\omega$ ,

$$U_{filtered} = \int_{-\Delta\omega}^{\Delta\omega} A(\omega + \omega_0) e^{i\omega t} d\omega \simeq A(\omega_0) 2\Delta\omega. \quad (30.26)$$

Such techniques are widely used in lock-in amplifiers (see Sec. 30.4.3).

### 30.3.3 Exercises

#### 30.3.3.1 Ex: Phase modulation

- Show that it is not possible to construct a periodic phase modulation function such that the signal has only two sidebands.
- Compare the spectra  $\sum_{k=-\infty}^{\infty} J_k(M) e^{ik\Omega t} = e^{iM \sin \Omega t}$  and  $\sum_{k=-\infty}^{\infty} |J_k(M)| e^{ik\Omega t}$ . Can you detect phase modulation of a photodetector signal on a spectrum analyzer? How about amplitude modulation?

### 30.3.4 *Experiment: Creating sidebands on a radiofrequency*

In this exercise, we will understand the origin of sidebands as we'll see them emerge from a modulation spectrum when we gradually increase the modulation index <sup>3</sup>.

- Take a VCO, for example, ZOS-100+ from MiniCircuits. Study the datasheet and drive the VCO with an AC voltage. Vary the amplitude and the frequency of the voltage and observe the output signal of the VCO on a spectrum analyzer.
- Try to understand the spectrum observing the limiting cases  $\Omega \gg \Delta\omega$  and  $\Omega \ll \Delta\omega$ . How can you read  $\Omega$  and  $\Delta f$  from the spectra in both cases?
- Write a MATLAB program to simulate the spectrum.

## 30.4 Measurement instrumentation

### 30.4.1 Sample-and-hold circuit

*sample-and-hold circuit* Solder on euroboard

### 30.4.2 Box-car integrator

*box-car integrator* Solder on euroboard

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<sup>3</sup>Datasheet for the VCO see appendix Fig. 34.15,  
data sheet for the variable attenuator see appendix Fig. 34.16,  
data sheet for the mixer see appendix data sheet Fig. 34.18.



### 30.4.3 Lock-in amplifier

An *lock-in amplifier* (also called a phase-sensitive rectifier or *mixer*) is an amplifier that can measure a weak electrical signal by modulating the signal by a reference signal with a known frequency and phase. The device represents a bandpass filter with an extremely narrow bandwidth and, therefore, improves the signal-to-noise ratio (SNR). DC or AC noise components are efficiently filtered.

Download an illustration of the working principle of a *lock-in amplifier* here.

### 30.4.4 Experiment: Building a lock-in amplifier

Let's now build a lock-in amplifier. The principle is illustrated in Fig. 30.15(a). The sinusoidal signal discriminated at a non-linear line is switched on and off in the lock-in by a switch. At the same time, the inverted signal (i.e., phase shifted by  $180^\circ$ ) is turned off and on. Both signals are combined and low-pass filtered. As Fig. 30.15(b) shows, the sign of the filtered signal depends on the phase between the discriminator and the TTL signal controlling the switch <sup>4</sup>

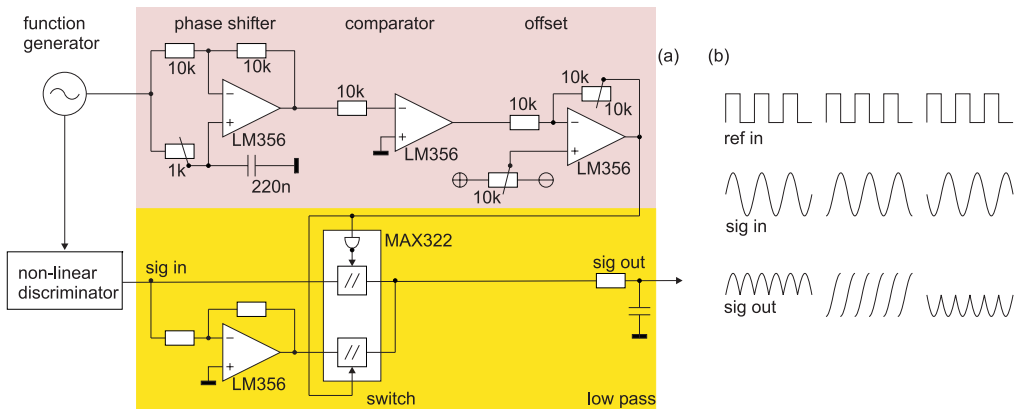


Figure 30.15: (a) Principal scheme of a lock-in amplifier. (b) Mode of operation.

1. Create the circuit sketched in Fig. 30.15(a) on a circuit board and test it by varying the phase between the modulated output signal and the TTL signal provided by a function generator.

## 30.5 Further reading

P. Horowitz et al., *The art of electronics* [DOI]

U. Tietze et al., *Halbleiterschaltungstechnik* [DOI]

<sup>4</sup>Datasheets for the operational amplifier see appendix Fig. 34.23, data sheet for the switch see appendix Fig. 34.22.

# Chapter 31

## Quantum optics and optical interferometry

The objective of this chapter is to introduce the basics of optical *interferometry*. We will see, how to match the light modes in optical cavities and fibers, and to phase-match the wavefronts of two laser beams in order to detect their frequency beating with a photodetector. Furthermore, he will learn how to handle essential tools of *quantum electronics*, such as a piezo-electric transducer, an electro-optic modulator, and an acousto-optic modulator, used in interferometry, as discussed in Secs. 31.4.1 to 31.4. Interferometers have versatile applications such as 1. for the detection of very small length variations (as for example caused by gravitational waves), 2. as vibration and inertial sensors, or in 3. the transmission of information (radio).

### 31.1 Introduction to interferometry

#### 31.1.1 Beam splitter

The essential component of any interferometer is the (non-polarizing) *beam splitter*.

We consider a classical lossless beam splitter with electric fields incident at both its inputs. The two output fields  $E_c$  and  $E_d$  are linearly related to the inputs through

$$\begin{pmatrix} \mathcal{E}_c \\ \mathcal{E}_d \end{pmatrix} = \begin{pmatrix} r_{ac} & t_{bc} \\ t_{ad} & r_{bd} \end{pmatrix} \begin{pmatrix} \mathcal{E}_a \\ \mathcal{E}_b \end{pmatrix}, \quad (31.1)$$

where the  $2 \times 2$  element is the beam splitter matrix.  $r$  and  $t$  are the reflectance and transmittance along a particular path through the beam splitter, that path being indicated by the subscripts.

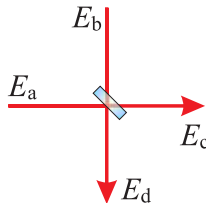


Figure 31.1: Beam splitter.

Assuming the beam splitter removes no energy from the light beams, the total output energy can be equated with the total input energy, reading

$$|\mathcal{E}_c|^2 + |\mathcal{E}_d|^2 = (|r_{ac}||\mathcal{E}_a| + |t_{bc}|\mathcal{E}_b)^2 + (|t_{ad}||\mathcal{E}_a| + |r_{bd}||\mathcal{E}_b)^2 = |\mathcal{E}_a|^2 + |\mathcal{E}_b|^2 . \quad (31.2)$$

This can only be true for any field amplitudes, if the following relationships between reflectance and transmittance are satisfied,

$$|r_{ac}|^2 + |t_{ad}|^2 = 1 = |r_{bd}|^2 + |t_{bc}|^2 \quad \text{and} \quad r_{ac}t_{bc}^* + t_{ad}r_{bd}^* = 0 . \quad (31.3)$$

We write each  $r$  and  $t$  as a complex number having an amplitude and phase factor accounting for possible phase shifts of a beam as it reflects or transmits at the beam splitting surface. From the second equation (31.3) we obtain,

$$\frac{|r_{ac}|}{|t_{ad}|} = -\frac{|r_{bd}|}{|t_{bc}|} e^{i(\phi_{ad} - \phi_{bd} + \phi_{bc} - \phi_{ac})} \quad (31.4)$$

which is true when  $\phi_{ad} - \phi_{bd} + \phi_{bc} - \phi_{ac} = \pi$ . Squaring both sides of the expression (31.4) and comparing this with the first equation (31.3) we obtain the result

$$|t_{ad}| = |t_{bc}| \equiv \sqrt{T} \quad \text{and} \quad |r_{ac}| = |r_{bd}| \equiv \sqrt{R} . \quad (31.5)$$

It follows that

$$\boxed{R + T = 1} . \quad (31.6)$$

The above result holds for any type of beam splitting device. For beam splitting at dielectric interfaces in particular we know that the electric field amplitude does not suffer phase shifts upon transmission and no phase shifts upon reflection at an optical more dilute medium. But it suffers a  $180^\circ$  phase shift upon reflection at an optical denser medium. For the situation depicted in Fig. 31.1, we conclude  $\phi_{ac} = \phi_{bd} = \phi_{bc} = 0$  and  $\phi_{ad} = \pi$ . With this constraints the matrix describing a lossless beam splitter reads,

$$\boxed{\begin{pmatrix} \mathcal{E}_c \\ \mathcal{E}_d \end{pmatrix} = \begin{pmatrix} \sqrt{R} & \sqrt{T} \\ -\sqrt{T} & \sqrt{R} \end{pmatrix} \begin{pmatrix} \mathcal{E}_a \\ \mathcal{E}_b \end{pmatrix}} . \quad (31.7)$$

### 31.1.2 Piezo-electric actuator

The piezo-electricity effect describes the reciprocal action between mechanical pressure (from Greek: *piézein* - press) and electrical voltage in solids. It is based on the phenomenon that occurs in the regular deformation of certain piezoelectric materials: at the surface occur displacements of electric charges creating microscopic dipoles inside the unit cells. The sum over all the unit cells of the crystal leads to a macroscopically measurable electrical voltage. The deformation should be directed, which means, that the pressure is not applied from all sides on the crystal, but for example only on opposite sides.

On the other hand, by applying an electric voltage, a crystal (or piezo-ceramic element) may be deformed. Like any other solid body, piezo-electric crystals can execute mechanical vibrations. In a *piezo-electric actuator* (or piezo transducer PZT), these vibrations can be electrically excited. The frequency of the vibrations depend

only on the speed of sound (which is a constant of the material) and the dimensions of the actuator. Therefore, actuators are also suitable for realizing oscillators (for example, quartz crystals). The piezo-electric effect can only occur in non-conductive materials (e.g., lead titanate zirconate).

When a voltage is applied to the piezo-ceramic in the direction of polarization, we observe an expansion in this direction and a perpendicular contraction. Depending on the employed material and the coefficient for piezo-electric strain  $d$ , stretches up to  $\Delta l/l = 0.15\%$  can be obtained:

$$\Delta l = d\mathcal{E}l_0 , \quad (31.8)$$

where  $l_0$  is the length of the actuator and  $E = U/l_0$  the amplitude of the electric field. The elongation effect is therefore proportional to the field strength and the overall length of the actuator. To achieve large stretches with manageable electrical voltages, actuator discs are often stacked (mechanical circuit in series and electric circuit in parallel).

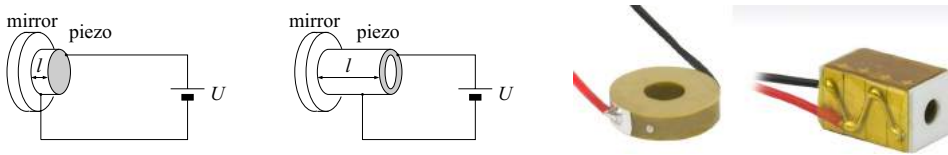


Figure 31.2: (Left) Scheme of mirrors mounted on a piezo actuator having the shape of a disc or a ring. (Right) Photos of a ring piezo and a piezo stack.

Negative voltages with respect to the orientation of the discs cause a contraction. However, negative voltages can also cause a change in the polarization state of the piezo and should therefore be avoided! In electrical circuits, piezoelectric actuators introduce a capacitance with a relative dielectric constant between 600 and 5000 and an internal resistance of about  $10^8 \Omega$  depending on the material. See Exc. 31.1.10.1.

### 31.1.3 Michelson and Mach-Zehnder interferometer

Interferometry is a technique exploiting the interference of waves coherently split and recombined by beam splitters. Sufficiently stable interferometers allow to visualize variations of the path lengths of two or more partial waves following different pathways as an alteration of constructive and destructive interference.

The two most common types of interferometers are the *Michelson interferometer* and the *Mach-Zehnder interferometer* are depicted in Fig. 31.3. The advantages of the Michelson interferometer are an easy alignment and the need of only one beamsplitter. The advantage of the Mach-Zehnder interferometer is a direct optical access to both output ports of the interferometer. The following treatment applies to both types.

The field amplitude of a laser beam,  $\mathcal{E}_i$ , with frequency,  $\omega = ck$ , is divided by a beam splitter (reflectivity  $\sqrt{R}$ ) into a transmitted  $\mathcal{E}_t$  and a reflected beam  $\mathcal{E}_r$ ,

$$\mathcal{E}_r = \sqrt{R_1}\mathcal{E}_i \quad \text{and} \quad \mathcal{E}_t = \sqrt{1 - R_1}\mathcal{E}_i , \quad (31.9)$$

where we disregard possible phase-shifts upon reflection at optically dilute interface. The energy is obviously conserved,  $|\mathcal{E}_r|^2 + |\mathcal{E}_t|^2 = \mathcal{E}_i^2$ .

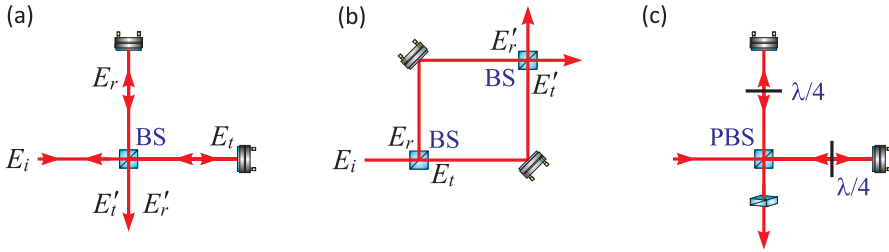


Figure 31.3: Principle of a two-beam interferometer: (a) Michelson interferometer and (b) Mach-Zehnder interferometer using non-polarizing beamsplitters. (c) Michelson interferometer using a polarizing beamsplitter.

We consider the Mach-Zehnder interferometer sketched in Fig. 31.3 with one arm of length  $L_r$ , which can be varied by a piezo, and the other arm of length  $L_t$ ,

$$\mathcal{E}'_r = \mathcal{E}_r e^{2ikL_r} \quad \text{and} \quad \mathcal{E}'_t = \mathcal{E}_t e^{2ikL_t} . \quad (31.10)$$

The beams are recombined on a second beam splitter and sent to a photodetector, whose signal is,

$$\begin{aligned} I &\propto |\sqrt{R_2}\mathcal{E}'_r + \sqrt{1-R_2}\mathcal{E}'_t|^2 \\ &= |\sqrt{R_2}\sqrt{R_1}e^{2ikL_r} + \sqrt{1-R_2}\sqrt{1-R_1}e^{2ikL_t}|^2 \mathcal{E}_i^2 . \end{aligned} \quad (31.11)$$

Hence,

$$I \propto R_2 R_1 + (1-R_2)(1-R_1) + 2\sqrt{R_2}\sqrt{R_1}\sqrt{1-R_2}\sqrt{1-R_1} \cos[2k(L_t - L_r)] . \quad (31.12)$$

For reflectivities of  $R_1 = R_2 = 50\%$ , we get,

$$I \propto \frac{1}{2} + \frac{1}{2} \cos[2k(L_t - L_r)] . \quad (31.13)$$

It is important to realize that, while superpositions of light field amplitudes in the same mode interfere, *superpositions of light field amplitudes in different modes do not*. For example, the superposition of two plane waves with equal frequency and polarization interferes,

$$\left| \begin{pmatrix} \mathcal{E}_1 + \mathcal{E}_2 \\ 0 \end{pmatrix} \right|^2 = |\mathcal{E}_1 + \mathcal{E}_2|^2 , \quad (31.14)$$

while the superposition of two plane waves with equal frequency but different polarizations does not,

$$\left| \begin{pmatrix} \mathcal{E}_1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \mathcal{E}_2 \end{pmatrix} \right|^2 = |\mathcal{E}_1|^2 + |\mathcal{E}_2|^2 . \quad (31.15)$$

Solve the Excs. 31.1.10.2 to 31.1.10.4.

### 31.1.4 Coherence and spectrum of a light field

We have seen above that interferometers probe the electric field amplitude rather than the intensity. For this reason, they are suited to measure the first-order correlation function  $g^{(1)}(\tau)$  and the emission spectrum, which are defined by,

$$g^{(1)}(\tau) \equiv \frac{\langle \mathcal{E}^-(t)\mathcal{E}^+(t+\tau) \rangle}{\langle \mathcal{E}^-(t)\mathcal{E}^+(t) \rangle} \quad \text{and} \quad S_{\mathcal{E}}(\omega) \equiv \mathcal{F}[g^{(1)}(\tau)]. \quad (31.16)$$

As an example, Fig. 31.4 shows the aurocorrelation function and spectrum of a simultaneously amplitude- and phase-modulated laser beam,  $\mathcal{E}(t) = (1+n \cos \omega_n t)e^{im \sin \omega_m t}$ .

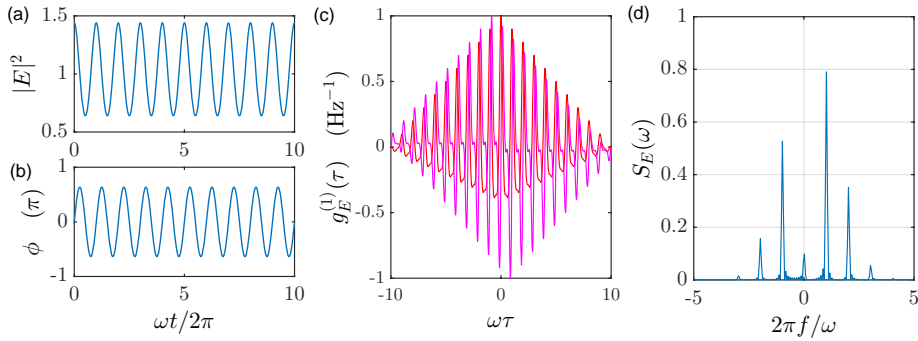


Figure 31.4: (code) (a) Amplitude and (b) phase of the electric field, with  $n = 0.2$ ,  $m = 1$ , and  $\omega_n = \omega_m = (2\pi) 1$  Hz. (c) Aurocorrelation function and (d) spectrum of the light field.

### 31.1.5 Birefringent interferometer

A *birefringent interferometer* or *Lyot filter* consists of one or more birefringent crystals mounted onto a rotation frame between two polarizers. Let  $n_o$  and  $n_e = n_o + \Delta n$  be the refractive indices of the normal and the extraordinary axis, respectively. The corresponding Jones matrix is then,

$$\mathcal{M} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} e^{ik_o L} & 0 \\ 0 & e^{ik_e L} \end{pmatrix} \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (31.17)$$

Such that,

$$\begin{pmatrix} \mathcal{E}_{out} \\ 0 \end{pmatrix} = \mathcal{M} \begin{pmatrix} \mathcal{E}_{in} \\ 0 \end{pmatrix} = \begin{pmatrix} (e^{ik_o L} \cos^2 \phi + e^{ik_e L} \sin^2 \phi) \mathcal{E}_{in} \\ 0 \end{pmatrix}. \quad (31.18)$$

By trigonometric transformations it is possible to show, that the transmission  $T \equiv |\mathcal{E}_{out} / \mathcal{E}_{in}|^2$  is,

$$\boxed{T(\lambda, \phi) = |e^{ik_o L} \cos^2 \phi + e^{ik_e L} \sin^2 \phi|^2 = 1 - \sin^2 2\phi \sin^2 \frac{\pi L \Delta n}{\lambda}}. \quad (31.19)$$

For  $\phi = 45^\circ$  the transmission becomes simply,

$$T(\lambda, \frac{\pi}{4}) = \cos^2 \frac{\pi L \Delta n}{\lambda} . \quad (31.20)$$

In practice Lyot filters are often used, placed under the Brewster angle inside ring cavity lasers, as frequency selective elements. Frequently, birefringent plates of different thicknesses are stacked,

$$T(\lambda) = T_1(\lambda)T_2(\lambda) , \quad (31.21)$$

in order to increase the frequency selectivity. Furthermore, when the axis of the birefringent plates are rotated by fixed angles  $\Delta\alpha$  with respect to each other,

$$T(\lambda, \alpha) = T_1(\lambda, \alpha)T_2(\lambda, \alpha + \Delta\alpha) , \quad (31.22)$$

the frequency of maximum transmission can be tuned by simply rotating the stack as a whole by an angle  $\alpha$ . See 31.1.10.5.

A Lyot filter can be considered an interferometer, because it splits and recombines the polarization vector of a light beam in two parts following the ordinary and the extraordinary axis of the birefringent crystal. This is somewhat analogous to the Michelson interferometer depicted in Fig. 31.3(c).

### 31.1.6 Optical resonators

Optical cavities consist of an arrangement of mirrors reflecting the light beams in such a way, that they form a closed path. Since light that entered the cavity is performing there many round trips before it is transmitted again or absorbed, the light power is considerably enhanced, i.e. cavities can store light.

Light which is to resonate in the cavity must satisfy the boundary condition, that the mirror surfaces coincide with standing wave nodes. Therefore, in a cavity with length  $L$  only a discrete spectrum of wavelengths  $N\frac{\lambda}{2} = L$  can be resonantly amplified, where  $N$  is a natural number. Because of this property, cavity are often used as frequency filters or optical spectrum analyzers: Only frequencies  $\nu = N\delta_{f_{sr}}$  are transmitted, where

$$\boxed{\delta_{f_{sr}} = c/2L} \quad (31.23)$$

is the free spectral range of the cavity.

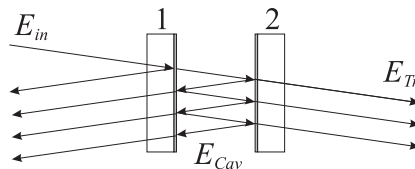


Figure 31.5: Multiple interference in an optical cavity.

Cavities are characterized on one hand by their geometry, i.e. the curvature and the distance of their mirrors, and on the other hand by their finesse, which is given by the reflectivity of their mirrors. Let us first study the finesse. Regarding the cavity as a multipass interferometer [186], we can derive expressions for the reflected and

transmitted intensity as a function of frequency <sup>1</sup>. The so-called *Airy formula* for transmission and reflection are,

$$\frac{\mathcal{E}_{refl}}{\mathcal{E}_{in}} = r_1 - \frac{t_1^2 r_2 e^{2ikL}}{1 - r_1 r_2 e^{2ikL}} \quad \text{and} \quad \frac{\mathcal{E}_{trns}}{\mathcal{E}_{in}} = \frac{t_1 t_2 e^{ikL}}{1 - r_1 r_2 e^{2ikL}}. \quad (31.24)$$

In terms of intensity, assuming identical mirrors,  $r_1 = r_2 = \sqrt{R}$  and  $t_1 = t_2 = \sqrt{T}$ , and neglecting possible absorptive losses,  $A = 1 - R - T = 0$ ,

$$\boxed{\frac{I_{refl}}{I_{in}} = \frac{\left(\frac{2F}{\pi}\right)^2 \sin^2 \frac{\Delta}{2\delta_{f_{sr}}}}{1 + \left(\frac{2F}{\pi}\right)^2 \sin^2 \frac{\Delta}{2\delta_{f_{sr}}}} \quad \text{and} \quad \frac{I_{trns}}{I_{in}} = \frac{1}{1 + \left(\frac{2F}{\pi}\right)^2 \sin^2 \frac{\Delta}{2\delta_{f_{sr}}}},} \quad (31.25)$$

where  $R$  is the reflectivity of a mirror and  $\delta = 4\pi L/\lambda = 2\pi\nu/\delta_{f_{sr}}$ . The transmission curve of a cavity has a finite transmission bandwidth  $\Delta\nu$ , which depends on the reflectivity of the mirrors. The finesse of a cavity is defined by

$$\boxed{F \equiv \frac{2\pi\delta_{f_{sr}}}{\kappa} = \frac{\pi\sqrt{R}}{1-R}}. \quad (31.26)$$

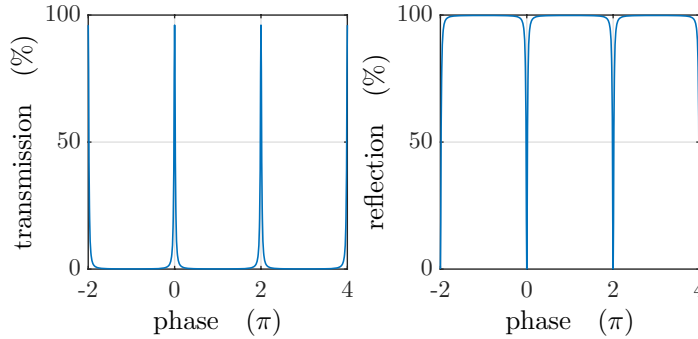


Figure 31.6: (code) Transmission and reflection through a resonator.

Note that factors others than the finite reflectivity may degrade the finesse of a cavity. For example, an imperfect mirror flatness (commonly specified as  $\lambda/F_{surf}$ ) reduces the finesse to [186],

$$F_{tot} = \left( \frac{1}{F} + \frac{1}{F_{surf}} \right)^{-1}. \quad (31.27)$$

The geometry of a cavity must satisfy certain conditions, in order to be stable [402]. Besides the main longitudinal modes a cavity possesses transverse modes of the order  $TEM_{mn}$ , whose frequencies are given by <sup>2</sup>,

$$\nu/\delta_{f_{sr}} = (q+1) + \frac{m+n+1}{\pi} \arccos \sqrt{\left(1 - \frac{L}{\rho_1}\right) \left(1 - \frac{L}{\rho_2}\right)}. \quad (31.28)$$

<sup>1</sup>See script on *Electrodynamics* (2020), Exc. 7.3.6.16.

<sup>2</sup>See script on *Electrodynamics* (2020), Sec. 7.4.2.2.



A *confocal cavity* with degenerate transverse modes,  $\rho_1 = \rho_2 = L$ , is particularly suited as optical spectrum analyzer.

The diameter of the beam waist in the cavity is,

$$w_0 = \sqrt[4]{\left(\frac{\lambda}{\pi}\right)^2 \frac{L(\rho_1 - L)(\rho_2 - L)(\rho_1 + \rho_2 - L)}{(\rho_1 + \rho_2 - 2L)^2}}. \quad (31.29)$$

For an optimal coupling of the light into the cavity the Gaussian laser beam must be matched to the cavity's geometry of the cavity, i.e. diameter and divergence of the laser beam must be adapted to the cavity mode with a suitable arrangement of lenses [187, 402]. See Excs. 31.1.10.6 to 31.1.10.11.

### 31.1.7 Dielectric mirrors and filters

*Dielectric mirrors* and filters are multiple beam interferometers in a similar sense as Fabry-Pérot cavities. They consist of stacks of thin dielectric layers with alternating refraction indices <sup>3</sup>.

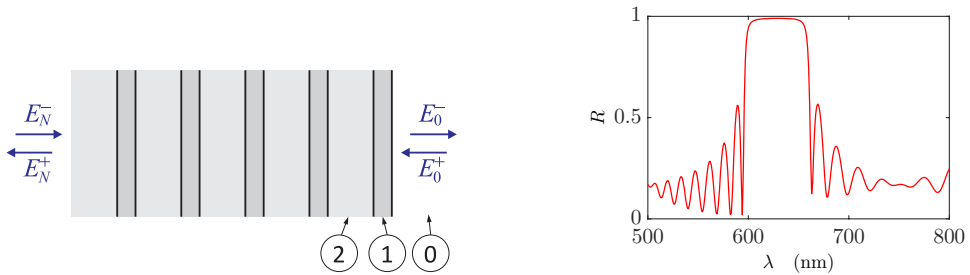


Figure 31.7: (code) Reflection by a high reflecting mirror made of 10 layers with  $n_1 = 2.4$  and  $\Delta z_1 = 80$  nm alternating with 10 layers with  $n_2 = 1.5$  and  $\Delta z_2 = 500$  nm. The absorption coefficient for each layer is supposed to be  $\alpha = 0.2\%$ . The beam impinges from vacuum,  $n_0 = 1$ .

Reflections of  $R = 99.999\%$  can be reached which, applied of superpolished mirrors, allow for the construction of cavities with finesse  $F > 300000$ . On the other anti-reflection coatings can be applied to surfaces reducing their reflections to below  $R = 0.1\%$ . See Excs. 31.1.10.12 and 31.1.10.13 [187, 433].

### 31.1.8 Optical fibers

An *optical fiber* is a waveguide in which light is guided by internal total reflection. The total reflection occurs between layers with different refractive indices called *fiber core* and *fiber cladding*. The core is the central region of the optical fiber where the light is guided. In order to create guiding conditions, the refractive index of the core must be higher than the one of the cladding. The cladding diameter is typically 8 to 10 times the *mode field diameter* (MFD) of the fundamental mode. In general, MFD

<sup>3</sup>See script on *Electrodynamics* (2020), Sec. 7.1.7.

is greater than the physical diameter of the fiber core, which means that some optical power is always guided by the fiber cladding as an evanescent wave.

The *cut-off wavelength*  $\lambda_{co}$  of an optical fiber is the wavelength above which a guided mode of a waveguide ceases to exist. For wavelength longer than  $\lambda_{co}$  an optical fiber becomes single-mode. At wavelengths shorter than  $\lambda_{co}$  several optical modes may propagate and the fiber becomes multi-mode. The cut-off wavelength is directly related to the core diameter of the fiber  $\lambda_{co} \propto \emptyset$ . For

$$\frac{\lambda}{2} < \emptyset < \lambda \quad \text{or equivalently} \quad \emptyset < \lambda < 2\emptyset \quad (31.30)$$

the fiber is single-mode. For  $\lambda > 2\emptyset$  no guided mode exists and for  $\emptyset > \lambda$  the fiber becomes multimode.

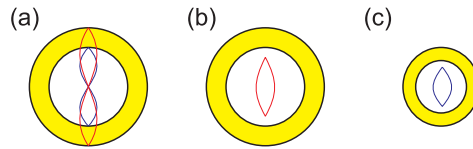


Figure 31.8: Mono-mode waveguiding by optical fibers.

The *numerical aperture* is a measure of the acceptance angle of the fiber. It is very important because it determines how strongly a fiber guides light, and so how resistant it is to bend-induced losses. The numerical aperture can be defined by the acceptance angle of the fiber, though as this is highly diverging in space it is rather complicated to reach a simple definition. It is most convenient to define the NA in terms of the relative indices of core and cladding glass forming the fiber waveguide:

$$NA = \sin \frac{\theta_a}{2} = \sqrt{n_{core}^2 - n_{clad}^2} \simeq \sqrt{2n_{core}^2 \delta n}, \quad (31.31)$$

where  $\delta n$  is the index difference between the core and cladding. An optical fiber with 'high' numerical aperture will confine light more strongly in the core, and so support guidance further above cut-off. This attribute has two important effects: (a) it will be single-mode over a greater range of wavelengths than is possible with a fiber with a 'low' numerical aperture fiber and (b) it will still guide a single-mode when coiled or bent to a smaller diameter.

### 31.1.8.1 Multi-mode, mono-mode, and polarization maintaining fibers

Many types of fibers are currently available for a large variety of applications.

### 31.1.9 Laser gyroscope and the Sagnac effect

*Gyroscopes* are based on the *Sagnac effect*. They are based on a ring cavity mounted on a rotating stage, as shown in Fig. 31.10(a). Let us, for simplicity first consider a circular path for the light beam (e.g. a fiber-based ring cavity) rotating at an angular velocity  $\Omega$ . Then the time needed for the light beam to travel in either one of the two directions is,

$$t_{\pm} = \frac{(2\pi \pm \Omega t_{\pm})r}{c} = \frac{2\pi r}{c \mp \Omega r}, \quad (31.32)$$

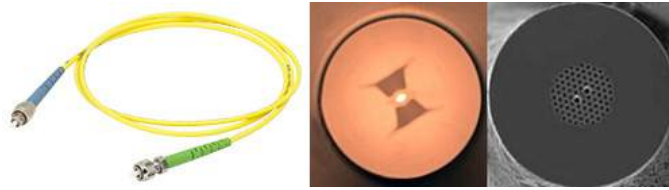


Figure 31.9: (Left) Fiber patch cord, (center) cross section of a bow-tie polarization maintaining fiber, and (right) cross section of a photonic crystal fiber.

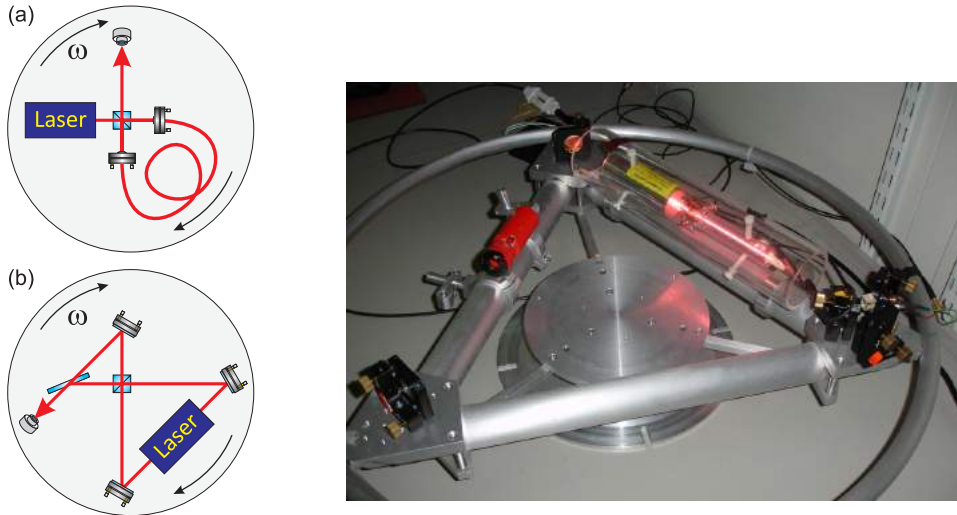


Figure 31.10: (a) Principle scheme of a fiber-based Sagnac interferometer. (b,c) Laser gyroscope realized with a HeNe gain tube.

that is,

$$\Delta t \equiv t_+ - t_- = \frac{4\pi r^2 \Omega}{c^2 - \Omega^2 r^2} \simeq \frac{4\pi r^2 \Omega}{c^2} \equiv \frac{4A\Omega}{c^2}, \quad (31.33)$$

where  $A$  is the area enclosed by the path. This formula can be generalized to arbitrary paths.

For example, assuming an interferometer with  $A = 1 \text{ m}^2$  at rest in an Earth-based system,  $\Omega \simeq 2\pi/24 \text{ h}$ , the time difference for light propagating along the two directions is  $\Delta t \approx 3 \cdot 10^{-21} \text{ s}$  and the path difference  $\Delta L = c\Delta t \approx 100 \text{ fm}$ . The frequency shift is,

$$\Delta\nu = k(v_+ - v_-) = k(2\Omega r) = \frac{\sqrt{4\pi A}\Omega}{\lambda}, \quad (31.34)$$

yielding for the given example of an Earth-based interferometer  $\Delta\nu \approx 400 \text{ Hz}$ .

### 31.1.10 Exercises

**31.1.10.1 Ex: Characterizing a piezo actuator**

In order to characterize a recently purchased piezo actuator (Thorlabs, TA0505D024W) a Scientific Initiation student sets up a Michelson interferometer driven by a HeNe laser beam. Scanning the voltage applied to the piezo through the entire permitted range, he observes 8.8 oscillations of the interference fringes. What is the piezo displacement per volt?

**31.1.10.2 Ex: Michelson interferometer**

The figure 31.11 shows a Michelson interferometer containing in one arm an airtight 5 cm long cell with glass windows. Light with wavelength  $\lambda = 500$  nm is used. After the cell has been evacuated, the interference pattern shifts by 60 fringes. Use this information to calculate the refractive index of air at atmospheric pressure. With what accuracy can you determine the refractive index with this method?

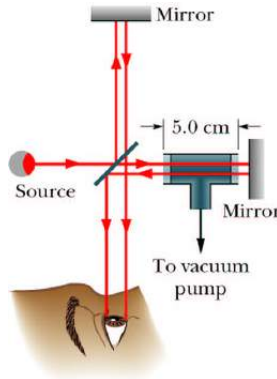


Figure 31.11:

**31.1.10.3 Ex: Michelson interferometer**

Assume that a signal-to-noise ratio of 50 has been achieved in measuring the fringe pattern of a Michelson interferometer with one continuously moving mirror. Estimate the minimum path length  $\Delta L$  that the mirror has to travel in order to reach an accuracy of  $\Delta\lambda = 10^{-4}$  nm in the measurement of a laser wavelength at  $\lambda = 600$  nm.

**31.1.10.4 Ex: Rotating the polarization with a Mach-Zehnder interferometer**

Using the Jones matrix formalism demonstrate how to use the Mach-Zehnder interferometer setup sketched in the figure to rotate the polarization of a linearly polarized laser beam in an electronically controlled way using a piezo actuator mounted in one of the interferometer arms.

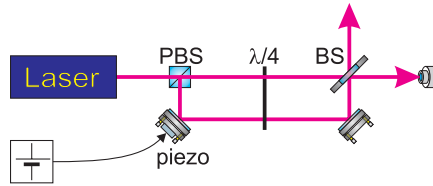


Figure 31.12:

### 31.1.10.5 Ex: Lyot filter

Consider a Lyot filter with two plates ( $L_1 = 1$  mm and  $L_2 = 4$  mm) with the refraction indices  $n_o = 1.40$  in the fast axis and  $n_e = 1.45$  in the slow axis.

- Calculate the transmission peaks of the Lyot filter as a function of  $\lambda$  for the rotation angle  $\phi = 45^\circ$ .
- Determine the transmitted intensity  $I(\phi)$  as a function of the rotation angle  $\phi$  for a fixed wavelength  $\lambda$ . What is the contrast of the transmitted intensity for arbitrary values of  $\lambda$  if the absorption losses are 2%?

### 31.1.10.6 Ex: Wedge-shaped etalon

A beam of light of wavelength  $\lambda = 683$  nm with large diameter is incident perpendicularly on the first of two quadratic plates. Each plate has the edge length 120 mm; at the left edge the plates touch each other, at the right edge they are separated by a wire of  $d_w = 0.048$  mm in diameter. The air between the plates acts as a thin layer.

- How many interference fringes does an observer see from above this arrangement?
- Now suppose that the incident light be white. Will the interference pattern at the far left be bright or dark?
- Starting from the left edge there will be a series of interference minima, whose position depend on the wavelength of the light. For what light color (blue or red) will the minimum be closer to the edge?

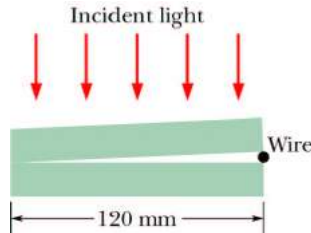


Figure 31.13:

### 31.1.10.7 Ex: Fabry-Perot interferometer

The dielectric coatings of each plate of a Fabry-Perot interferometer have the following specifications:  $R = 98\%$ ,  $A = 0.3\%$ . The flatness of the surfaces is  $\lambda/100$  at  $\lambda = 500$  nm.

- Estimate the finesse from (31.24) and (31.27), the maximum transmission, and the spectral resolution of the FPI for a plate separation of 5 mm.
- Show that, for a given absorption, the transmitted intensity decreases with increasing reflectivity. Explain why. **Note:** A trade-off between high finesse and high transmission at a given absorption  $A > 0$ , called *impedance matching*, is reached by maximizing the intracavity intensity. For a symmetric cavity, it can be shown that impedance matching is reached for  $A = T$ .

**31.1.10.8 Ex: Confocal and concentric cavities**

- Calculate the spectrum of longitudinal and transverse modes for (i) a confocal cavity ( $\rho_a = \rho_b = L$ ) and (ii) a concentric cavity ( $\rho_a = \rho_v = L/2$ ). Interpret the results.
- Assuming radii of curvature  $\rho_a = \rho_b = 5$  cm and a finesse of  $F = 500$  for the cavity, how precise must the length of the cavity be adjusted in order to observe only longitudinal modes in the transmission spectrum?

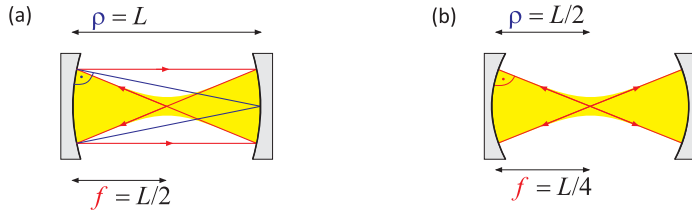


Figure 31.14: (a) Confocal cavity and (b) concentric cavity.

**31.1.10.9 Ex: Thermal drift of a laser cavity**

Estimate the frequency drift of a laser oscillating at  $\lambda = 500$  nm because of thermal expansion of the resonator at a temperature drift of  $1^\circ\text{C}/\text{h}$ , when the resonator mirrors are mounted on distance-holder rods a. made of invar and b. made of fused quartz.

**31.1.10.10 Ex: Stability of a supercavity**

Consider a non-confocal optical cavity of 10 cm length whose spacer is made of (i) aluminum, (ii) stainless steel, (iii) invar steel, (iv) fused quartz, (v) Zerodur, and (vi) ULE. The cavity is maintained at constant temperature with a precision of 0.001 C. What maximum drift do you estimate for its resonance frequency at 633 nm?

**31.1.10.11 Ex: Fabry-Perot interferometer as optical spectrum analyzer**

A confocal FPI shall be used as optical spectrum analyzer, with a free spectral range of  $\delta_{f_{sr}} = 3$  GHz. Calculate the mirror separation  $L$  and the finesse that is necessary to resolve spectral features in the laser output within  $\Delta\nu = 10$  MHz. What is the minimum reflectivity  $R$  of the mirrors, if the surface finesse is  $F_S = 500$ ?

**31.1.10.12 Ex: Interference and colors filters**

Strontium atoms resonantly driven by two lasers at 461 nm and 689 nm emit fluorescence light at both wavelengths. Because the red transition is 5000 times narrower than the blue one, the red fluorescence is much weaker and difficult to detect. Find a suitable low-pass filter in the Thorlabs<sup>®</sup> catalogue suppressing the blue light sufficiently to be sure that any fluorescence recorded after the filter must be resulting from the red transition. What signal ratios can you achieve with a single filter? Consider interference filters as well as color filters.

**31.1.10.13 Ex: Interference filter**

An interference filter shall be designed with peak transmission at  $\lambda = 550$  nm and a bandwidth of 5 nm. Estimate the reflectivity  $R$  of the dielectric coatings and the thickness of the etalon, if no further transmission maximum is allowed between 350 and 750 nm.

**31.1.10.14 Ex: Cut-off wavelength of a single-mode fiber**

You want to transport 461 nm light via a polarization maintaining single-mode fiber. How do you need to choose the cut-off wavelength of the fiber? Assuming a 50% coupling efficiency, how much power can you get through the 5 m long fiber? Choose a model from the Thorlabs catalog and justify your choice.

**31.1.10.15 Ex: Exc Numerical aperture of a fiber**

Calculate the numerical aperture of a step-index fiber with core refractive index  $n_{core}$  and cladding refractive index  $n_{cladding}$  considering the scheme 31.15.

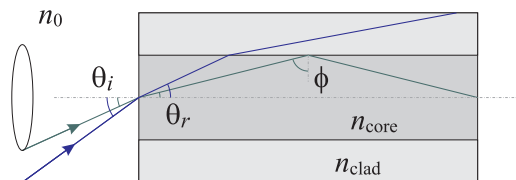


Figure 31.15:

**31.1.10.16 Ex: Tuning by tilting an etalon**

- It is a common method to tune an etalon (or dielectric mirror or waveplate) to a certain transmission wavelength by tilting it as a whole with respect to the optical axis (without changing its intrinsic alignment). Does the tilt increase or decrease the wavelengths of the transmission peaks? Justify your answer. What is the implication for a dielectric mirror to be used under a non-normal angle of incidence?
- A narrow band interference filter consisting of a glass plate coated on both surfaces has the following characteristics: thickness  $L = 0.5$  mm, refractive index  $n_{r,fr} = 1.45$ , central wavelength  $\lambda_{eff} = 706$  nm, and bandwidth  $\Delta\lambda = 0.3$  nm. Considering the filter as Fabry-Pérot etalon, calculate its free spectral range, its finesse, and the

reflectivity of its surfaces.

c. Assuming that the filter of part (b) can be tilted from normal incidence up to an angle  $\theta_{max} = 35^\circ$ , how far will the center frequency shift. Prepare a graph showing  $\lambda_{eff}$  as a function of  $\theta$ .

### 31.1.10.17 Ex: Double MZI as a model for Coherent Back-Scattering

Consider the setup shown in Fig. 31.16 and calculate the signal observed on the photodetector for arbitrary phase shifts  $\phi$  and arbitrary rotation angles  $\alpha$  by the  $\lambda/2$ -waveplate.

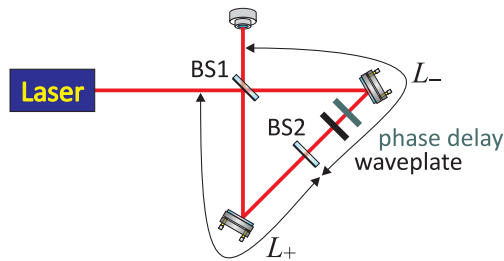


Figure 31.16: Double Mach-Zehnder interferometer.

### 31.1.11 Experiment: Mach-Zehnder interferometer

The Mach-Zehnder interferometer and the Michelson interferometer are the two most common two-beam interferometers. For the realization of the following project prior knowledge of 1. Gaussian beams (see Sec. 29.2), 2. photodetectors (see Sec. 30.2.1), and 3. piezo-electric transducers (see Sec. 31.1.2) is required.

1. Set up a Mach-Zehnder interferometer with a piezo in one of the arms according to Fig. 31.3(a). Optimize the phase matching of the two beams onto a photodetector and the rotation of the  $\lambda/2$ -waveplates until you obtain visible interference patterns.
2. Vary the length of one arm of the interferometer using the piezo. Measure the contrast of the interference fringes and discuss from which parameters it depends and how it can be maximized.
3. Rotate the first  $\lambda/2$ -waveplate (behind the laser). What do you observe? Explain the observation!
4. Remove the PBS in front of the photodetector. What do you observe? Explain the observation!
5. If a piezo is used, vary the voltage applied to the piezo-electric actuator and measure the voltage expansion coefficient  $d$ .



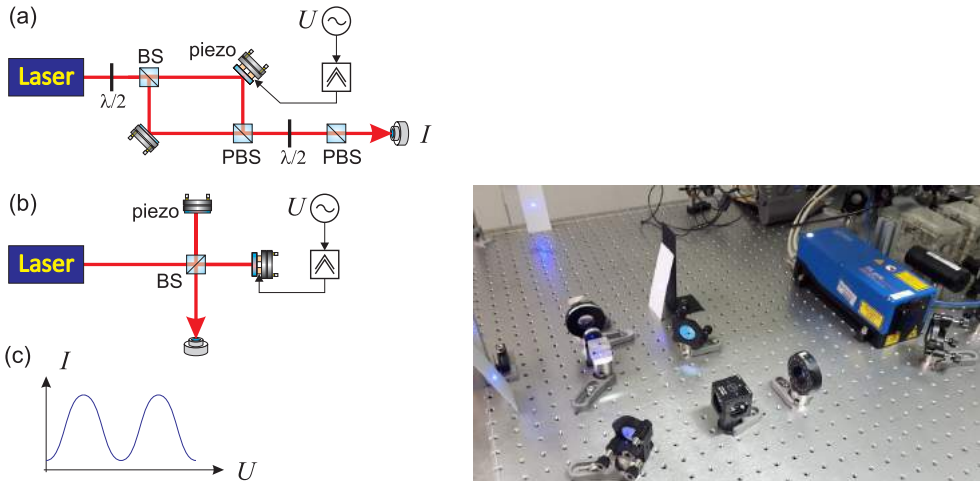


Figure 31.17: Setup for (a) a Mach-Zehnder interferometer or (b) a Michelson interferometer. (BS) non-polarizing beamsplitter, (PBS) polarizing beamsplitter. (c) Signal on the photodetector as a function of the length variation of an arm of the interferometer.

### 31.1.12 Experiment: Fabry-Pérot cavity

A Fabry-Pérot cavity is a typical multi-beam interferometer.

1. Set up a Fabry-Pérot cavity according to Fig. 31.18 and mode-match a laser beam into the cavity. Scan the cavity length using a piezo and observe the transmitted spectrum on an oscilloscope. What do you observe?
2. If an ECDL is used, vary the current and the temperature of the laser diode. What do you observe? Vary the frequency of the diode laser by scanning the piezo transducer of the laser cavity. Observe the mode spectrum of the laser in the transmission signal of the cavity. Measure its free spectral range, the transmission linewidth, and the finesse of the cavity.

Optical cavities are frequently used as *optical spectrum analyzers*. For this application, it is helpful to simplify the intrinsic mode spectrum of the cavity by using a confocal design, where all transverse modes are degenerated. We will now set up an optical cavity and characterize it by its free spectral range and its finesse. Then we will analyze its mode spectrum and modify its geometry to make it confocal.

1. Couple a laser beam into a cavity as shown in Fig. 31.18. The cavity provided by this tinker course consists of a plane incoupler ( $\rho_1 = \infty$ ,  $R_1 = 98\%$ ) and a high reflector ( $\rho_2 = 25$  mm,  $R_2 = 99.8\%$ ). Position the mirror at a distance  $L$ , where the cavity is stable. Calculate the free spectral range, the finesse, the diameter of the beam waist.
2. Optimize the phase-matching of the laser beam to the cavity. In order to do this, (a) measure the diameter of the diode laser beam, (b) determine the lens

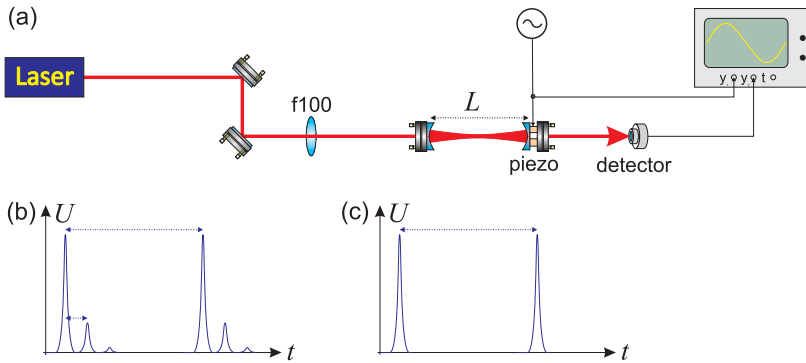


Figure 31.18: (a) Setup for aligning a confocal resonator. (b) Transmission spectrum of the cavity for non-confocal alignment. (c) Same as (b) but for the case of confocal alignment.

which can be used to focus down to the beam waist of the cavity. How does the transmission spectrum change upon the beam matching?

### 31.1.13 Experiment: Fizeau interferometer

A *Fizeau interferometer* is a device allowing to analyze the rugosity of surfaces.

1. Set up a Fizeau interferometer according to Fig. 31.18.

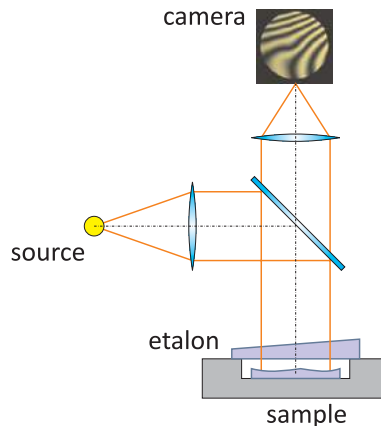


Figure 31.19: Principle of operation of a Fizeau interferometer.

### 31.1.14 Experiment: Coupling light into an optical fiber

Coupling a laser beam into an optical fiber is a delicate task, requiring a good collimation optics and full control over the 6 degrees of freedom defining a laser beam: horizontal and vertical position, horizontal and vertical tilt, beam diameter and divergence.

1. Redirect the light of a HeNe laser via two adjustable mirrors into a fiber collimator in such a way that the beam is not deviated from the optical axis by the collimator.
2. Now connect (a) a multimode fiber and (b) a single mode fiber to the collimator. Optimize the coupling by walking the laser beam and by adjusting the focus of the fiber collimator. What differences do you observe for multi- and single mode fibers?

## 31.2 Conventional light sources and lasers

The laser is a light emitting device with unsurpassed properties, which have enabled fantastic scientific and technical advances, only comparable to those due to the invention of the transistor. See also [\(watch talk\)](#).

The laser produces light through an optical quantum amplification process based on the stimulated emission of electromagnetic radiation. The term 'laser' is an acronym for 'Light Amplification by Stimulated Emission of Radiation'. A laser differs from other light sources in that it emits *coherent* light. Its spatial coherence allows the light to be focused on a very tiny spot, where the concentration of energy is sufficient for applications such as laser cutting and lithography. The spatial coherence also allows it to collimate a laser beam over large distances, that is, the light forms a concentrated beam propagating in a straight line. Lasers can also have a very high temporal coherence, which corresponds to a very narrow spectrum, that is, lasers usually emit a single very well defined color of light. The extreme temporal coherence can be used to produce pulses of light as short as a femtosecond. In addition, laser light is polarized.

In 1917, Albert Einstein established the theoretical foundations of the laser in an article 'Zur Quantentheorie der Strahlung' through a rederivation of Max Planck's radiation law. He proposed a mechanism explaining how light is absorbed and emitted from atoms. The fundamental ingredient is that the photon can be emitted in two different ways, by spontaneous emission, an indeterministic process that occurs without physical reason, or by stimulated emission. This latter emission process occurs because of stimulation by light, which is already present in the system and represents the fundamental mechanism of the laser. In the following decade German and American researchers experimentally confirmed the phenomena of stimulated emission and negative absorption, that is, gain. In 1950, Alfred Kastler (French physicist and Nobel Prize in Physics of 1966) proposed the method of optical pumping, confirmed experimentally two years later by other French physicists.

In 1953, Charles Townes produced the first microwave amplifier called *maser*, a device that operates similarly to the laser but amplifies microwave radiation instead of visible or infrared radiation. However, Townes' maser was unable to emit light continuously. In 1955, in the Soviet Union, Nikolay Basov and Aleksandr Prokhorov solved the problem of continuous operation using atoms with more than two energy levels. These level systems were able to sustain a permanent population inversion of an energetic level decaying to a less energetic system by releasing light via stimulated emission. Despite the fact that several prominent physicists, including Niels Bohr,

John von Neumann, and Isidor Rabi, argued that the maser violates Heisenberg's uncertainty principle and therefore could not work, in 1964, Charles Townes, Nikolay Basov and Aleksandr Prokhorov shared the Nobel Prize in Physics for fundamental work in the field of quantum electronics that led to the realization of oscillators and amplifiers based on the maser principle.

In 1957, Charles Townes and Arthur Schawlow, from the Bell labs, began to seriously study feasibility of an 'optical maser'. In 1958, the Bell labs submitted a patent proposing a scheme for optical radiation, and Schawlow and Townes presented a scientific paper. Simultaneously, at the Columbia University, the PhD student Gordon Gould was working on the energy levels of excited thallium. In 1957-8, Gould and independently Prokhorov, Schawlow and Townes proposed the use of an open resonator, which later became an essential component of the laser. Gould also proposed several possible applications for a laser, such as spectrometry, interferometry, the radar, and nuclear fusion. He continued to develop the idea, and filed a patent application in April 1959. The United States Patent Office dismissed his application, and granted a patent to the Bell Labs in 1960. Gould won his first minor patent in 1977 after a 28-year fight, and it took him until 1987 to win his first significant process in the struggle, when a federal judge ordered the United States Patent Office to issue to Gould patents for optical pumping and the invention of a laser based on the principle of electrical gas discharge.

It was Theodore Maiman, who on May 16, 1960, operated the first working laser at the Hughes Research Laboratories, Malibu, California, evincing several other research teams, including the ones of Townes at Columbia University, of Schawlow at Bell Labs, and Gould at the company TRG (Technical Research Group). Maiman's laser used a synthetic solid-state ruby crystal pumped by a flash lamp to produce red laser light at 694 nm wavelength; however, the device was only capable of pulsed operation due to its three-level pumping scheme. Later in 1960, the first gas laser was built, using a helium-neon mixture, which was capable of continuous operation in the infrared spectrum. Basov and Javan proposed the concept of a semiconductor laser diode. In 1962, the first laser diode device, made of gallium arsenide, was realized emitting near-infrared light. Nowadays, laser diodes are available in various spectral regimes up to the UV.



Figure 31.20: First suggested application in 1964 of a (left) HeNe laser and (right) a diode laser.

Interestingly, despite many attempts, it has not yet been possible to manufacture yellow or green laser diodes.

### 31.2.1 Features and operation of lasers

To understand how a laser operates, we consider the process of absorption and emission of light by an atom. Following Bohr's model an absorbed photon raises an electron from a lower orbit to a higher orbit, and when the electron returns back to the ground state, it re-emits a photon in an arbitrary direction.

When we illuminate a sample of  $N$  atoms,  $N_1$  atoms of which are in the ground state, by a radiation field, the absorption rate depends on the field intensity  $I(\nu)$  and a constant  $B_{12}$ , which is characteristic for the transition,

$$R_{abs} \propto B_{12}I(\nu)N_1 . \quad (31.35)$$

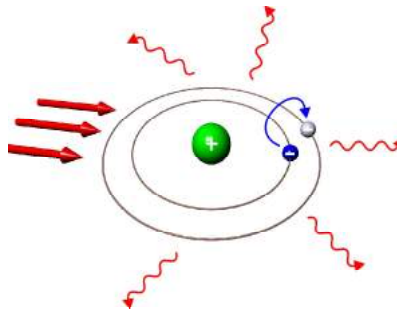


Figure 31.21: Bohr's model of photon absorption.

The emission rate depends on the number of atoms  $N_2$  in the excited state, such that,

$$R_{sp} \propto A_{21}N_2 . \quad (31.36)$$

As the excited state has more energy, it can decay by itself (i.e. spontaneously) to a lower energy state. Einstein's brilliant idea now was to postulate a third process, which he called stimulated emission,

$$R_{st} \propto B_{21}I(\nu)N_2 . \quad (31.37)$$

In this process, an incident photon stimulates an excited atom to transfer the electron to a lower orbit. The released energy is then used to form a second photon, which is in all respects identical to the first. This process is necessary to ensure that, in thermal equilibrium, the population of the states follows Boltzmann's law.

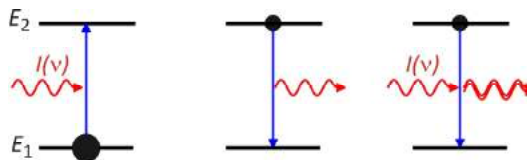


Figure 31.22: Einstein's model of absorption and spontaneous and stimulated emission.

Obviously, absorption decreases the intensity of a light beam crossing the atomic sample, while stimulated emission amplifies it. In order to amplify incident light, the gain in intensity must overcome the losses. Therefore, we need the absorption processes to be less frequent than the stimulated emission processes, i.e. the number of atoms in the excited state  $N_2$  must exceed the number of atoms in the ground state  $N_1 < N_2$ .

We can easily write the rate equation,

$$\frac{dN_2}{dt} = -A_{21}N_2 - B_{21}I(\nu)N_2 + B_{21}I(\nu)N_1 = -\frac{dN_1}{dt}, \quad (31.38)$$

with  $N = N_1 + N_2$ . It is easy to solve this equation. The result is,

$$N_2 = \frac{I(\nu)B_{21}N}{A + 2B_{21}I(\nu)} [1 - e^{-(A_{21} + 2B_{21}I(\nu))t}] < N_1. \quad (31.39)$$

The graphical representation 31.23 shows the temporal behavior of the populations

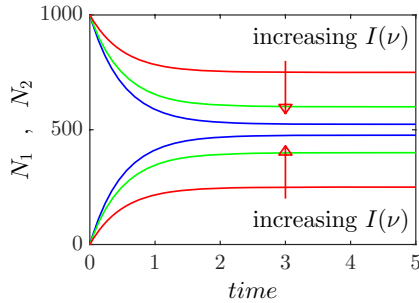


Figure 31.23: (code for download) Impossibility of achieving inversion. in a two-level system.

$N_1$  (in green in the figure) and  $N_2$  (in blue), reaching a state of equilibrium after a certain time. By increasing the intensity of the incident light, we observe that the curves approach each other but never cross. That is, in a two-level system, we always get  $N_1 > N_2$  and the populations are never inverted. Therefore, amplification of light as in the laser does not happen.

Fortunately, we can resort to a trick by inserting a third level. Ensuring that the decay rate of the (metastable) state  $E_3$  is much slower than the optical pumping to this state via the driven transition  $E_1 \rightarrow E_2$  followed by a rapid decay  $E_2 \rightarrow E_3$ , we can reach the situation  $N_3 > N_1$ . Now it is possible to amplify light, which is resonant with the transition  $E_2 \rightarrow E_3$ .

What are the minimum requirements for the realization of a laser? The first condition is that the *pumping cycle is irreversible* to ensure that the processes of stimulated emission and absorption do not compensate. Spontaneous emission is irreversible and can be incorporated into a three-level system.

The second condition is the existence of a *stimulated emission process*, because we want the amplified photon to be an exact copy of the incident photon.

The third requirement is a *feedback mechanism* that synchronizes the amplification processes by different atoms in a disordered environment, such as a gas. Mirrors are

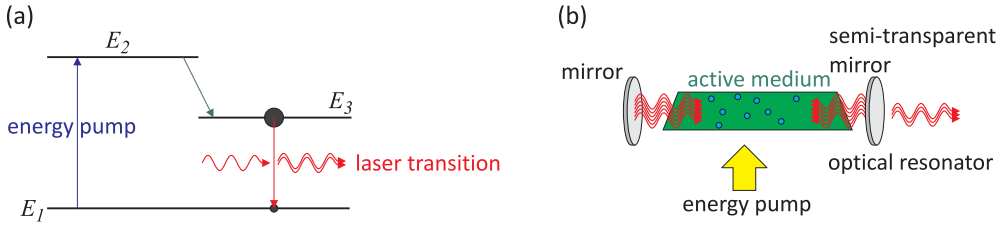


Figure 31.24: Basics of a laser: (a) Level system and (b) principle scheme.

ideal because they increase the effective gain path, i.e. the distance within which inverted atoms can amplify light. Also, the mirrors define the phase of the light wave, since the standing wave formed by the counterpropagating light fields must have nodes on the surfaces of the mirrors.

### 31.2.1.1 Threshold condition

According to the *Lambert-Beer law* the intensity of a monochromatic laser beam evolves, on its way through a gas of two-level atoms with energies  $E_2 - E_1 = \hbar\omega_0$  like,

$$I(z, \nu) = I(0, \nu)e^{-\alpha(\nu)z} , \quad (31.40)$$

where the frequency-dependent absorption coefficient,

$$\alpha(\nu) = [N_1 - \frac{g_1}{g_2} N_2] \sigma(\nu) , \quad (31.41)$$

is determined by the absorption cross section  $\sigma(\nu)$  for the transition and by the inversion,

$$\Delta N \equiv \frac{g_1}{g_2} N_2 - N_1 , \quad (31.42)$$

which determines whether stimulated emission prevails or absorption: For  $\Delta N > 0$ , the absorption coefficient  $\alpha(\nu)$  becomes negative and the incident wave is amplified instead of attenuated [186].

If the active medium is placed between two mirrors [Fig. 31.24(b)], the wave is reflected back and forth, and traverses the amplifying medium many times, which increases the total amplification. With the length  $L$  of the active medium the total gain factor per single round-trip without losses is,

$$G(\nu) = \frac{I(\nu, 2L)}{I(\nu, 0)} = e^{-2\alpha(\nu)L} . \quad (31.43)$$

A mirror with reflectivity  $R$  reflects only the fraction  $R$  of the incident intensity. The wave therefore suffers at each reflection a fractional reflection loss of  $(1 - R)$ . Furthermore, absorption in the windows of the cell containing the active medium, diffraction by apertures, and scattering due to dust particles in the beam path or due to imperfect surfaces introduce additional losses. When we summarize all these losses by a loss coefficient  $\gamma$ , which gives the fractional energy loss  $\Delta W/W$  per round-trip time  $T$ , the intensity  $I$  decreases without an active medium per round-trip as,

$$I(2d, \nu) = I(0, \nu)e^{-\gamma} . \quad (31.44)$$

Including the amplification by the active medium with length  $L$ , we obtain for the intensity after a single round-trip through the resonator with length  $d$ , which may be larger than  $L$ :

$$I(2d, \nu) = I(0, \nu)e^{-2\alpha(\nu)L - \gamma} . \quad (31.45)$$

The wave is amplified if the gain overcomes the losses per round-trip. This implies that,

$$-2L\alpha(\nu) = 2L\Delta N\sigma(\nu) > \gamma , \quad (31.46)$$

which yields the threshold condition for the population difference,

$$\Delta N > \Delta N_{thr} = \frac{\gamma}{2L\sigma(\nu)} . \quad (31.47)$$

If the inverted population difference  $\Delta N$  of the active medium is larger than  $\Delta N_{thr}$ , a wave that is reflected back and forth between the mirrors will be amplified in spite of losses, therefore its intensity will increase.

The wave is initiated by spontaneous emission from the excited atoms in the active medium. Those spontaneously emitted photons that travel into the right direction (namely, parallel to the resonator axis) have the longest path through the active medium and therefore the greater chance of creating new photons by induced emission. Above the threshold they induce a photon avalanche, which grows until the depletion of the population inversion by stimulated emission just compensates the repopulation by the pump. Under steady-state conditions the inversion decreases to the threshold value  $\Delta N_{thr}$ , the saturated net gain is zero, and the laser intensity limits itself to a finite value  $I_L$ . This laser intensity is determined by the pump power, the losses  $\gamma$ , and the gain coefficient  $\alpha(\nu)$ .

The frequency dependence of the gain coefficient  $\alpha(\nu)$  is related to the line profile  $g(\nu - \nu_0)$  of the amplifying transition. Without saturation effects (i.e. for small intensities),  $\alpha(\nu)$  directly reflects this line shape, for homogeneous as well as for inhomogeneous profiles. According to (31.41) and we obtain with the Einstein coefficient  $B_{ik}$ ,

$$\alpha(\nu) = \Delta N\sigma(\nu) = -\Delta N(h\nu/c)B_{12}(\nu - \nu_0) , \quad (31.48)$$

which shows that the amplification is largest at the line center  $\nu_0$ . For high intensities, saturation of the inversion occurs, which is different for homogeneous and for inhomogeneous line profiles.

The loss factor  $\gamma$  also depends on the frequency  $\nu$  because the resonator losses are strongly dependent on  $\nu$ . The frequency spectrum of the laser therefore depends on a number of parameters.

### 31.2.1.2 Applications of lasers in industry and fundamental research

Among their many applications, lasers are nowadays used in compact disc players, laser printers, and bar code scanners, optical fibers and optical communication, laser surgery and skin treatments, welding, cutting and machining, military devices, distance and velocity measurements, projectors, laser pointers, etc..

In fundamental research (in particular on atomic gases, metamaterials, etc.), the laser plays elementary roles in the areas of photonics, quantum computers, metrology,



frequency combs, and atomic clocks (laser-based clocks are up to 1000 times more stable than the best state-of-the-art microwave clocks).

We all know that light is a wave. With the invention of the laser we found a process and a device to make this light coherent. On the other hand, since de Broglie's assertion we know that *matter is a wave, as well*. Is it conceivable to construct a matter laser? Yes, it is! The first coherent matter wave was in fact observed in 1995. This state of matter, also called Bose-Einstein condensate, was predicted by Bose and Einstein in 1924. To create a Bose-Einstein condensate, we need, similarly to the laser, that the matter waves interfere constructively in a way that they amplify each other. For this, the Broglie wavelength of the particles, which constitute the matter, must be longer than the distance between them. Assuming a typical average distance on the order of  $\mu\text{m}$ , this corresponds to an average velocity of the particles of mm/s or a temperature of some 100 nK.

### 31.2.2 HeNe laser

HeNe lasers are gas lasers, whose gain medium consists of a mixture of 90% helium and 10% neon at a total pressure of about 1 Torr excited by a small electrical discharge. The most widely used transition wavelength is at 632.8 nm.

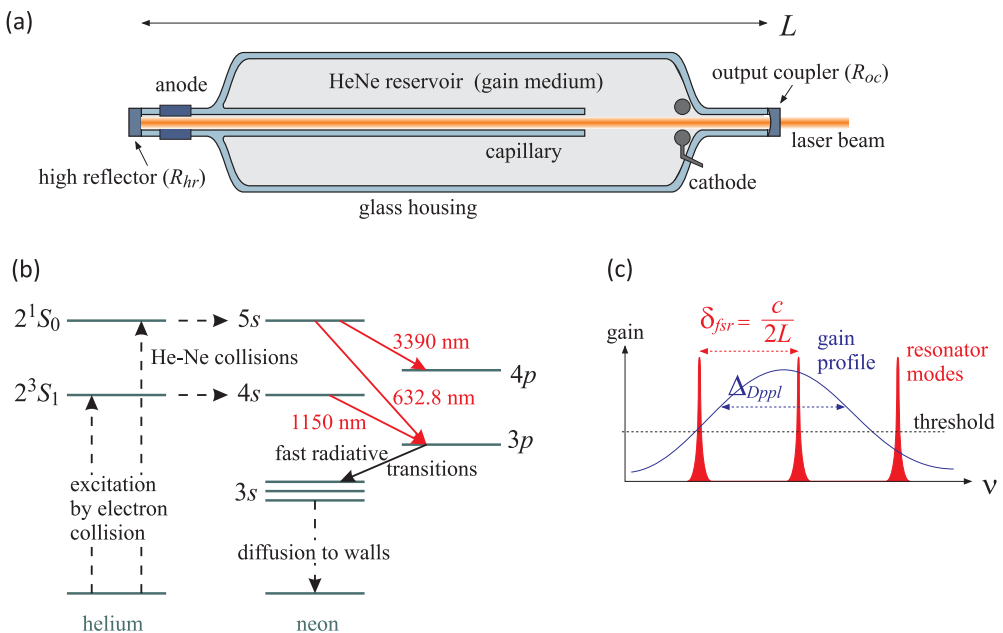


Figure 31.25: (a) Construction scheme of a HeNe laser. (b) Gain and emission profile. (c) Optical pumping scheme.

Fig. 31.25(a) shows the principle scheme of a commercial HeNe laser. The distance between the high-reflecting mirror ( $R_{hr}$ ) and the output coupler ( $R_{oc}$ ) determines the free spectral range  $\delta_{fsr}$ . Typically, a HeNe laser operates on two or three longitudinal modes separated by  $\delta_{fsr}$ . As illustrated in Fig. 31.25(b), the numbers of lasing modes

above threshold depends on the ratio of gain-to-loss. Fig. 31.25(c) shows the optical pumping scheme to reach inversion on three of the lasing transitions at 632.8 nm, 1.15  $\mu\text{m}$ , and 3.39  $\mu\text{m}$ .

### 31.2.3 Diode laser

A laser diode is electrically a *pin*-diode. The active region of the laser diode is in the intrinsic (*i*) region, and the carriers (electrons and holes) are pumped into that depletion region from the *n*- and *p*-doped regions respectively. The depletion region, devoid of any charge carriers, forms as a result of the difference in electrical potential between *n*- and *p*-type semiconductors wherever they are in physical contact. Unlike a regular diode, the goal for a laser diode is to recombine all carriers in the *i* region, and produce light.



Figure 31.26: (Left) Laser diode with protective housing removed, e.g. using a can opener. (Right) Laser diode collimator.

#### 31.2.3.1 Generation of light

Electrons and holes present in the same region may recombine or 'annihilate' by spontaneous emission of photons with energy equal to the difference between the electron's original state and hole's state (see Fig. 30.9). This is in contrast to a conventional semiconductor junction diode, where the energy released from the recombination is carried away as phonons, i.e. lattice vibrations. Spontaneous emission below the lasing threshold is the operating mode of an LED. While spontaneous emission is necessary to initiate laser oscillation, it contributes to reduce the efficiency of a laser operating above threshold.

One condition for lasing is that, in the absence of stimulated emission, electrons and holes may coexist in proximity to one another without recombining immediately. For typical diode laser materials the 'upper-state lifetime' or 'recombination time' is on the order of a nanosecond. A nearby photon with energy equal to the recombination energy can cause recombination by stimulated emission. This generates another photon of the same frequency, polarization, and phase, traveling in the same direction as the first photon. In this way stimulated emission will cause gain for an optical wave in the injection region, and the gain increases as the number of electrons and holes injected across the junction increases.

### 31.2.3.2 Optical cavity and laser modes

As in other lasers, the gain region needs to be surrounded by an optical cavity providing optical feedback. In its simplest form, a laser diode is made in the shape of a narrow optical waveguide on the surface of a crystal. The two ends of the crystal are cleaved to form perfectly smooth, parallel edges, forming a Fabry-Pérot resonator. Emitted photons will travel along the waveguide, be amplified by stimulated emission and reflected several times from each end face before exiting. If the losses due to absorption and incomplete reflection from the end facets are smaller than the gain, the diode begins to 'lase'.

Important properties of laser diodes are determined by the geometry of the optical cavity. If the waveguide is thick compared to the wavelength of the light, it can support higher-order transverse optical modes. The laser is then called 'multi-mode'. These transversely multi-mode lasers are adequate for application where high power is needed, for example, in printing, activating chemicals, or pumping other types of lasers.

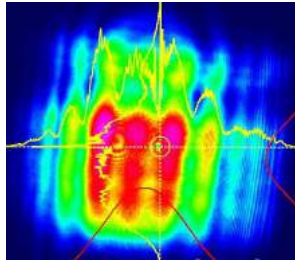


Figure 31.27: Typical beam profile of a multimode laser diode (Thorlabs, L450P1600MM).

For applications requesting small focused beams the waveguide must be made narrow, on the order of the optical wavelength, such that only a single transverse mode is supported, and one ends up with a diffraction-limited beam. Such single spatial mode devices are used for optical storage, laser pointers, and fiber optics. Note that these lasers may still support multiple longitudinal modes, and thus can lase simultaneously at multiple wavelengths. The wavelength emitted is a function of the band-gap of the semiconductor material and the modes of the optical cavity. In general, the maximum gain will occur for photons with energy slightly above the band-gap energy, and the modes nearest the peak of the gain curve will lase most strongly. The width of the gain curve will determine the number of additional 'side modes' that may also lase, depending on the operating conditions. Single spatial mode lasers that can support multiple longitudinal modes are called Fabry-Pérot (FP) lasers. A FP laser will lase at multiple cavity modes within the gain bandwidth of the lasing medium. The number of lasing modes in an FP laser is usually unstable, and can fluctuate due to changes in current or temperature.

Single spatial mode diode lasers can be designed so as to operate on a single longitudinal mode. These single frequency diode lasers exhibit a high degree of stability, and are used in spectroscopy and metrology, and as frequency references. Single frequency diode lasers are classed as either distributed feedback (DFB) lasers or distributed Bragg reflector (DBR) lasers.

Due to diffraction, the beam diverges (expands) rapidly after leaving the chip, typically at 30 degrees vertically by 10 degrees laterally. A lens must be used in order to form a collimated beam like that produced by a laser pointer. If a circular beam is required, cylindrical lenses and other optics are used. For single spatial mode lasers, using symmetrical lenses, the collimated beam ends up being elliptical in shape, due to the difference in the vertical and lateral divergences.

### 31.2.3.3 Distributed Bragg reflector lasers and distributed feedback lasers

The simple diode described above has been heavily modified in recent years to accommodate modern technology, resulting in a variety of types of laser diodes. One example is the distributed Bragg reflector laser (DBR). It consists of a monolithic single frequency laser diode, characterized by an optical cavity consisting of an electrically or optically pumped gain region between two mirrors to provide feedback. One of the mirrors is a broadband reflector and the other mirror is wavelength selective so that gain is favored on a single longitudinal mode, resulting in lasing at a single resonant frequency. The broadband mirror is usually coated with a low reflectivity coating to allow emission. The wavelength selective mirror is a periodically structured diffraction grating with high reflectivity. The diffraction grating is etched into the semiconductor within a non-pumped, or passive region of the cavity.

A distributed feedback laser (DFB) is a monolithic single frequency laser diode with a diffraction grating etched close to the  $pn$ -junction of the diode aiming at stabilizing the lasing wavelength. This grating acts like an optical filter, causing a single wavelength to be fed back to the gain region and lase. Since the grating provides the feedback that is required for lasing, reflection from the facets is not required. Thus, at least one facet of a DFB is anti-reflection coated. The DFB laser has a stable wavelength that is set during manufacturing by the pitch of the grating, and can only be tuned slightly with temperature. DFB lasers are widely used in optical communication applications, where a precise and stable wavelength is critical.

### 31.2.3.4 ECDL

An *extended-cavity diode laser* (*ECDL*) is an optical setup based on a laser diode chip, which typically has one end anti-reflection (AR) coated, and the laser resonator is completed with a collimating lens and a mirror, as shown in Fig. 31.28(a). The extended external laser resonator introduces various new features and options: Compared to a standard laser diode, the longer resonator increases the damping time of the intracavity light according to Eq. (31.26), and thus allows for lower phase noise and a smaller emission linewidth (in single-frequency operation). Furthermore, it opens the way for inserting frequency-selective optical components into the extended laser resonator, such as narrow-band Fabry-Pérot etalons or diffraction gratings, which can further *reduce the linewidth* and even allow to *tune and control the frequency* of the laser.

Tunable ECDLs based on diffraction grating as the wavelength-selective element are also called grating-stabilized diode lasers. The common Littrow configuration Fig. 31.28(b) generates optical feedback to the laser diode chip by retro-reflecting the first-order diffracted beam from the grating. The emission wavelength can be tuned by slightly tilting the diffraction grating. A disadvantage of this configuration is, that

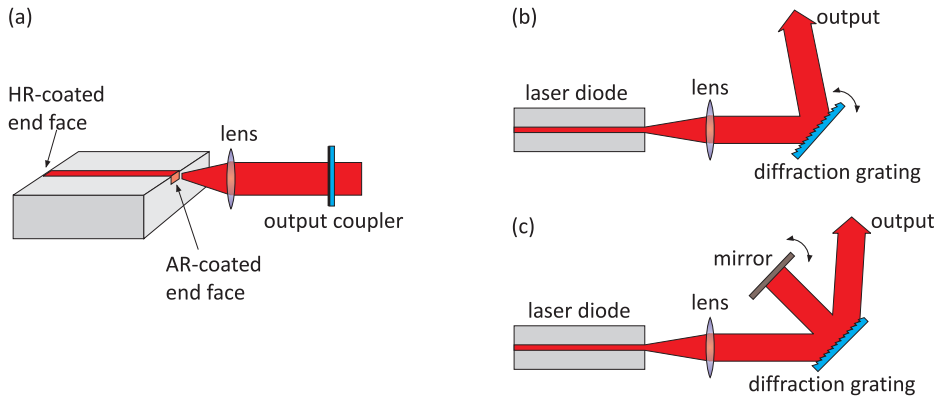


Figure 31.28: (a) ECDL with an AR-coated laser diode and an external mirror. (b) Littrow configuration. (c) Littmann configuration.

the tilt also changes the direction of the output beam, which is inconvenient for many applications.

In the Littman-Metcalf configuration Fig. 31.28(c), the grating angle is held fixed, and an additional mirror is used to reflect the first-order beam back into the laser diode. The wavelength can be tuned by rotating that mirror. This configuration offers a fixed direction of the output beam, and also tends to exhibit a smaller linewidth, as the wavelength selectivity is stronger, because the wavelength-dependent diffraction occurs twice per resonator round trip. A disadvantage is that the zero-order reflection of the beam reflected by the tuning mirror is lost, so that the output power is lower than that of a Littrow laser.

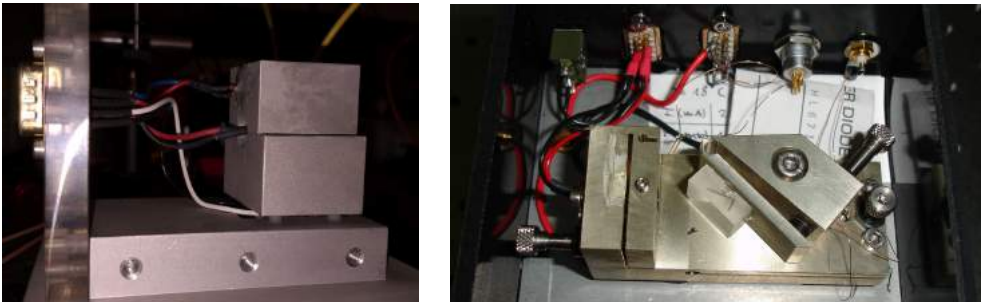


Figure 31.29: (Left) Side view of a 'free-running' laser diode mounted in a collimator (Thorlabs, LT110P-B) clamped in an aluminum block cooled by a Peltier element (Thorlabs, TEC3-6) and whose temperature is measured by a thermistor (Thorlabs, TH10K). (Right) Top view of a home-built ECDL laser in Littrow configuration. The diode collimator is clamped into the left mount. a holographic grating (Newport, 10HG2000-475-1) is glued to the right mount, whose angle can be adjusted mechanically and via a piezo. The whole setup is cooled by a Peltier element mounted on the bottom of the base plate.

New concepts have recently become popular, such as the so-called *cat-eye laser* [40,

266, 61], where the frequency-selective element is an extremely narrow-band (0.3 nm) optical filter<sup>4</sup>.

By adjusting the tilt angle of a grating or a narrow-band filter by means of a piezo an extremely fine tuning of the emission frequency is possible, while coarse tuning of the frequency over a range of several nanometers is typically achieved by changing the temperature and the laser current. Typical linewidths of free-running ECDLs are well below 5 MHz. Controlling the laser temperature, current, and piezo voltage by active feedback circuits (e.g. within a Pound-Drever-Hall servo electronics) emission bandwidths in the milliHertz range have been achieved, which corresponds to quality factors of the laser oscillator of up to  $10^{18}$ .

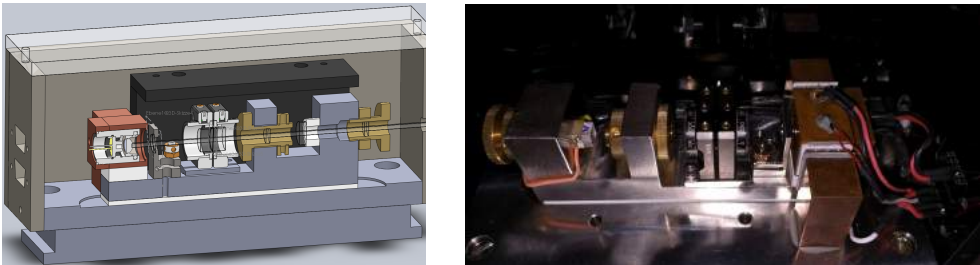


Figure 31.30: (Left) Construction plan of a home-built ECDL lasers in cat-eye configuration. (Right) Side view of the cat-eye laser.

In comparison to other laser types, a *diode laser* exhibits, the advantage of a very small size and a compact design. They are, in general, easy to handle and can be controlled conveniently via current and temperature. However, they also have the disadvantage of a large beam divergence and a broad emission spectrum. The beam divergence can be compensated by a collimation optics in front of the laser diode.

The temperature has an impact on the band structure of the *pn*-transition of the laser diode and hence on the frequency. Therefore, it is stabilized via a Peltier element, which is mounted underneath the laser diode holder. The degree of freedom is used for tuning the laser frequency in wide steps.

### 31.2.3.5 Pulsed diode lasers

Diode lasers can be used for generating ultrashort pulses either with various techniques of mode locking or with gain switching. Typically, pulses with durations between 0.5 and 5 ps and pulse repetition rates between 1 GHz and hundreds of giga-Hertz are generated with mode locking. In extreme cases, the repetition rate can even be above 1 THz. The main application of ultrafast diode lasers is in optical fiber communications systems, where such lasers function as pulse sources of fast data transmitters or for all-optical signal processing.

Common techniques for mode locking of diode lasers are active or passive mode locking. Active mode locking can be accomplished with an optical modulator in the laser resonator. This is usually either an electro-absorption modulator in the form of an unpumped region with some modulated voltage, or an amplifying section where

<sup>4</sup>Available from Semrock or Laseroptik.

the drive current is modulated. Passive mode locking relies on a saturable absorber in the resonator. This can simply be an unpumped section of the device. It is common to apply an electrical bias for adjusting the absorber properties. However, the recovery time of that kind of absorber is fairly long. Shorter recovery times are achieved e.g. by implanting nitrogen ( $N^+$  or  $N_2^+$ ) ions from one facet. This introduces crystal defects, where carriers can recombine. The absorber is often placed at a resonator end, but it can also be placed somewhere within the resonator so that different pulses can meet in the absorber (colliding pulse mode locking).

For pulse repetition rates roughly below 10 GHz, an external cavity setup is usually required, as a monolithic device would become too long. The extended cavity may be an ECDL setup. Another technical approach is to incorporate the semiconductor chip into a ring laser resonator made of optical single-mode fiber. In the latter case, the resonator is typically much longer, and allows the use of fiber-optic components. The semiconductor device may then be a fiber-coupled semiconductor optical amplifier (SOA).

External-cavity lasers have various advantages: The pulse repetition rate can be chosen in a wide range, and can easily be tuned e.g. by moving the end mirror, or with a fiber resonator by stretching a piece of fiber with a piezo transducer. It is possible to insert an optical filter for fixing the emission wavelength, or use a diffraction grating as the end mirror (Littrow configuration; see the article on external-cavity diode lasers). Even for higher pulse repetition rates, where harmonic mode locking is required, external-cavity devices can be advantageous, because they have a potential for lower laser noise, e.g. in the form of timing jitter. Therefore, mode-locked external-cavity diode lasers sometimes compete with mode-locked fiber lasers in areas where monolithic laser diodes would not be suitable. On the other hand, a monolithic setup with fundamental mode locking can be very compact, much cheaper to manufacture, and can exhibit very robust pulse emission.

On the other hand, mode-locked diode lasers are subject to various limitations, which do not allow them to reach the full performance potential of, e.g., mode-locked fiber lasers: The pulse energy is fairly limited often far below 1 pJ. Average output powers are often below 1 mW. Due to the short upper-state lifetime, ultrafast semiconductor lasers are generally not suitable for lower repetition rates of e.g. well below 1 GHz, except with synchronous pumping. Although the gain bandwidth of semiconductors would be compatible with pulse durations of a few tens of femtoseconds, the pulse durations achieved are usually much longer at least hundreds of femtoseconds, and often picoseconds. The pulse formation dynamics are relatively complicated, e.g. due to nonlinear phase changes associated with gain saturation, and difficult to optimize. The pulse quality is normally not as good as e.g. for mode-locked fiber lasers. In particular, there are often additional satellite pulses, caused e.g. by imperfections of the anti-reflection coating. Also, the pulses are often chirped, i.e. they are not bandwidth-limited. The timing jitter and the noise of other pulse parameters are higher than for other mode-locked lasers. This is partly a consequence of the low power level.

### 31.2.3.6 Tapered amplifiers and injection locking

Other ways to amplify the power of a laser without altering its coherence properties are using a *tapered amplifier* or via *injection locking* also called *master-slave locking* [109, 438] (see Fig. 31.31).

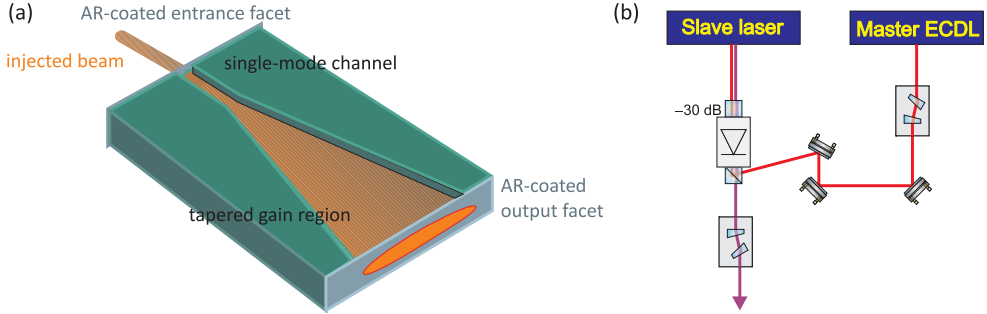


Figure 31.31: (a) Tapered amplifiers are available e.g. from Eagleyard. (b) Principle of injection locking.

The description presented here uses semi-classical laser rate equations [437]. Assuming that the master and the slave laser field are given by, respectively,

$$E_{inj} = A_{inj} e^{-i\omega_{inj}t} e^{i\phi_{inj}(t)} \quad \text{and} \quad E = A e^{-i\omega_s t} e^{i\phi_s(t)}, \quad (31.49)$$

The phase difference between the both fields is denoted by  $\phi(t) = \phi_s(t) - \phi_m(t)$ . Now, Considering the semi-classical laser rate equations we can describe the impact of the master laser field in the slave laser,

$$\begin{aligned} \frac{dA(t)}{dt} &= \frac{1}{2}g[N(t) - N_{th}]A(t) + \kappa A_{inj} \cos \phi(t) \\ \frac{d\phi(t)}{dt} &= \frac{\alpha}{2}[N(t) - N_{th}] - \kappa \frac{A_{inj}}{A(t)} \sin \phi(t) - \Delta\omega \\ \frac{dN(t)}{dt} &= J - \gamma_N N(t) - [\gamma_p + g[N(t) - N_{th}]A(t)^2], \end{aligned} \quad (31.50)$$

where  $A(t)$  is the field amplitude normalized as  $A^2(t) = S(t)$ , and  $S(t)$  is the photon number.  $N(t)$  is the number of carriers in the slave laser, and the other parameters are  $g$  laser gain coefficient,  $N_{th}$  threshold carrier number,  $\kappa$  coupling coefficient,  $\alpha$  linewidth enhancement factor,  $\gamma_p$  photon decay rate,  $N$  carrier recombination rate,  $J$  pump current normalized by electron charge,  $\Delta\omega$  frequency difference between the master and the free running slave  $\omega_m - \omega_s$ . The parameter  $\kappa$  describes the rate at which the photons of the master laser enter into the slave laser cavity and is given in terms of the cavity quality factor,

$$\kappa = \frac{\omega_s}{2Q}. \quad (31.51)$$

From the steady state solutions of above equations, we can obtain the frequency locking range,

$$-\kappa \sqrt{(1 + \alpha^2)} \sqrt{\frac{P_{inj}}{P_s}} < \Delta\omega < \kappa \sqrt{\frac{P_{inj}}{P_s}}, \quad (31.52)$$



where  $P_{inj}/P_s$  is the master laser fraction power used for the injection locking and  $P_s$  is the power of slave laser. From equation 4.25 we can see that the locking range is determined by the amplitude ratio between the fields and by the cavity quality factor since  $\kappa \propto Q^{-1}$ . Therefore, lasers with low  $Q$  are easier to lock. On the other hand, this leads to increased laser linewidth that reduces the phase noise performance of the injection locking systems. For higher injection ratio  $P_{inj}/P_s$  also results in a large locking range, which also makes the lock easier to achieve.

### 31.2.4 Exercises

#### 31.2.4.1 Ex: Conventional light sources and lasers

Compare the properties of an incandescent light and a laser.

#### 31.2.4.2 Ex: Threshold inversion for lasing 1

Calculate the necessary threshold inversion of a gas laser transition at  $\lambda = 500$  nm with the transition probability  $A_{ik} = 5 \cdot 10^7$  s<sup>-1</sup> and a homogeneous linewidth  $\Delta\nu_{hom} = 20$  MHz. The active length is  $L = 20$  cm and the resonator losses per round-trip are  $\gamma = 5\%$ .

#### 31.2.4.3 Ex: Threshold inversion for lasing 2

A laser medium has a Doppler-broadened gain profile of halfwidth  $\delta\nu = 2$  GHz and central wavelength  $\lambda = 633$  nm. The homogeneous width is 50 MHz, and the transition probability  $A_{ik} = 10^8$  s<sup>-1</sup>. Assume that one of the resonator modes ( $L = 40$  cm) coincides with the center frequency  $\nu_0$  of the gain profile. What is the threshold inversion for the central mode, and at which inversion does oscillation start on the two adjacent longitudinal modes if the resonator losses are 10%?

#### 31.2.4.4 Ex: Mode pulling in an active resonator

The frequency of a passive resonator mode ( $L = 15$  cm) lies  $0.5\Delta\nu_D$  away from the center of the Gaussian gain profile of a gas laser at  $\lambda = 632.8$  nm. Estimate the mode pulling if the cavity resonance width is 2 MHz and  $\Delta\nu_D = 1$  GHz.

#### 31.2.4.5 Ex: Spatial hole-burning

Assume a laser transition with a homogeneous width of 100 MHz, while the inhomogeneous width of the gain profile is 1 GHz. The resonator length is  $d = 200$  cm and the active medium with length  $L \ll d$  is placed  $a = 20$  cm from one end mirror. Estimate the spacing of the spatial hole-burning modes. How many modes can oscillate simultaneously if the unsaturated gain at the line center exceeds the losses by 10%?

#### 31.2.4.6 Ex: Optimizing the transmission of laser output mirrors

Estimate the optimum transmission of the laser output mirror if the unsaturated gain per round trip is 2 and the internal resonator losses are 10%.

**31.2.4.7 Ex: Mode selection in a HeNe laser**

A HeNe laser with an unsaturated gain of  $G(\nu_0) = 1.3$  per round trip at the center of the Gaussian gain profile with halfwidth  $\Delta\nu_D = 1.5$  GHz has a resonator length of  $d = 50$  cm and total losses of 4%. Single-mode operation at  $\nu_0$  is achieved with a coated tilted etalon inside the resonator. Design the optimum combination of etalon thickness and finesse.

**31.2.4.8 Ex: Mode hopping in a HeNe laser**

A single-mode HeNe laser with resonator length  $L = 15$  cm is tuned by moving a resonator mirror mounted on a piezo. Estimate the maximum tuning range before a mode hop will occur, assuming an unsaturated gain of 10% at the line center and resonator losses of 3%. What voltage has to be applied to the piezo (expansion 1 nm/V) for this tuning range?

**31.2.4.9 Ex: Mode selection with an intracavity etalon**

Mode selection in an argon laser is often accomplished with an intracavity etalon. What is the frequency drift of the transmission maximum

- for a solid fused quartz etalon with thickness  $d = 1$  cm due to a temperature change of  $2^\circ\text{C}$ ?
- For an air-space etalon with  $d = 1$  cm due to an air pressure change of 4 mbar?
- Estimate the average time between two mode hops (cavity length  $L = 100$  cm) for a temperature drift of  $1^\circ\text{C}/\text{h}$  or a pressure drift of 2 mbar/h.

**31.2.4.10 Ex: Frequency and intensity noise of a laser**

A single-mode laser is frequency stabilized onto the slope of the transmission maximum of an external reference Fabry-Perot interferometer made of invar with a free spectral range of 8 GHz. Estimate the frequency stability of the laser

- against temperature drifts, if the FPI is temperature stabilized within  $0.01^\circ\text{C}$ ,
- against acoustic vibrations of the mirror distance  $L$  in the FPI with amplitudes of 100 nm.
- Assume that the intensity fluctuations are compensated to 1% by a difference amplifier. Which frequency fluctuations are still caused by the residual intensity fluctuations, if a FPI with a free spectral range of 10 GHz and a finesse of 50 is used for frequency stabilization at the slope of the FPI transmission peak?

**31.2.5 Experiment: Analyzing the mode structure of a HeNe laser**

Here we will analyze the mode structure of a HeNe laser via (i) an optical spectrum analyzer and (ii) a radiofrequency spectrum analyzer. We will also try to unravel the polarization of the laser light.

- Couple the light of a HeNe laser simultaneously into an optical spectrum analyzer and a radiofrequency spectrum analyzer. What do you observe when you

slightly heat the laser housing? Calculate from your observations the length of the laser cavity.

2. Pass the light through a  $\lambda/4$ -plate and then through a polarizing beam splitter. What do you observe in the two output ports of the PBS?

### 31.2.6 *Experiment: Adjusting the threshold of an ECDL laser*

Here we will construct a diode laser in Littmann configuration.

1. Take a laser diode, a Peltier cooler, a thermistor, a piezo transducer, and a diffraction grating. Put everything together.
2. Optimize the threshold. Analyze the emission spectrum with an optical spectrum analyzer.

## 31.3 Introduction to optical phase and frequency modulation

### 31.3.1 Acousto-optic modulator

The *acousto-optic modulator AOM* permits fast frequency and amplitude variations of a laser beam. Because it does not incorporate mechanical parts, it works without fatigue. AOMs are used, for instance, in laser printers, where the gray tone of a pixel can be adjusted via the intensity of the laser beam, while its position (rows and columns) is varied by a rotating mirror and the drum propagating the paper sheet. In quantum optics labs they are frequently used for fast (down to  $\mu\text{s}$ ) switching on and off, intensity control, and super-fine frequency-tuning of laser beams. The angular deflection of the first-order diffracted beam upon frequency tuning, which is often perceived as an inconvenience, can be circumvented by double-passage through the AOM.

The acousto-optic modulator consists of a piece of crystal (or glass) excited by an acoustic wave with frequency  $f$  produced by a piezo-electric transducer (see Sec. 31.3.1) mounted perpendicularly to propagation direction of the laser beam. The sound waves propagate through the crystal as density fluctuations periodically changing the refraction index  $n$ . The incident light is diffracted through Brillouin scattering at the spatial modulation of the refraction index. In a wave picture, the process can be interpreted as Bragg scattering of a light wave (with its wavelength inside the crystal  $\lambda_n = 2\pi/k_n = c/n\nu$ ) from a density grating.  $c/n$  is the propagation velocity of light inside the crystal. Since phonons (with their wavelength  $\lambda_f = 2\pi/k_f = c_f/f$ , where  $c_f$  is the sound velocity in the crystal) are quantized and can only be emitted and absorbed entirely, the frequency of the first-order diffraction is  $\nu_1 = \nu + f$ . In case of an ideal adjustment of the Bragg angle, the *Bragg condition* results in  $\theta_1 = \theta$  (see Fig. 31.32),

$$\sin \theta = \frac{k_f}{2k} = \frac{f\lambda_n}{2c_f} . \quad (31.53)$$

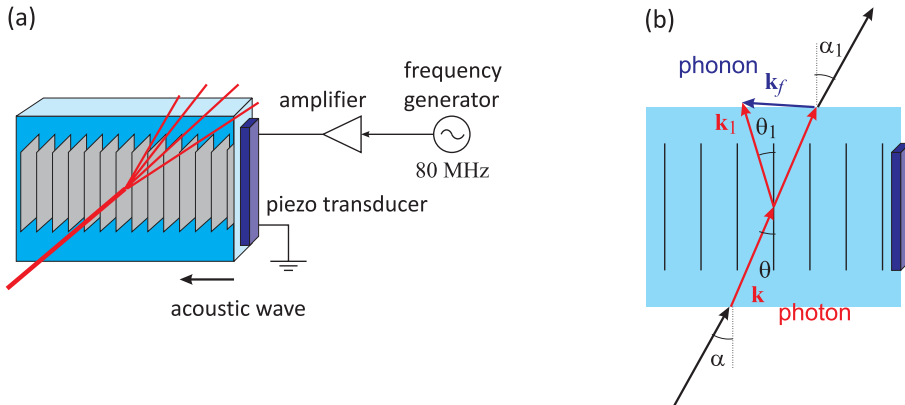


Figure 31.32: (a) Principle of the acousto-optic modulator. (b) Scheme of the diffraction in an acousto-optic modulator: A photon with wavevector  $\mathbf{k}$  is scattered by a phonon with wavevector  $\mathbf{k}_1$  resulting in a photon with wavevector  $\mathbf{k}_f$ .

Since the laser beam is refracted when it enters the crystal, the relation between the incidence and exit angle is given by *Snell's law*,  $\sin \alpha = n \sin \theta$ . With this, the Bragg condition can be written,

$$\boxed{\sin \alpha = \frac{f \lambda}{2c_f}} . \quad (31.54)$$

The angle between the 0<sup>th</sup> and the 1<sup>st</sup> order is, hence,  $2\alpha$ .

In a corpuscular picture, the process can be understood as a *four-wave mixing* (*4WM*) between photons and phonons. The deflection of the laser beam is a consequence of momentum,  $\mathbf{k}_1 = \mathbf{k} + \mathbf{k}_f$ . The frequency shift corresponds exactly to the Doppler shift induced by the Brillouin scattering (absorption and reemission of a phonon in reverse direction), and we obtain a relationship that is equivalent to the Bragg condition,

$$f = \nu_1 - \nu = 2\nu \frac{c_f \sin \theta}{c/n} . \quad (31.55)$$

From the Bragg condition, knowing the deflection angle and the (fixed) frequency shift, we can calculate the sound velocity. A typical value is  $c_f \simeq 4200$  m/s<sup>5</sup>

An AOM works best (highest diffraction efficiency in to the first Bragg order, which may reach more than 90%) at a specific radiofrequency, which typically is located somewhere in the range  $f = 40 \dots 800$  MHz, the most common one being 80 MHz. Deviations from this 'center frequency' are possible within a range of typical  $\pm 10\%$  of the center frequency.

<sup>5</sup>The result (31.55) can be derived from conservations laws for energy  $\omega_1 = \omega + \omega_f$  and momentum  $\mathbf{k}_1 = \mathbf{k} + \mathbf{k}_f$ . Defining  $\omega \equiv 2\pi\nu$ ,  $\omega_1 \equiv 2\pi\nu_1$  and  $\omega_f \equiv 2\pi f$  we find,

$$\frac{\omega_f^2}{c_f^2} = \mathbf{k}_f^2 = (\mathbf{k}_1 - \mathbf{k})^2 = k_1^2 + k^2 - 2\mathbf{k}_1 \cdot \mathbf{k} = \frac{\omega_1^2}{c_n^2} + \frac{\omega^2}{c_n^2} - \frac{2\omega\omega_1}{c_n^2} \cos(2\theta) \simeq \frac{4\omega\omega_1}{c_n^2} \sin^2 \theta .$$

With  $\omega_1 \simeq \omega$  we reproduce the result [742, 743].

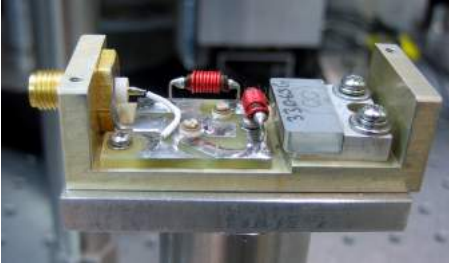


Figure 31.33: Image of an AOM without cover.

### 31.3.2 Electro-optic modulator

An *electro-optic modulator* is an optical device with which, by an applied voltage, the phase, frequency, amplitude or direction of a light beam can be modulated. Modulation bandwidths in the GHz regime are possible. In the simplest case, the EOM consists of a crystal (e.g., lithium niobate), whose refractive index depends on the amplitude of the local electric field. That is, when a lithium niobate crystal is exposed to an electric field the speed of light propagation is reduced. One can thus control the phase of a light beam at the output of a crystal by inserting it into a plate capacitor and applying a voltage. The phase shift of the light depends linearly on the applied voltage.

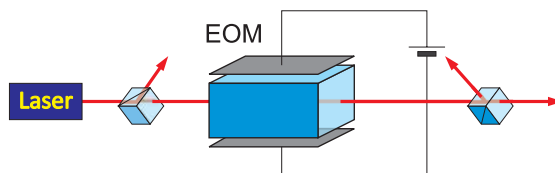


Figure 31.34: Electro optic modulator.

EOMs are often used to generate sidebands in a monochromatic laser beam. They are also used as *Pockels cell*, i.e., as a voltage-controlled phase-plate. The Pockels effect produces in a medium a *birefringence*, which depends linearly on the applied electric field. This is in contrast to the *Kerr effect* Kerr, in which the birefringence depends in a quadratic form of the electric field.

Suppose the optically inactive axis is  $x$ . In this case, the influence of EOM on the polarization of a laser beam is described by

$$\mathcal{M}_{EOM}(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}. \quad (31.56)$$

For operation as a Pockels cell, the EOM is inserted between two crossed polarizers

oriented, e.g., along the  $x$  and  $y$  axis. The EOM itself is rotated by an angle  $\phi$ ,

$$\begin{aligned} \mathcal{M}_{Pockels}(\theta, \phi) &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix} \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ &= 2ie^{i\theta/2} \sin \frac{\theta}{2} \sin \phi \cos \phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \end{aligned} \quad (31.57)$$

For  $\phi = \pi/4$  we get,

$$\mathcal{M}_{Pockels}(\theta, \frac{\pi}{4}) = ie^{i\theta/2} \sin \frac{\theta}{2} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (31.58)$$

That is, an incident beam of light,  $\mathbf{E} = E\hat{\mathbf{e}}_x$ , linearly polarized in  $x$ -direction is rotated into the  $y$ -direction and, depending on the phase shift  $\theta$ , it is completely blocked or transmitted through the Pockels cell [see Fig. 31.35(a)],

$$I_{tr} = I_0 \sin^2 \frac{\theta}{2}. \quad (31.59)$$

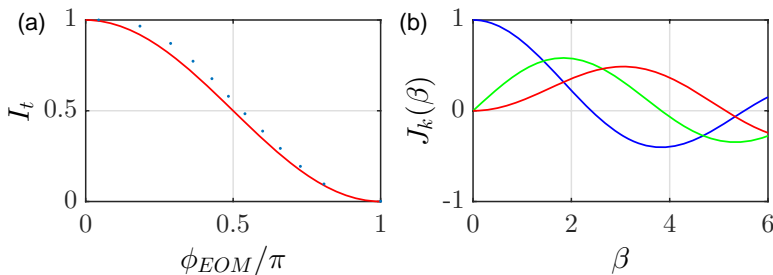


Figure 31.35: (code) (a) Effect of a Pockels cell. The solid line was calculated with the Eq. (31.57), the dotted was measured experimentally. (b) Lowest-order Bessel functions.

### 31.3.3 Optical phase modulation

The frequency and the phase of a laser beam can be influenced and modulated similarly to radiofrequency signals. We can therefore use the calculation of Sec. 30.3.1 completely, only changing the carrier frequency to be the frequency of the light: The Fourier expansion of a complex-valued periodic function  $s(x)$  into a series is defined as,

$$s_N(x) = \sum_{k=-N}^N c_k e^{ikx} \quad \text{where} \quad c_k = \frac{1}{2\pi} \int_{2\pi} s(x) e^{-ikx} dx. \quad (31.60)$$

Applying this to the modulated phase shift factor  $s(\Omega t) = e^{i\theta(t)}$  with  $\theta(t) \equiv \beta \sin \Omega t$ , we get,

$$s_N(\Omega t) = \sum_{k=-\infty}^{\infty} c_k e^{ik\Omega t} \quad \text{where} \quad c_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i\beta \sin \Omega t} e^{-ik\Omega t} d\Omega t, \quad (31.61)$$

but the Fourier coefficients are nothing else than the integral definition of the  $k$ -th order Bessel function,

$$J_k(\beta) \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i(\beta \sin \tau - k\tau)} d\tau, \quad (31.62)$$

where  $J_{-k}(\beta) = -J_k(\beta)$ . Hence, we may write the electric field,

$$\begin{aligned} E(t) &= e^{i[kz - \omega t + i\theta(t)]} = e^{i(kz - \omega t)} \sum_{k=-\infty}^{\infty} J_k(\beta) e^{ik\Omega t} \\ &\simeq J_0(\beta) e^{i\omega t} + J_1(\beta) e^{i\omega t + i\Omega t} + J_{-1}(\beta) e^{i\omega t - i\Omega t} \end{aligned} \quad (31.63)$$

For small modulation indices  $\beta$  only the lowest-order Bessel function contribute noticeable amplitudes, as illustrated in Fig. 31.35(b).

The interpretation of this is, that *phase modulation* imprints sidebands onto a monochromatic laser beam. These sidebands are independent modes which can be resolved, e.g. with an optical spectrum analyzer, as illustrated in Fig. 31.36.

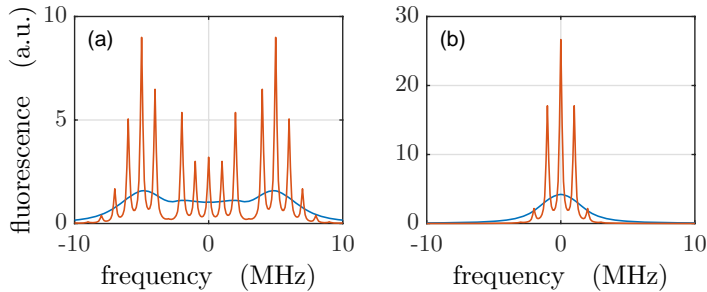


Figure 31.36: (code) Phase modulation sidebands with high (left) and low (right) modulation index resolved by a narrow (red) or broad (blue) filter.

Technically the phase can be modulated by means of an electro-optical modulator, as shown in Fig. 31.37(b). Alternatively, one may apply a periodic modulation of the current which controls a diode laser, as shown in Fig. 31.37(a), which can be done e.g. by inductive coupling using a *bias-T*.

From (31.63) we immediately see that phase modulation remains invisible for a photodetector measuring  $|E(t)|^2$ . Imagine, however, that the light passes through a frequency-selective absorber, as illustrated in Fig. 31.37(b), such that the sidebands suffer unequal losses. Then the photodetector will record (apart from a constant offset) a signal oscillating at the frequency  $\Omega$ ,

$$\begin{aligned} |E(t)|^2 &= \left| J_0(\beta) e^{i\omega t} + a J_1(\beta) e^{i\omega t + i\Omega t} + b J_{-1}(\beta) e^{i\omega t - i\Omega t} \right|^2 \\ &= J_0(\beta)^2 + (a + b) J_1(\beta)^2 + (a - b) J_0(\beta) J_1(\beta) 2 \cos \Omega t + \dots \end{aligned} \quad (31.64)$$

This idea is at the heart of powerful spectroscopic techniques, such as *frequency modulation spectroscopy*, *modulation transfer spectroscopy*, and the *Pound-Drever-Hall* frequency stabilization technique.

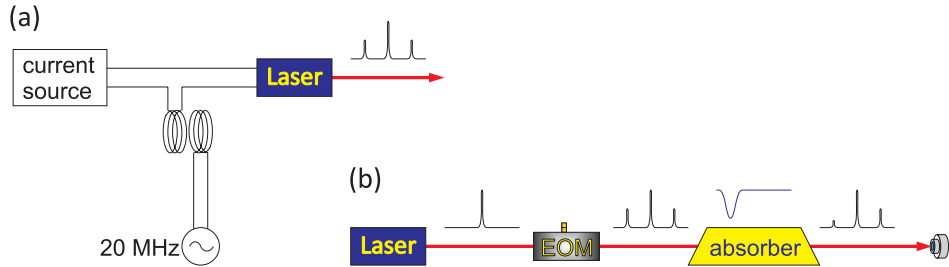


Figure 31.37: (a) Scheme for phase modulation of a diode laser by modulating the drive current. (b) Phase modulation with an external EOM followed by frequency-selective absorption of the lower sideband.

### 31.3.4 Exercises

#### 31.3.4.1 Ex: Response time of an AOM

A beam of light at 689 nm focused to a waist of  $100\ \mu\text{m}$  passes through the crystal of an 80 MHz AOM, characterized by a sound velocity of  $c_s = 4200\ \text{m/s}$ .

a. By how much the first diffraction order is deflected by the AOM? Regarding the beam divergence of the Gaussian beam, will it be possible to spatially separate the diffraction orders?

b. An experimentalist ramps the driving frequency between 70 and 90 MHz by means of a voltage-controlled oscillator. What is the range of diffraction angles covered?

c. Estimating the response time of the AOM by the time that the traveling sound wave needs to cover a distance corresponding to the focus of the light beam, how fast can the experimentalist switch off the light beam by suddenly interrupting the driving signal? What is the modulation bandwidth of the AOM?

d. The light beam passes through the AOM at a distance of  $d = 2\ \text{mm}$  from the piezo transducer generating the sound wave. How will this fact limit response time?

#### 31.3.4.2 Ex: Intensity stabilization with a Pockels cell

Assume that the output power of a laser shows random fluctuations of about 5%. Intensity stabilization is accomplished by a Pockels cell with a halfwave voltage of 600 V. Estimate the ac output voltage of the amplifier driving the Pockels cell that is necessary to stabilize the transmitted intensity if the Pockels cell is operated around the maximum slope of the transmission curve.

#### 31.3.4.3 Ex: Generating sidebands with an EOM

An EOM (e.g. Thorlabs, EO-PM-NR-C1) characterized by a half-wave voltage of  $U_{hvw} = 230\ \text{V}$  at 689 nm is to be used to generate optical sidebands at 20 MHz.

a. Estimate numerically, how much voltage amplitude at what frequency a frequency generator must provide in order to generate optical sidebands having half the light power as the carrier?

b. How high must the finesse of a 5 cm confocal Fabry-Pérot spectrum analyzer be in order to resolve the sidebands.



### 31.3.4.4 Ex: Reflection of a phase-modulated signal from an optical cavity

A phase-modulated light beam (modulation frequency  $f = 20$  MHz) is reflected from an optical cavity and recorded by a fast photodetector, whose bandwidth is larger than  $f$ . Using the Airy formulae for the electric field of a light beam reflected from a cavity (31.24) calculate the reflection spectrum, that is, the intensity of reflected light as a function of detuning  $\Delta = \omega - \omega_c$ , where  $\omega$  is the frequency of the light and  $\omega_c$  a resonant frequency of the cavity. What frequency components does the photodetector signal contain.

### 31.3.5 Experiment: Characterizing an AOM

Fig. 31.38 illustrates the setup, use, and test of an AOM. It is recommended familiarizing with the operation principle of a *voltage-controlled oscillator (VCO)* (see Sec. 30.3.1) and a voltage-controlled *variable attenuator*. We will also learn how to use a spectrum analyzer <sup>6</sup>.

1. Optimize a diffraction efficiency of the AOM. What are the impacts of the Bragg angle, the radiofrequency power, and the laser beam diameter.
2. Measure the deflection angle as a function of the applied radiofrequency. Based on this result, calculate the sound velocity in the crystal.
3. Measure the diffraction efficiency as a function of the applied radiofrequency power at a fixed Bragg angle. Repeat the measurement optimizing the Bragg angle for every value of the radiofrequency.
4. Reduce the radiofrequency power using the variable voltage-controlled attenuator. Determine the diffraction efficiency as a function of radiofrequency power.

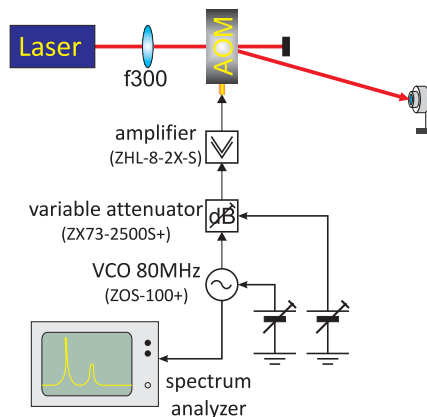


Figure 31.38: Setup for testing an acousto-optic modulator.

<sup>6</sup>Data sheet for the VCO see appendix Fig. 34.15, data sheet for the AOM see appendix Fig. 34.19

### 31.3.6 *Experiment: EOM in a Mach-Zehnder interferometer*

Here we will learn to operate an EOM as Pockels cell and as phase modulator.

1. Align a laser beam through an electro-optic modulator. Supply a voltage between 0 V and 500 V to the EOM. Test its operation by beating the ordinary with the extraordinary beam. Modulate the supply voltage at a low frequency.
2. Set up a Mach-Zehnder interferometer by phase-matching the exit beam of the EOM with a part of the input beam.
3. The interferometer provides a mean to convert a phase modulation into an amplitude modulation. Describe this feature theoretically using the Eqs. (30.12) and (30.13).
4. Use the EOM as a Pockels cell. Rotate the EOM by  $45^\circ$  around the optical axis. Probe the polarization of the outgoing beam with a polarization filter.
5. Modulate the EOM and show that the light acquires sidebands.

### 31.3.7 *Experiment: Creating sidebands with an EOM*

EOMs can be used to generate optical sidebands <sup>7</sup>.

1. Apply the required voltages to a VCO (MiniCircuits, ZOS100), until it generates a variable frequency between 40 and 60 MHz. Attenuate the power with a variable attenuator up to -20 dBm. Check the amplitude and frequency with a spectrum analyzer.
2. Add a bias-T to the power supply of a laser diode. Observe the transmission spectrum of a Fabry-Pérot cavity for various frequencies and modulation amplitudes. Determine the modulation index. Use the known distance of the sidebands to estimate the finesse of the Fabry-Pérot cavity.

## 31.4 Radiofrequency techniques and the transfer of information

It often happens that information is coded within a frequency band corresponding to wavelengths which are not easily transported to other locations. For example, audio frequencies (speech or music), once they are converted to electromagnetic vibrations, correspond to wavelengths of hundreds of kilometers. Such waves are very difficult to radiate and are subject to diffraction.

For this reason, audio frequencies are often used to *modulate* so-called carriers, which in turn are chosen in frequency ranges which are easy to radiate by antennas. This is the basic idea of the radio, where the carrier frequencies are typically chosen in the MHz regime. But information can as well be encoded into laser beams, as illustrated in Fig. 31.39.

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<sup>7</sup>Datasheet for the VCO see appendix Fig. 34.15, data sheet for the power divider see appendix Fig. 34.17, data sheet for the mixer see appendix Fig. 34.18

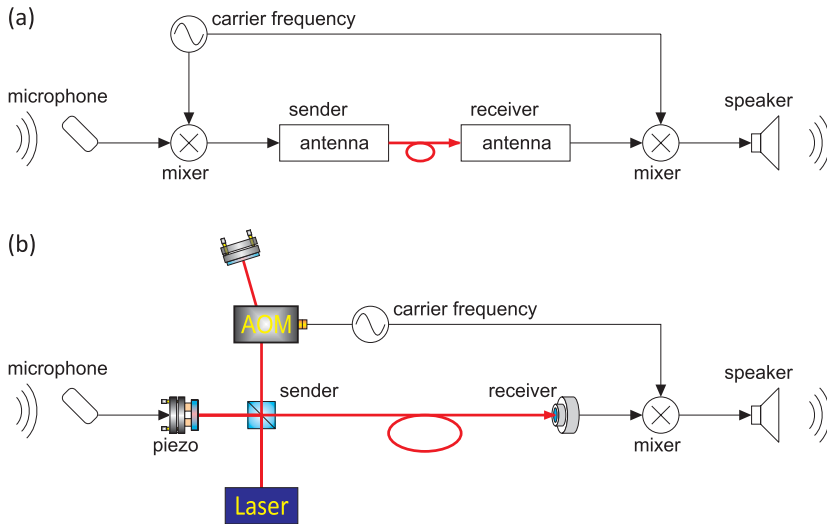


Figure 31.39: Analogy between radio transmission (a) and heterodyne techniques with a laser (b).

### 31.4.1 Measurement of a frequency beat

Interferometry is always based on the splitting and recombination of a wave, e.g., a laser beam or a matter wave. The recombination of laser beams is always a little technical challenge, as it requires a perfect phase matching of the Gaussian laser modes. Let us consider two plane waves  $\mathcal{E}_1 = Ae^{i\omega_1 t}$  and  $\mathcal{E}_2 = Ae^{i\omega_2 t}$  impinging on a photodiode. We suppose that they are phase-matched, such that their wavevectors are parallel. The photodiode then generates a *beat signal*,

$$I = |\mathcal{E}_1 + \mathcal{E}_2|^2 = AB[2 + 2\cos(\omega_1 - \omega_2)t]. \quad (31.65)$$

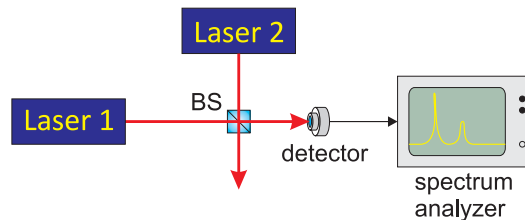


Figure 31.40: Principle of a beat frequency measurement.

In practice, laser beams are usually not plane waves, but have a finite diameter and radius of curvature. In order to get a high contrast signal, a good phase-matching of the beams is important in order to obtain a strong photodiode signal.

### 31.4.2 Homodyne method

For the *homodyne method* the field amplitude of a laser beam,  $E_i$ , with frequency,  $\omega = ck$ , is divided by a beam splitter (reflectivity  $R = |\eta|^2 \simeq 50\%$ ) into a reference beam (reflection at an optically dilute medium) and a probe beam, exactly as we have done for the Michelson interferometer in Sec. 31.1.3, when we obtained the formula (31.13)<sup>8</sup>,

$$I \propto 1 + \cos[k(L_t - L_r)] . \quad (31.66)$$

However, we will now modulate the path length of one interferometer arm, e.g. using an EOM,  $L_r = L_r(t)$ . The modulation can, but does not need to be sinusoidal. In fact it may be an arbitrary radiofrequency signal, e.g. generated by acoustic sound. Restricting to small modulation amplitudes,  $kL_r \ll \pi$ , and choosing the length of the interferometer arms such that,

$$I(t) \propto \sin kL_r \simeq kL_r(t) , \quad (31.67)$$

we see, that the photodetector signal will reproduce the modulation signal. In other words, we encoded information on a laser beam, which carries it (e.g. through an optical fiber) to another place.

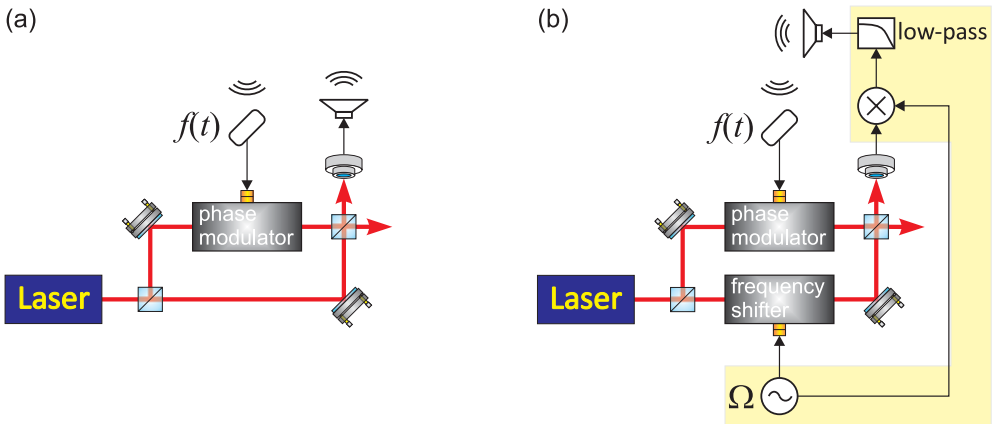


Figure 31.41: Principle scheme of the (a) homodyning and (b) heterodyning technique at the example of a Mach-Zehnder interferometer. The components in the yellow area of (b) constitute a Lock-In amplifier.

### 31.4.3 Heterodyne method

The *heterodyne method* is similar to the homodyne one, except that the probe beam is frequency-shifted (e.g., by the passage through an AOM operated at frequency  $\Omega$ ),

$$\mathcal{E}'_t = \mathcal{E}_t e^{i k L_t + i \Omega t} . \quad (31.68)$$

<sup>8</sup>Here, we call  $L_{t,r}$  the total length of the interferometer arm (back and forth for Michelson, one-way for Mach-Zehnder).

The photodetector signal generated by the beams after their recombination at the beam splitter is,

$$\begin{aligned}
 I &\propto |(1-\eta)\mathcal{E}_r e^{ikL_r} + \eta\mathcal{E}_t e^{ikL_t + i\Omega t}|^2 \\
 &= |-(1-\eta)\eta\mathcal{E}_i e^{ikL_r} + \eta(1-\eta)\mathcal{E}_i e^{ikL_t + i\Omega t}|^2 \\
 &= |(1-\eta)\eta\mathcal{E}_i|^2 |-e^{2ikL_r} + e^{ikL_t + i\Omega t}|^2 .
 \end{aligned} \tag{31.69}$$

This signal is now demodulated with the AOM frequency,

$$I e^{i\Omega t} \propto |-e^{ikL_r} + e^{ikL_t + i\Omega t}|^2 e^{i\Omega t} = e^{2i\Omega t} - e^{ik(L_t - L_r) + 2i\Omega t} - e^{-ik(L_t - L_r)} . \tag{31.70}$$

A low-pass filter cuts all ac-components of the signal,

$$\boxed{I_{filtered}(t) \propto -e^{-ik(L_t - L_r)} \simeq -1 + ik[L_t - L_r(t)]} , \tag{31.71}$$

for small signal amplitudes  $L_r(t)$ .

### 31.4.4 Measuring the quadrature components of an electric field

Photodetectors measure intensities  $I \propto |\vec{\mathcal{E}}|^2$ . Sometimes, however, we are interested in the electric field itself, for example, when we want to get the correlation function  $g^{(1)}(\tau)$  and the spectrum  $S_E(\omega)$  of a signal. A frequently used procedure consists in beating the signal of interest with a frequency-shifted local oscillator and demodulating the *quadrature components* of the beat signal.

Let us consider a signal of interest  $\mathcal{E}_{sig}(t) = |\mathcal{E}_{sig}| e^{i\phi(t)}$  with information encoded in the temporal behavior of the phase  $\phi(t)$ . The first step consists in beating this signal on a photodetector with a frequency-shifted local oscillator  $\mathcal{E}_{lo}(t) = |\mathcal{E}_{lo}| e^{i\omega_{lo} t}$ , yielding a photocurrent,

$$S \propto |\mathcal{E}_{sig} + \mathcal{E}_{lo}|^2 = |\mathcal{E}_{sig}|^2 + |\mathcal{E}_{lo}|^2 + 2|\mathcal{E}_{lo}||\mathcal{E}_{sig}| \cos[\omega_{lo} t - \phi(t)] . \tag{31.72}$$

Now, demodulating this signal simultaneously with the local oscillator frequencies  $\cos \omega_{lo} t$  and  $\sin \omega_{lo} t$ , we get,

$$\begin{aligned}
 U_c &= S \cos \omega_{lo} t = |\mathcal{E}_{lo}||\mathcal{E}_{sig}| \cos \phi(t) + \text{oscillating terms} \\
 U_s &= S \sin \omega_{lo} t = |\mathcal{E}_{lo}||\mathcal{E}_{sig}| \sin \phi(t) + \text{oscillating terms} ,
 \end{aligned} \tag{31.73}$$

where the oscillating terms can be removed by a low-pass filtering. Finally, we calculate,

$$|\mathcal{E}_{sig}| = \frac{\sqrt{U_c^2 + U_s^2}}{|\mathcal{E}_{lo}|} \quad \text{and} \quad \tan \phi(t) = \frac{U_s}{U_c} , \tag{31.74}$$

and obtain the electric field via,

$$\boxed{\mathcal{E}_{sig} = |\mathcal{E}_{sig}| e^{i\phi(t)} = \frac{\sqrt{U_c^2 + U_s^2}}{|\mathcal{E}_{lo}|} e^{i \arctan \frac{U_s}{U_c}}} . \tag{31.75}$$

### 31.4.5 Exercises

#### 31.4.5.1 Ex: Pound-Drever-Hall signal

Consider the photodetector signal of Exc. 31.3.4.4. What signal do you observe when demodulating the signal with an oscillation of frequency  $f$ ? Calculate the derivative of the signal close to resonance; from which parameters does the slope depend, and how must you choose the modulation index to maximize it?

#### 31.4.6 Experiment: Beating two lasers

In this exercise, we will ...

1. Take two independent lasers operating at nearly the same frequency (within  $\sim 1$  GHz) and overlap them at a (non-polarizing) beam splitter.
2. Focus one of the ports of the beam splitter on a photodetector with large bandwidth ( $\sim 1$  GHz).
3. Analyze the beat signal on a spectrum analyzer.
4. Focus a helium-neon laser onto a fast photodetector and determine the free spectral range of the laser resonator.

#### 31.4.7 Experiment: Homo- and heterodyning with a Michelson interferometer

In this exercise, we will ...

1. Set up a Michelson interferometer.

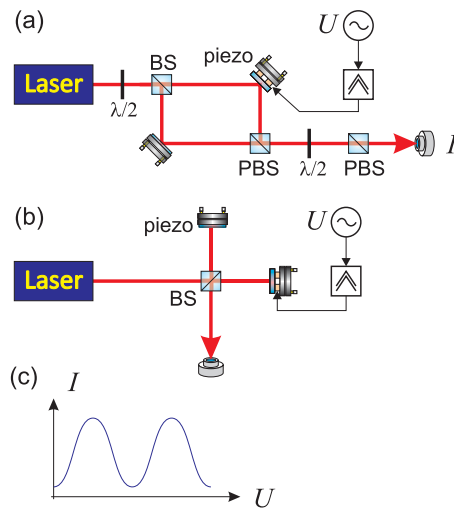


Figure 31.42: Homo- and heterodyning with a Michelson interferometer.

## 31.5 Further reading

C.J. Buczek et al., *Laser injection locking* [\[DOI\]](#)

Zhixin Liu et al., *Optical Injection Locking: From Principle to Applications* [\[DOI\]](#)

H. Kogelnik et al., *Laser Beams and Resonators* [\[DOI\]](#)

A. Yariv, *Quantum Electronics* [\[DOI\]](#)

A. Yariv et al., *Optical waves in crystals* [\[DOI\]](#)

W. Demtröder, *Atoms, Molecules and Photons: An Introduction to Atomic- Molecular- and Quantum Physics* [\[DOI\]](#)

W. Lichten, *Precise Wavelength Measurements and Optical Phase Shifts: I. General Theory* [\[DOI\]](#)

W.W. Chow, *The ring laser gyro* [\[DOI\]](#)

# Chapter 32

## Optical spectroscopy

Modern 'optics' is to be understood as 'physics of light-matter interaction' in the optical energy regime. In this sense, this area of physics comprises quantum optics, photonics, atomic physics, and atom optics. Since the invention of the laser the field of optics has seen a huge technological progress leading to the development of extremely powerful and precise tool for investigating and manipulating matter. The femtosecond laser, the frequency comb, atomic interferometers and clocks, and Bose-Einstein condensation are just a few examples.

Spectroscopy is the art of taking and interpreting spectra, i.e. frequency-dependent response functions. The variety of spectroscopic techniques is so overwhelming that a survey is hopeless. As the course also aims at familiarizing the student with applications, a major part of this course will concentrate on techniques employed and available in quantum optics labs. These techniques are mostly oriented toward ultra-high resolution spectroscopy and techniques of manipulating the motion of atoms.

In Sec. 32.1 to 32.4.3, we will try various spectroscopic techniques applied to atomic or cavity resonances.

### 32.1 Spectrometer and monochromator

Typical dispersive devices are *prisms* and *gratings*.

- lateral displacement as a function of  $\lambda$
- spectral resolving power  $R = |\lambda/\Delta\lambda| = |\nu/\Delta\nu|$
- Rayleigh criterion

#### 32.1.1 Prism spectrometer

For a symmetrical arrangement ( $\alpha_1 = \alpha_2 = \alpha$ ) it is easy to see from Fig. 32.1 that,  $\beta = \frac{1}{2}\epsilon$  and  $\theta = 2(\alpha - \beta)$ . Snell's law the yields,

$$n = \frac{\sin \alpha}{\sin \beta} = \frac{\sin \frac{1}{2}(\theta + \epsilon)}{\sin \frac{1}{2}\epsilon} . \quad (32.1)$$

Hence,

$$\frac{dn}{d\theta} = \frac{1}{2} \frac{\cos \frac{1}{2}(\theta + \epsilon)}{\sin \frac{1}{2}\epsilon} , \quad (32.2)$$



or

$$\frac{d\theta}{dn} = \frac{\sin \frac{1}{2}\epsilon}{1 - n^2 \sin^2 \frac{1}{2}\epsilon} . \quad (32.3)$$

The angular dispersion is therefore,

$$\frac{d\theta}{d\lambda} = \frac{\sin \frac{1}{2}\epsilon}{1 - n^2 \sin^2 \frac{1}{2}\epsilon} \frac{dn}{d\lambda} . \quad (32.4)$$

The spectral dispersion of typical transparent materials is on the order of  $-dn/d\lambda \approx 10^{-4}$ .

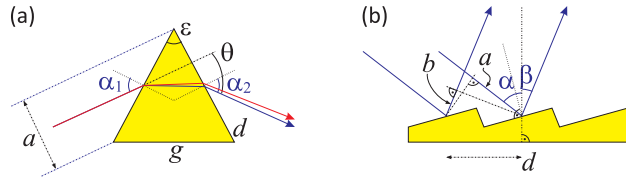


Figure 32.1: Illustration of (a) the prism spectrometer and (b) the grating spectrometer.

**Example 128 (Prism spectrometer):** We calculate the angular dispersion for an equilateral prism ( $\sin \frac{1}{2}\epsilon = 0.5$ ) made of BK7 for two superposed wavelength  $\lambda_1 = 461 \text{ nm}$  ( $n_{\lambda_1} = 1.5243$ ) and  $\lambda_2 = 633 \text{ nm}$  (with  $n_{\lambda_2} = 1.5151$ ) to be,

$$d\theta = \frac{1}{\sqrt{1 - (n/2)^2}} dn \approx 0.8^\circ .$$

The resolving power can be calculated, once we have expressed the limiting aperture  $a = d \cos \alpha$  where  $d = g/(2 \sin \frac{\epsilon}{2})$ ,

$$\left| \frac{\lambda}{\Delta\lambda} \right| = a \frac{d\theta}{d\lambda} = \frac{g \cos \alpha}{1 - n^2 \sin^2 \frac{1}{2}\epsilon} \frac{dn}{d\lambda} = g \frac{dn}{d\lambda} . \quad (32.5)$$

Solve Exc. 29.2.3.14.

### 32.1.2 Grating spectrometer

Destructive interference occurs for,

$$\Delta s = m\lambda = a - b = d \sin \alpha - d \sin \beta . \quad (32.6)$$

Frequently used is the so-called *Littrow configuration* for which  $\alpha = -\beta$ .

The grating represents a multiple beam interferometer, because the beams reflected from every groove of the grating are phase-shifted by amounts (setting  $\alpha = 0$ ,

$$\delta = \frac{2\pi}{\lambda} \Delta s = -2\pi \frac{d}{\lambda} \sin \beta . \quad (32.7)$$

The sum of the reflections from  $N$  grooves of an incident plane wave  $E_{in} = E_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$  is therefore,

$$\mathcal{E}_r = \sqrt{R}\mathcal{E}_0 \sum_{m=0}^N e^{i\mathbf{k}_r\cdot\mathbf{r}-\omega t} e^{im\delta} = \sqrt{R}E_0 e^{i\mathbf{k}_r\cdot\mathbf{r}-\omega t} \frac{1 - e^{iN\delta}}{1 - e^{i\delta}}. \quad (32.8)$$

Consequently, the intensity is,

$$I_r = RI_0 \frac{\sin^2 \frac{N}{2}\delta}{\sin^2 \frac{1}{2}\delta}. \quad (32.9)$$

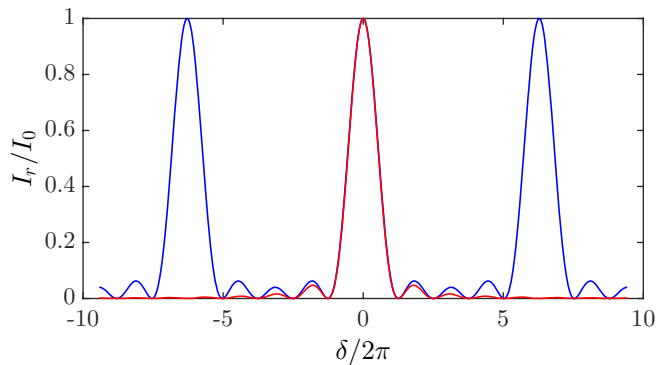


Figure 32.2: (code) Reflection curve of a diffraction grating.

The angular dispersion is, using Eqs. (32.7) and (32.6),

$$\frac{d\beta}{d\lambda} = \left( \frac{d\lambda}{d\beta} \right)^{-1} = -\frac{m}{d \cos \beta} = -\frac{\sin \alpha - \sin \beta}{\lambda \cos \beta}. \quad (32.10)$$

The resolving power is,

$$\left| \frac{\lambda}{\Delta\lambda} \right| = \frac{Nd(\sin \alpha - \sin \beta)}{\lambda} = mN. \quad (32.11)$$

Solve Exc. 32.1.3.1, 32.1.3.2, and 32.1.3.3.

### 32.1.3 Exercises

#### 32.1.3.1 Ex: Resolution of a grating spectrometer

Calculate the spectral resolution of a grating spectrometer with an entrance slit width of  $10 \mu\text{m}$ , focal lengths  $f_1 = f_2 = 2 \text{ m}$  of the mirrors M1 and M2, a grating with 1800 grooves/mm and an angle of incidence  $\alpha = 45^\circ$ . What is the useful minimum slit width if the size of grating is  $100 \times 100 \text{ mm}^2$ ?

### 32.1.3.2 Ex: Grating spectrometer

The spectrometer in Exc. 32.1.3.1 shall be used in first order for a wavelength range around 500 nm. What is the optimum blaze angle, if the geometry of the spectrometer allows an angle of incidence  $\alpha$  about  $20^\circ$ ?

### 32.1.3.3 Ex: Littrow grating

Calculate the number of grooves/mm for a Littrow grating for a  $25^\circ$  incidence at  $\lambda = 488$  nm (i.e., the first diffraction order is being reflected back into the incident beam at an angle  $\alpha = 25^\circ$  to the grating normal).

### 32.1.3.4 Ex: Combining spectrometers

A fluorescence spectrum shall be measured with a spectral resolution of  $10^{-2}$  nm. The experimenter decides to use a crossed arrangement of grating spectrometer (linear dispersion: 0.5 nm/mm) and FPI of Exc. 31.1.10.7. Estimate the optimum combination of spectrometer slit width and FPI plate separation.

## 32.1.4 Experiment: Separating bichromatic light by prisms and gratings

In this experiment we will study the dispersive power of a prism and a grating.

1. Combine the beams of a helium-neon laser and a laser at 461 nm via a beam-splitter. Pass this combination through a prism and quantify the dispersion.
2. Calculate the minimum angle between the two beams.
3. Shine the combination onto a reflection grating and quantify the dispersion.

## 32.1.5 Experiment: Thorlabs optical spectrum analyzer

CCS175, characterization, Thorlabs <sup>®</sup> tour.

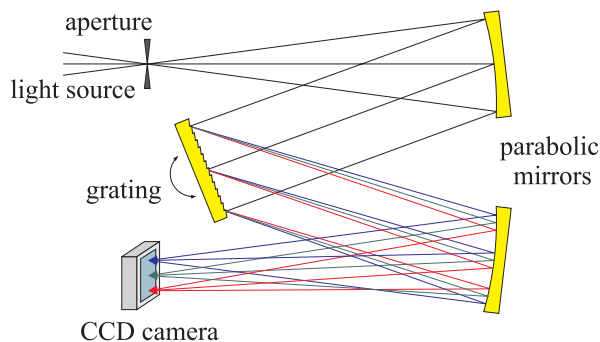


Figure 32.3: Principle of operation of a Czerny-Turner monochromator.

Czerny-Turner CCD spectrometer

1. Irradiate light on OSA and observe the spectrum.

### 32.1.6 Experiment: HighFinesse wavemeter

Wavemeters measure the wavelength of monochromatic light sources by interference. One type of wavemeter is based on a Michelson interferometer, where the length of one interferometer arm is uniformly increased while the interference fringes are counted. Counting the fringes of a known reference laser simultaneously and comparing the counts of the unknown and the reference laser, the wavelength of the unknown laser can be determined with high precision (down to 2 MHz resolution).

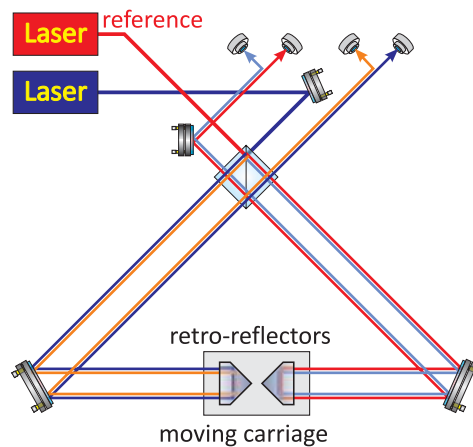


Figure 32.4: Principle of operation of a Michelson-type wavemeter.

1. HighFinesse WSU30, characterization.

## 32.2 Fluorescence, excitation, and absorption spectroscopy

Depending on the information we want to extract from a sample and on the available instrumentation various types of spectroscopic techniques are possible, which will be discussed on the following sections.

### 32.2.1 Classification of spectroscopic methods

It is important to distinguish *fluorescence spectra* from *excitation spectra*: Fluorescence spectra are taken by processing the light emitted from a radiator in a monochromator. That is, the light is shone onto a spectral band filter, which only transmits a narrow fraction of the fluorescence spectrum. The power of the transmitted light is measured with a detector. Upon changing the center frequency of the band filter,

different components of the fluorescence spectrum are measured, thus yielding a curve  $u(\nu)$ , which represents the spectral energy density of the radiator [see Fig. 32.5(a,d)].

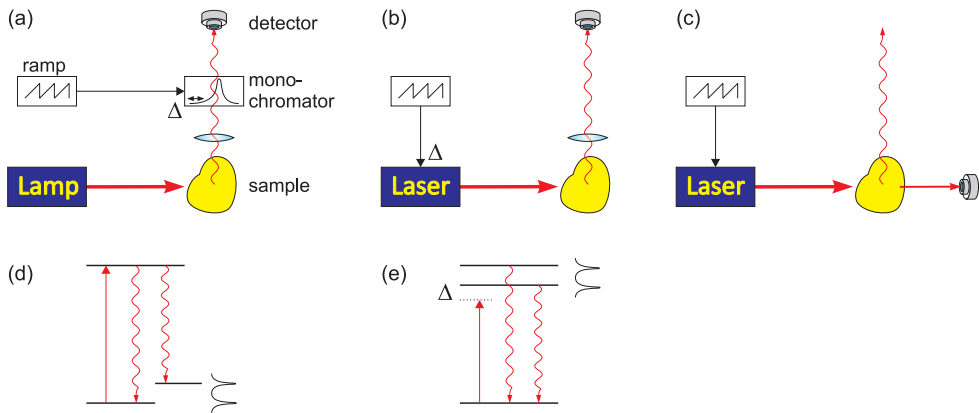


Figure 32.5: (a) Taking a fluorescence spectrum, (b) an excitation spectrum, and (c) an absorption spectrum. Typical level schemes for (d) fluorescence spectroscopy and (e) excitation or absorption spectroscopy.

In contrast to fluorescence spectroscopy, excitation or absorption spectra are taken by varying the frequency of the light exciting a sample. The reemitted light is then measured by a detector without discriminating its frequency components. Obviously, both methods yield very different information about the scatterer [see Fig. 32.5(b,c,e)]. Depending on whether the scattered or the transmitted light is detected, we speak of excitation and absorption spectroscopy.

### 32.2.2 Saturated absorption spectroscopy

One of the most popular spectroscopic techniques is *saturation spectroscopy*, as it is simple, robust, and allows to avoid Doppler-broadening. There are, however, many

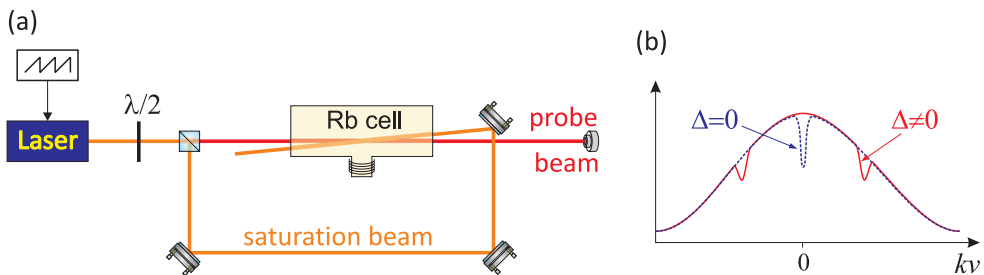


Figure 32.6: (a) Experimental scheme for saturated absorption spectroscopy. (b) Spectral hole burning by the counter-propagating saturation and probe beams for (red) detuned and (blue) resonant light.

possible implementations of saturation spectroscopy, f.ex. *frequency modulation spec-*

*troscopy* or *modulation transfer spectroscopy*, which we will present in the following.

### 32.2.2.1 Calculation of the Lamb-dip

The scheme known as *Lamb-dip spectroscopy* and which is illustrated in Fig. 32.6(a), consists in a cell filled with a gas [for example, atomic rubidium whose resonance frequency is  $\omega_0 = ck = 2\pi c/780$  nm and decay rate is  $\Gamma = (2\pi) 6$  MHz] and two laser beams with the same frequency  $\omega$ , but propagating in opposite directions. One is called the saturating beam, the other probe beam.

The basic idea is that, if the laser frequency is detuned from resonance,  $\omega \neq \omega_0$ , the counter-propagating beams will interact with different velocity classes (i.e. atomic velocities projected on the optical axis,  $v = \mathbf{v} \cdot \hat{\mathbf{e}}_{\mathbf{k}}$ ), which results in two distinct 'holes' in the excitation profile [red curve in Fig. 32.6(b)]. Only for resonant light,  $\omega = \omega_0$ , will the counter-propagating beams interact with the same velocity class (i.e. atomic velocities with  $v = 0$ ). The 'holes' in the excitation profile then overlap thus leading to a deeper depression called Lamb-dip [blue curve in Fig. 32.6(b)].

For a quantitative description of the Lamb-dip we consider Maxwell's one-dimensional and normalized velocity distribution,

$$\rho(v)dv = \sqrt{\frac{m}{2\pi k_B T}} e^{-mv^2/2k_B T} dv . \quad (32.12)$$

As an example, we consider a gas at  $T = 300$  K temperature, where the partial pressure of rubidium is about  $P = 10^{-1}$  mbar, such that the particle density is,

$$n(T) = \frac{P}{k_B T} . \quad (32.13)$$

We also assume a cell length of  $L = 10$  cm.

The probe laser intensity is below saturation, such that the optical cross section for an atom moving with velocity  $v$ , is,

$$\sigma(v) = \frac{6\pi}{k^2} \frac{\Gamma^2}{4(\omega - \omega_0 - kv)^2 + \Gamma^2} , \quad (32.14)$$

where we considered the fact that the atoms moving with the velocity  $v$  along the optical axis perceive the probe laser beam as Doppler-shifted by an amount  $kv$ .

The saturating laser now has high intensity. Let us suppose here,  $\Omega \equiv 10\Gamma$ , where  $\Omega$  is the Rabi frequency caused by the saturating laser. In this way, it creates a population of  $N_e$  atoms in the excited state. Since this population is missing in the ground state,  $N_g = N - N_e$ , the absorption is reduced for the probe beam by a factor,

$$\frac{N_e}{N} = \frac{\Omega^2}{4(\omega - \omega_0 + kv)^2 + 2\Omega^2 + \Gamma^2} . \quad (32.15)$$

In contrast to (32.14), we now have to consider saturation broadening.

We will now calculate the spectrum of the optical density for the probe laser,  $O_D(\omega)$ , and the light intensity transmitted through the cell,  $\frac{I}{I_0} = e^{-O_D}$ , according to the Lambert-Beer law.

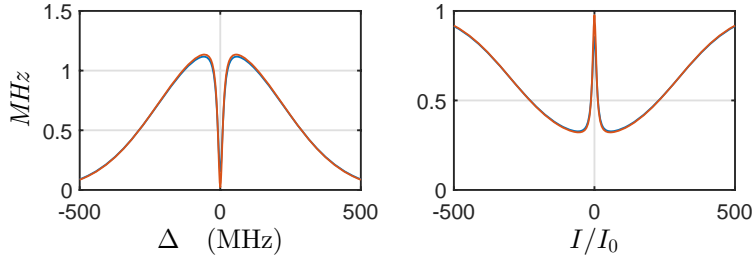


Figure 32.7: (code) (a) Optical density and (b) absorption. (Blue) Integral formula and (green) approximation for high temperature and high saturation.

The optical density with Doppler broadening is,

$$\begin{aligned}
 O_D(T, \omega) &= Ln(T) \int_{-\infty}^{\infty} \frac{N_g - N_e}{N} \sigma(v) \rho(v) dv & (32.16) \\
 &= L \frac{P}{k_B T} \sqrt{\frac{m}{2\pi k_B T}} \frac{6\pi}{k^2} \int_{-\infty}^{\infty} \left( 1 - \frac{2\Omega^2}{4(\Delta + kv)^2 + 2\Omega^2 + \Gamma^2} \right) \frac{\Gamma^2}{4(\Delta - kv)^2 + \Gamma^2} e^{-mv^2/2k_B T} dv,
 \end{aligned}$$

with  $\Delta \equiv \omega - \omega_0$  and substituting  $N_g - N_e = N - 2N_e$ . The widths of the three distribution functions are, respectively,

$$\begin{aligned}
 \delta\nu_{sat} &= \sqrt{\frac{1}{2}\Omega^2 + \frac{1}{4}\Gamma^2} \approx (2\pi) 68 \text{ MHz} && \text{for the saturating beam} \\
 \delta\nu_{Dpp} &= k \sqrt{\frac{k_B T}{m}} \approx (2\pi) 217 \text{ MHz} && \text{for the Doppler broadening} \\
 \delta\nu_{prb} &= \frac{1}{2}\Gamma \approx (2\pi) 3 \text{ MHz} && \text{for the probe beam}
 \end{aligned} \quad (32.17)$$

where  $\bar{v} = \sqrt{k_B T/m}$  is the mean atomic velocity (or the *rms* width) of Maxwell's distribution. Since the spectral width of the probe laser spectrum is much smaller, we can replace it by a  $\delta$ -function,

$$\frac{\Gamma^2}{4(\Delta - kv)^2 + \Gamma^2} \longrightarrow \frac{\pi\Gamma}{2} \delta(\Delta - kv), \quad (32.18)$$

which gives,

$$\begin{aligned}
 O_D(T, \omega) &\simeq L \frac{P}{k_B T} \sqrt{\frac{m}{2\pi k_B T}} \frac{6\pi}{k^3} \int_{-\infty}^{\infty} \left( 1 - \frac{2\Omega^2}{4(\Delta + kv)^2 + 2\Omega^2 + \Gamma^2} \right) \times & (32.19) \\
 &\quad \times \frac{\pi\Gamma}{2} \delta(\Delta - kv) e^{-mv^2/2k_B T} dkv \\
 &= L \frac{P}{k_B T} \sqrt{\frac{m}{2\pi k_B T}} \frac{6\pi}{k^3} \frac{\pi\Gamma}{2} \left( 1 - \frac{2\Omega^2}{8\Delta^2 + 2\Omega^2 + \Gamma^2} \right) e^{-m(\Delta/k)^2/2k_B T}.
 \end{aligned}$$

The *Lamb dip* is the narrow (Doppler-free) feature in the center of the spectrum exhibited in Fig. 32.7. Lamb-dip spectra are commonly serve as frequency references for laser frequency stabilization schemes.

### 32.2.3 Frequency modulation and modulation transfer spectroscopy

Variations of the saturation spectroscopic idea are the *frequency modulation spectroscopy* (FMS) and the *modulation transfer spectroscopy* (MTS). The basic scheme of those techniques is shown in Fig. 32.8. As in saturation spectroscopy, two counterpropagating beams interact with the same atoms of a molecular gas, but now one of the beams is frequency-modulated (e.g. using an electro-optic modulator). In the FMS configuration, the probe beam is modulated, and the sidebands are discriminated at the spectral feature generated by the saturation beam in a very similar way as for the Pound-Drever-Hall technique. The profile of the FMS signal is calculated in Exc. 32.2.4.2 [432, 73, 305, 645, 379, 122, 214, 633, 610, 340, 447].

In the MTS configuration, the saturation beam is modulated, and the sidebands are transferred to the probe beam via nonlinear four-wave mixing processes. In both cases, the sidebands are demodulated with the local oscillator frequency driving the EOM.

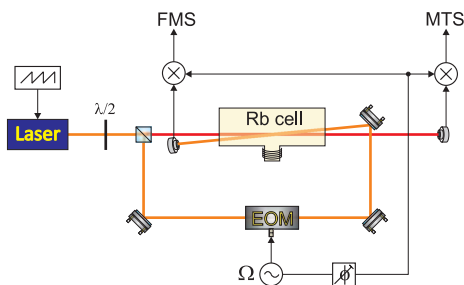


Figure 32.8: Schemes of frequency-modulation and modulation transfer spectroscopy.

The advantages of both techniques is, that they generate dispersive Doppler-free lineshapes. The FMS signal appears as a sharp feature on top of a large Doppler background (similarly to the Lamb-dip). In contrast, the MTS signal is free from Doppler background. The MTS signal recorded by the photodetector is given by,

$$I(\Delta) = \sum_{a,b} \frac{\mu_{ab}^2}{\gamma_j + i\delta} \left( \frac{1}{\gamma_{ab} + i(\Delta + \delta/2)} - \frac{1}{\gamma_{ab} + i(\Delta + \delta)} \right. \\ \left. + \frac{1}{\gamma_{ab} - i(\Delta - \delta)} - \frac{1}{\gamma_{ab} - i(\Delta - \delta/2)} \right), \quad (32.20)$$

where  $a$  and  $b$  denote the lower and upper levels,  $\mu_{ab}^2$  is the electric dipole moment,  $\gamma_{ab}$  is the optical relaxation rate,  $\gamma_j$  is the decay of the energy level  $j$  of the molecule, and  $\delta$  is the modulation frequency. Behind the mixer we see the electric signal,

$$S(\Delta, \vartheta) = \text{Re} [I(\Delta)e^{-i\varphi}], \quad (32.21)$$

where  $\vartheta$  is the demodulation phase [446]. The curves are shown in Fig. 32.8.

**Example 129 (Modulation transfer spectroscopy):** Modulation transfer spectroscopy is caused by four-wave mixing (4WM) processes, which have the



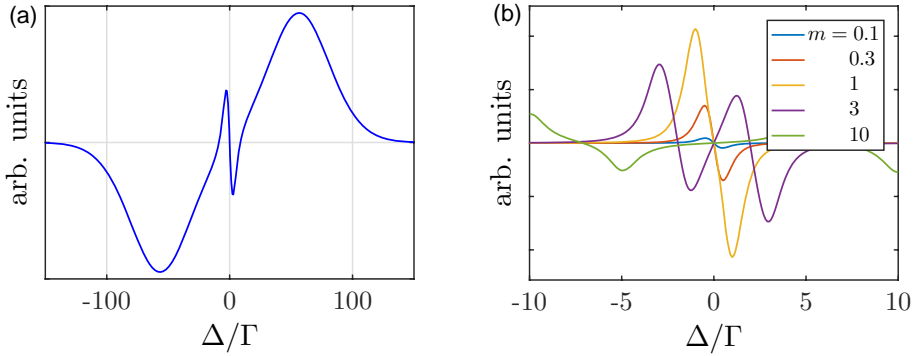


Figure 32.9: (code) (a) Calculated FMS signals and (b) MTS signals as a function of detuning for various modulation indices.

general form  $P(\omega + \Omega) = \chi^{(3)}(\omega + \Omega)E_s(\omega_s)E_p(\omega_s)E_s^*(\omega_s - \Omega)$ , or similar. When the beams  $\omega$  and  $\omega_s$  are counter-propagating, and the atoms are moving, their resonances shift toward  $\omega \mp \mathbf{k} \cdot \mathbf{v}$ , respectively in the atomic rest system. Resonant enhancement of 4WM occurs, when one of the intermediate levels coincides with  $\omega_0$ :

$$\begin{aligned} \omega - \mathbf{k} \cdot \mathbf{v} &= \omega_0 \\ (\omega - \mathbf{k} \cdot \mathbf{v}) - (\omega + \mathbf{k} \cdot \mathbf{v} - \Omega) &= 0 \\ (\omega - \mathbf{k} \cdot \mathbf{v}) - (\omega + \mathbf{k} \cdot \mathbf{v} - \Omega) + (\omega + \mathbf{k} \cdot \mathbf{v}) &= \omega_0 \\ (\omega - \mathbf{k} \cdot \mathbf{v}) - (\omega + \mathbf{k} \cdot \mathbf{v} - \Omega) + (\omega + \mathbf{k} \cdot \mathbf{v}) - (\omega - \mathbf{k} \cdot \mathbf{v} + \Omega) &= 0 . \end{aligned}$$

Assuming  $\omega = \omega_s = \omega - 0$ , these resonances reduced to,

$$\mathbf{k} \cdot \mathbf{v} = 0, \pm \Omega ,$$

and similarly for the other 4WM processes. This means, that the saturation beam burns holes in the velocity distribution at  $\mathbf{k} \cdot \mathbf{v} = 0, \pm \frac{1}{2}\Omega, \pm \Omega$ , which modulate the probe beam.

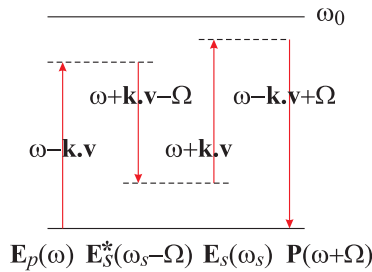


Figure 32.10: Levels involved in 4WM upon MTS.

### 32.2.4 Exercises

### 32.2.4.1 Ex: Lorentz and Gaussian profiles

At which detuning is a Doppler-broadened line dominated by Lorentzian profile of the transition?

### 32.2.4.2 Ex: Frequency-modulation spectroscopy

Calculate the FMS spectrum for a rubidium gas (describing the atoms as a two-level system) under the conditions specified in Sec. 32.2.2 and assuming a modulation frequency of  $f = 10$  MHz and a modulation index of  $\beta = 1$ .

### 32.2.5 Experiment: Rubidium Lamb-dips

In this exercise, we will spectroscopically identify the various lines of the rubidium  $D_2$ -transition of the isotopes  $^{87}\text{Rb}$  and  $^{85}\text{Rb}$ . The hyperfine splittings of the ground and excited states are reproduced in Fig. 32.11.

1. Set up the optics for a Lamb-dip spectroscopy as shown in Fig. 32.11.

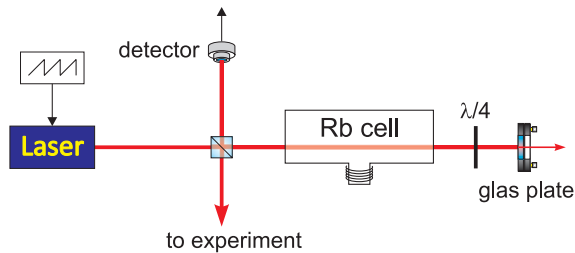


Figure 32.11: Saturation spectroscopy.

2. Fig. 32.12 shows a typical spectrum recorded with a rubidium gas cell. Find an interpretation for the various lines of the spectrum.

## 32.3 Polarization spectroscopy

The *Hänsch-Couillaud technique* uses the *birefringence* of certain materials, devices, or gases.

### 32.3.1 Birefringent cavity

We consider a birefringent cavity exhibiting slightly different path lengths for two axes that we will call, respectively, *ordinary* and *extraordinary*. Fig. 32.13(a) shows the optical setup. The detector signals may be calculated via a concatenation of the Jones matrices for a  $\lambda/2$ -plate, the transmissive response of the cavity, another

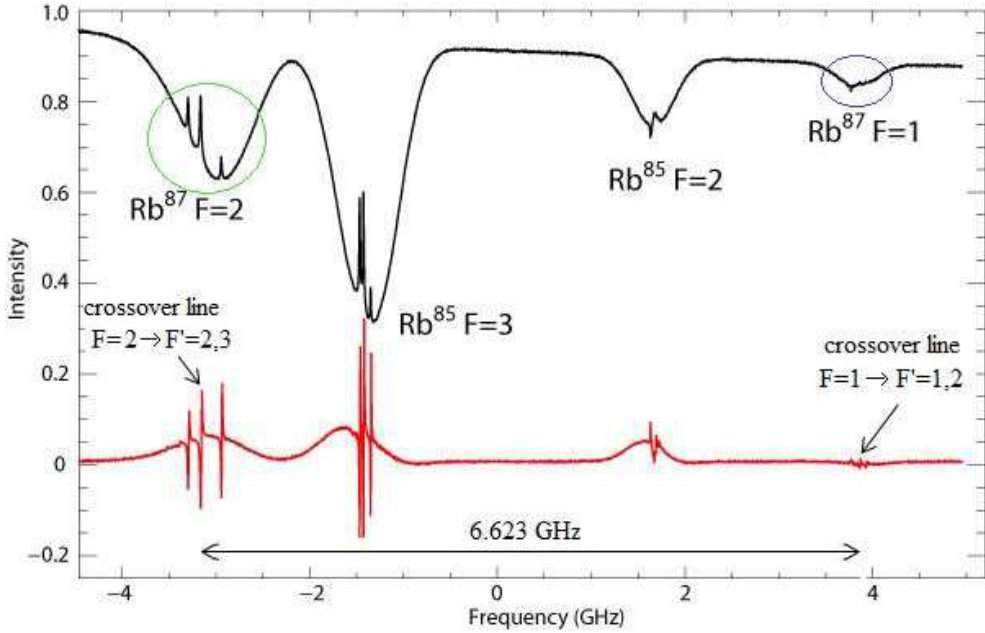


Figure 32.12: (Black) Lamb-dip spectroscopy of a rubidium gas (natural isotope mixture of  $^{85}\text{Rb}$  and  $^{87}\text{Rb}$ ) showing the hyperfine structure transitions of the D2-line. (Red) Derivative of the spectrum in (a).

$\lambda/2$ -plate, and finally a polarizing beam splitter,

$$\begin{pmatrix} E_o \\ E_e \end{pmatrix} = M \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{with} \quad (32.22)$$

$$M \equiv \begin{pmatrix} \cos \beta & \sin \beta \\ -\sin \beta & \cos \beta \end{pmatrix} \begin{pmatrix} \frac{T}{1-Re^{2ik_oL}} & 0 \\ 0 & \frac{T}{1-Re^{2ik_eL}} \end{pmatrix} \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix}. \quad (32.23)$$

For the particular polarization angles  $\alpha = \frac{\pi}{4}$  and  $\beta = 0$ , we derive the difference of the photodetector signals,

$$\Delta I = |E_o|^2 - |E_e|^2 = \frac{T^2}{2} \left[ \frac{1}{1-R^2-2R\cos 2k_oL} - \frac{1}{1-R^2-2R\cos 2k_eL} \right]. \quad (32.24)$$

As Fig. 32.13(b) demonstrates, the spectra corresponding to the axis, obtained by ramping the laser frequency are slightly shifted with respect to each other. Their subtraction leads to a dispersive lineshape that suits for laser locking purposes in the so-called *Hänsch-Couillaud* stabilization.

### 32.3.2 Experiment: Birefringence of a ring cavity

Birefringence automatically occurs in a ring cavities. In this exercise, we will analyze the birefringence observed in reflection of a such a ring cavity. In a *ring cavity*, the

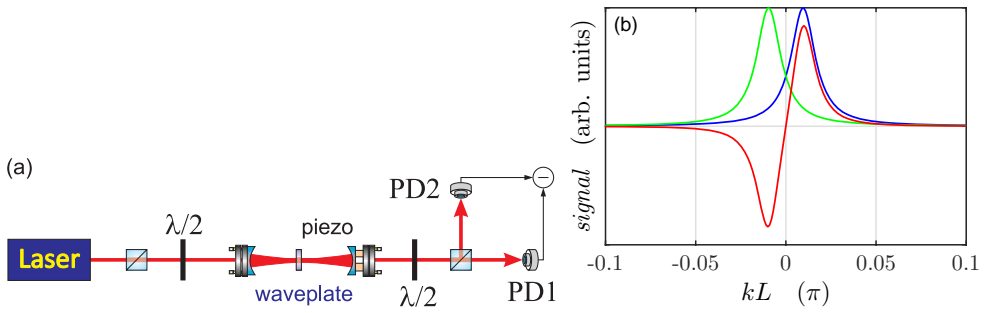


Figure 32.13: (code) (a) Generating a Hänsch-Couillaud error signal by transmission of a birefringent linear cavity. (b) Signals recorded by the two photodetectors (blue and green) and their difference (red).

resonance frequencies of the *s*-polarized and the *p*-polarized modes are slightly shifted from one another due to the different penetration depth of the *s*- and *p*-polarized light modes into the layers of the dielectric mirrors. For a moderate finesse of the cavity (say  $\mathcal{F} = 2000$ ), the modes actually overlap. This leads to a birefringence used in the

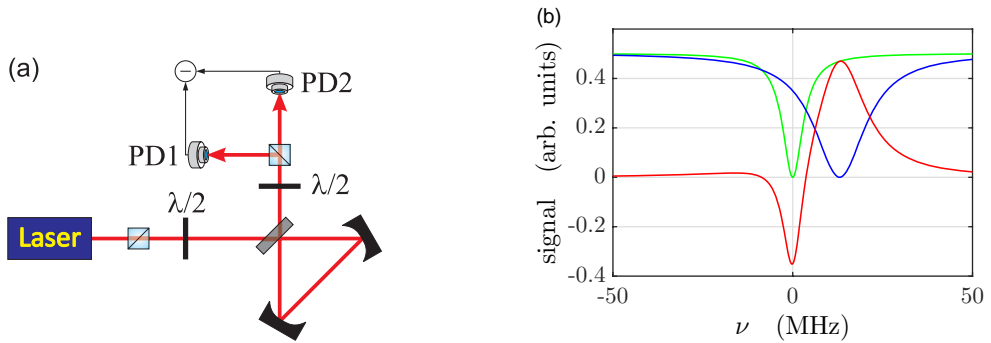


Figure 32.14: (code) (a) Generating a Hänsch-Couillaud error signal by (a) reflection from a ring cavity and (b) transmission of a linear cavity containing a Brewster plate. (b) Signals recorded by the two photodetectors (blue and green) and their difference (red). (a) Reflection signals  $|E_s|^2$  and  $|E_p|^2$  from a birefringent cavity with  $\delta_{fsr} = 8.2$  GHz,  $\varphi_s = 0$ ,  $R_{hr,s} = 99.97\%$ ,  $R_{ic,s} = 99.74\%$ ,  $F_s = \pi(R_{hr,s}^2 R_{ic,s})^{1/6} / [1 - (R_{hr,s}^2 R_{ic,s})^{1/3}]$ ,  $\varphi_p = 0.01$ ,  $R_{hr,p} = 99.92\%$ ,  $R_{ic,p} = 99.34\%$ , and  $F_p = \pi(R_{hr,p}^2 R_{ic,p})^{1/6} / [1 - (R_{hr,p}^2 R_{ic,p})^{1/3}]$ . (b) Difference  $|E_s|^2 - |E_p|^2$ .

famous Hänsch-Couillaud locking scheme. The detector signal in the scheme shown in the figure may be calculated via a concatenation of the Jones matrices for a  $\lambda/2$ -plate, the reflective response of the ring cavity, another  $\lambda/2$ -plate, and finally a polarizing

beam splitter,

$$\begin{pmatrix} E_s \\ E_p \end{pmatrix} = M \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{with} \quad (32.25)$$

$$M \equiv \begin{pmatrix} \cos \beta & \sin \beta \\ -\sin \beta & \cos \beta \end{pmatrix} \begin{pmatrix} \frac{1-e^{-2\pi i\omega/\delta_{fsr}+i\phi_s}}{1-R_s e^{-2\pi i\omega/\delta+i\phi_s}} & 0 \\ 0 & \frac{1-e^{-2\pi i\omega/\delta_{fsr}+i\phi_p}}{1-R_p e^{-2\pi i\omega/\delta+i\phi_p}} \end{pmatrix} \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix}.$$

Calculating  $|E_s|^2$  and  $|E_p|^2$  as a function of the laser frequency  $\omega$  reproduces the curves plotted in Fig. 32.14(a).

1. x

## 32.4 Other spectroscopic techniques

### 32.4.1 Mode-locked femtosecond laser

Mode-locking is a technique in optics by which a laser can be made to produce pulses of light of extremely short duration, down to the order of femtoseconds. The basis of the technique is to induce a fixed-phase relationship between the longitudinal modes of the laser's resonant cavity. Constructive interference between these modes can cause the laser light to be produced as a train of pulses.

In a simple laser, each of these cavity modes amplified within the bandwidth of the gain medium oscillates independently, with no fixed relationship between each other. The individual phase of the light waves in each mode is not fixed, and may vary randomly due to such things as thermal changes in materials of the laser. In lasers with only a few oscillating modes, interference between the modes can cause beating effects in the laser output, leading to fluctuations in intensity; in lasers with many thousands of modes, these interference effects tend to average to a near-constant output intensity.

If instead of oscillating independently, each mode operates with a fixed phase relation to the other modes. Instead of a random or constant output intensity, the modes of the laser will periodically constructively interfere with one another, producing an intense burst or pulse of light. Such a laser is said to be *mode-locked* or *phase-locked*. These pulses occur separated in time by  $\tau = 2L/c$ , where  $\tau$  is the laser cavity round trip time and corresponds to the cavity's inverse free spectral range.

#### 32.4.1.1 Active mode-locking

The most common active mode-locking technique places a standing wave electro-optic modulator (EOM) into the laser cavity. When driven with a sinusoidal electrical signal, this produces an amplitude modulation of the light in the cavity. Considering this in the frequency domain, if a mode has optical frequency  $\nu$ , and is amplitude-modulated at a frequency  $f$ , the resulting signal has sidebands at optical frequencies  $\nu \pm f$ . The modulation frequency is now chosen to coincide with the cavity's free spectral range,  $f = \delta_{fsr}$ , and since the sidebands are driven in-phase, the central mode and the adjacent modes will be phase-locked together. Further operation of the

modulator on the sidebands produces phase-locking of the  $\nu \pm 2f$  modes, and so on until all modes in the gain bandwidth are locked.

This process can also be considered in the time domain. The amplitude modulator acts as a weak 'shutter' to the light bouncing between the mirrors of the cavity, attenuating the light when it is 'closed', and letting it through when it is 'open'. If the modulation rate  $f$  is synchronized to the cavity round-trip time  $\tau$ , then a single pulse of light will bounce back and forth in the cavity. The actual strength of the modulation does not have to be large; a modulator that attenuates 1% of the light when 'closed' will mode-lock a laser, since the same part of the light is repeatedly attenuated as it traverses the cavity.

Related to this amplitude modulation (AM), active mode-locking is frequency modulation (FM) mode-locking, which uses a modulator device based on the acousto-optic effect. This device, when placed in a laser cavity and driven with an electrical signal, induces a small, sinusoidally varying frequency shift in the light passing through it. If the frequency of modulation is matched to the round-trip time of the cavity, then some light in the cavity sees repeated upshifts in frequency, and some repeated downshifts. After many repetitions, the upshifted and downshifted light is swept out of the gain bandwidth of the laser. The only light which is unaffected is that which passes through the modulator when the induced frequency shift is zero, which forms a narrow pulse of light.

The third method of active mode-locking is synchronous mode-locking, or synchronous pumping. In this, the pump source (energy source) for the laser is itself modulated, effectively turning the laser on and off to produce pulses.

### 32.4.1.2 Passive mode-locking

Passive mode-locking techniques are those that do not require a signal external to the laser to produce pulses. Rather, they use the light in the cavity to cause a change in some intracavity element, which will then itself produce a change in the intracavity light. A commonly used device to achieve this is a saturable absorber.

A saturable absorber is an optical device that exhibits an intensity-dependent transmission. For passive mode-locking, ideally a saturable absorber will selectively absorb low-intensity light, and transmit light which is of sufficiently high intensity. When placed in a laser cavity, a saturable absorber will attenuate low-intensity constant wave light (pulse wings). However, because of the somewhat random intensity fluctuations experienced by an un-mode-locked laser, any random, intense spike will be transmitted preferentially by the saturable absorber. As the light in the cavity oscillates, this process repeats, leading to the selective amplification of the high-intensity spikes, and the absorption of the low-intensity light. After many round trips, this leads to a train of pulses and mode-locking of the laser.

Considering this in the frequency domain, if a mode has optical frequency  $\nu$ , and is amplitude-modulated at a frequency  $nf$ , the resulting signal has sidebands at optical frequencies  $\nu \pm nf$  and enables much stronger mode-locking for shorter pulses and more stability than active mode-locking, but has startup problems.

Saturable absorbers are commonly liquid organic dyes, but they can also be made from doped crystals and semiconductors. Semiconductor absorbers tend to exhibit very fast response times ( $\sim 100$  fs), which is one of the factors that determines the

final duration of the pulses in a passively mode-locked laser. In a colliding-pulse mode-locked laser the absorber steepens the leading edge while the lasing medium steepens the trailing edge of the pulse.

There are also passive mode-locking schemes that do not rely on materials that directly display an intensity dependent absorption. In these methods, nonlinear optical effects in intracavity components are used to provide a method of selectively amplifying high-intensity light in the cavity, and attenuation of low-intensity light. One of the most successful schemes is called Kerr-lens mode-locking (KLM), also sometimes called 'self mode-locking'. This uses a nonlinear optical process, the optical Kerr effect, which results in high-intensity light being focussed differently from low-intensity light. By careful arrangement of an aperture in the laser cavity, this effect can be exploited to produce the equivalent of an ultra-fast response time saturable absorber.

### 32.4.2 Frequency comb

In optics, a frequency comb is a laser source whose spectrum consists of a series of discrete, equally spaced frequency lines. Frequency combs can be generated by a number of mechanisms, including periodic modulation (in amplitude and/or phase) of a continuous-wave laser, four-wave mixing in nonlinear media, or stabilization of the pulse train generated by a mode-locked laser. The invention of the *frequency comb* represents a breakthrough in ultrahigh resolution spectroscopy, which was honored with the Nobel price attributed to Theodor Hänsch in 2005 [745, 375, 341, 342, 511, 6, 677].

The frequency domain representation of a perfect frequency comb is a series of delta functions spaced according to,

$$f_n = f_{ceo} + n f_{rep} , \quad (32.26)$$

where  $n$  is an integer,  $f_{rep}$  is the comb tooth spacing (equal to the mode-locked laser's repetition rate or, alternatively, the modulation frequency), and  $f_{ceo}$  is the carrier offset frequency, which is less than  $f_{rep}$ . Combs spanning an octave in frequency (i.e., a factor of two) can be used to directly measure (and correct for drifts in)  $f_{ceo}$ . Thus, octave-spanning combs can be used to steer a piezoelectric mirror within a carrier-envelope phase-correcting feedback loop. Any mechanism by which the combs' two degrees of freedom ( $f_{rep}$  and  $f_{ceo}$ ) are stabilized generates a comb that is useful for mapping optical frequencies into the radio frequency for the direct measurement of optical frequency.

#### 32.4.2.1 Spectrum of a frequency comb

The field emitted by a pulsed laser characterized by its pump laser frequency  $\nu$ , the *repetition rate*  $f_{rep}$ , and the pulse width  $T$ , can be given as a temporal sequence of Gaussian shaped pulses. The repetition is mathematically described as a convolution of the Gaussian profile with a sum of temporal  $\delta$ -functions displaced in time,

$$E(t) = \cos 2\pi\nu t \left( \sum_n \delta\left(t - \frac{n}{f_{rep}}\right) \star e^{-t^2/T^2} \right) = \cos 2\pi\nu t \sum_n e^{-(t - \frac{n}{f_{rep}})^2/T^2} . \quad (32.27)$$

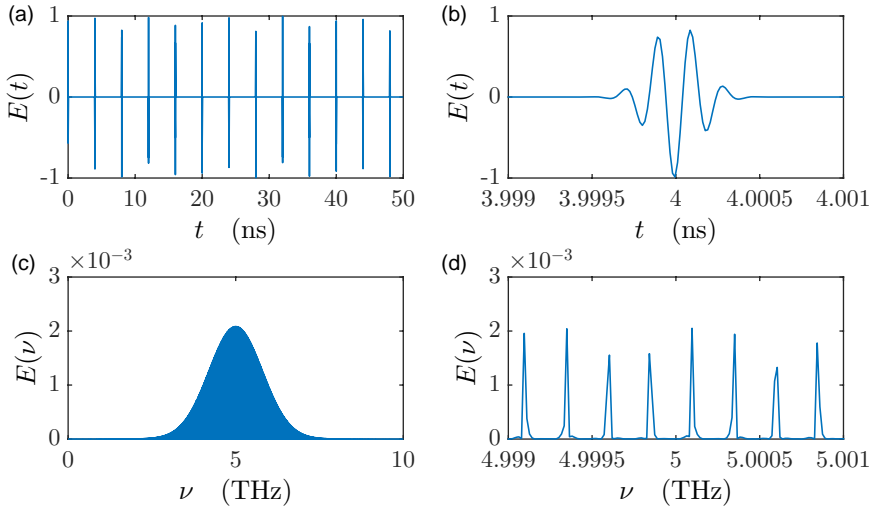


Figure 32.15: (code) Pulse train (a,b) and spectrum (b,c).

The carrier under each pulse is phase-shifted with respect to the adjacent pulse, except when the laser is mode-locked, that is, when,

$$\cos 2\pi\nu t = \cos 2\pi\nu\left(t + \frac{1}{f_{rep}}\right). \quad (32.28)$$

The Fourier transform of the laser field (32.27) is,

$$\begin{aligned} \mathcal{F}[E(t)] &= \int_{-\infty}^{\infty} e^{-i\omega t} \cos 2\pi\nu t \sum_n e^{-(t-n/f_{rep})^2/T^2} dt \\ &= \frac{1}{2} \sum_n \int_{-\infty}^{\infty} e^{-i(\omega-2\pi\nu)t} e^{-(t-n/f_{rep})^2/T^2} dt, \end{aligned} \quad (32.29)$$

where neglect negative frequency components. Using the rules,

$$\mathcal{F}[f(t)e^{i\Omega t}] = \int_{-\infty}^{\infty} e^{-i\omega t} f(t)e^{i\Omega t} dt = (\mathcal{F}f)(\omega - \Omega) \quad (32.30)$$

$$\text{and } \mathcal{F}[f(t-T)] = \int_{-\infty}^{\infty} e^{-i\omega t} f(t-T) dt = e^{-i\omega T} (\mathcal{F}f)(\omega)$$

$$\text{and } \mathcal{F}[e^{-t^2/T^2}] = \int_{-\infty}^{\infty} e^{-i\omega t} e^{-t^2/T^2} dt = T\sqrt{\pi} e^{-T^2\omega^2/4}$$

we get,

$$E(\omega) = \mathcal{F}[E(t)] = \frac{1}{2} T\sqrt{\pi} e^{-T^2(\omega-2\pi\nu)^2/4} \sum_n e^{-i(\omega-2\pi\nu)n/f_{rep}}. \quad (32.31)$$

We now write the pump laser frequency as,

$$\nu \equiv m f_{rep} + f_{ceo}, \quad (32.32)$$



where we set  $m \in \mathbb{N}$  and call  $|f_{ceo}| < f_{rep}$  the *carrier envelope offset*. We also express the Fourier frequency by,

$$\omega \equiv 2\pi(\eta f_{rep} + f_{ceo}), \quad (32.33)$$

firstly *without* specifying that  $\eta$  be an integer number. The spectrum is,

$$|E(\omega)|^2 = \frac{1}{4}\pi T e^{-T^2(\omega - 2\pi\nu)^2/2} \left| \sum_n e^{-2\pi i n(\eta - m)} \right|^2, \quad (32.34)$$

which only gives contributions for,

$$\eta = \frac{\omega - 2\pi f_{ceo}}{2\pi f_{rep}} \in \mathbb{N}. \quad (32.35)$$

I.e. the spectrum of comb frequencies is,

$$|E(\omega)|^2 = \frac{1}{4}\pi T e^{-T^2(\omega - 2\pi\nu)^2/2} \sum_n \delta[\omega - (n f_{rep} + f_{ceo})]. \quad (32.36)$$

The  $\delta$ -function comes from the fact that the sum of (32.35) over many oscillations  $e^{-2\pi i n(\eta - m)}$  vanishes by destructive interference, except when they are *in phase*, which is just the case when  $\omega = n f_{rep} + f_{ceo}$ .

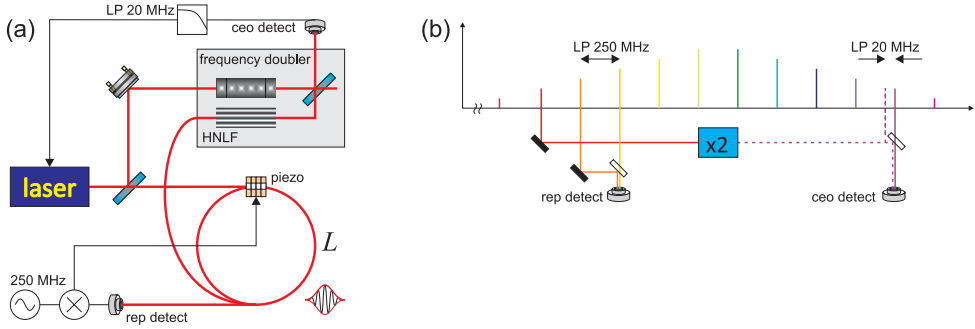


Figure 32.16: (a) Scheme and (b) operation principle of a frequency comb with control of the repetition rate and the carrier envelope offset.

### 32.4.2.2 Mode-locking of a frequency comb

From Eq. (32.28) we see that *mode-locking* is achieved when,

$$\frac{\nu}{f_{rep}} = m + \frac{f_{ceo}}{f_{rep}} \in \mathbb{N}, \quad (32.37)$$

which implies  $f_{ceo} = 0$ . Eq. (32.36) then becomes,

$$|E(\omega)|^2 = \frac{\pi T}{4} e^{-T^2(\omega - 2\pi\nu)^2/2} \sum_n \delta(\omega - n f_{rep}), \quad (32.38)$$

which means that all comb frequencies are locked.

### 32.4.2.3 Referencing radio and optical frequencies

In a frequency comb  $f_{rep}$  is easy to measure, as one just has to filter the beat of the comb light with a low pass filter cutting off frequency components higher than  $f_{rep}$ , as illustrated in Fig. 32.16. In contrast, measuring  $f_{ceo}$  is more complicated. Unless we have an octave spanning frequency comb, i.e. there are two frequencies in the comb,

$$\nu_1 = m_1 f_{rep} + f_{ceo} \quad \text{and} \quad \nu_2 = m_2 f_{rep} + f_{ceo} , \quad (32.39)$$

such that  $\nu_2 = 2\nu_1 + \Delta\nu$  with  $|\Delta\nu| < |f_{ceo}|$ , i.e.  $m_2 = 2m_1$ . We get,

$$m_2 f_{rep} + f_{ceo} = 2m_1 f_{rep} + 2f_{ceo} + \Delta\nu , \quad (32.40)$$

or,

$$f_{ceo} = -\Delta\nu . \quad (32.41)$$

### 32.4.2.4 Dual comb spectroscopy

Optical sensors are based on the interaction of light with matter and are often implemented like some kind of spectrometer. The ideal sensor should detect a given substance with great sensitivity, identify it (especially in the presence of many other substances or a noisy background) and quantify it. Add to these features the ability to perform measurements in real time, if possible remotely, in a compact and easy-to-use assembly at affordable price, and we have an absolutely non-trivial problem. Broadband sources allow to detect multiple substances, but have limitations in resolution, calibration or acquisition time. Monochromatic sources allow good resolution, but in general have limitations on tunability and spectral coverage. The sensitivity can be increased by increasing the optical path of interaction, requiring multi-pass cells or resonant optical cavities, which augment the complexity of the setup. Finally, the detection method places limits on the acquisition rate and also on the sensitivity. Particularly the Fourier transform spectroscopy uses broadband incoherent light sources and the time of acquisition and resolution are limited by the speed of translation of a mechanical stage, as well as the range of its displacement. Here, the use of optical frequency combs replacing the incoherent sources, combined with *dual comb spectroscopy*, brings important advantages [697, 329].

## 32.4.3 Multi-photon spectroscopy

### 32.4.4 Raman spectroscopy

Raman spectroscopy is a spectroscopic technique typically used to determine vibrational modes of molecules, although rotational and other low-frequency modes of systems may also be observed. Raman spectroscopy is commonly used in chemistry to provide a structural fingerprint by which molecules can be identified. Raman spectroscopy relies upon inelastic scattering of photons, known as Raman scattering. A source of monochromatic light, usually from a laser in the visible, near infrared, or near ultraviolet range is used, although X-rays can also be used. The laser light interacts with molecular vibrations, phonons or other excitations in the system, resulting in the energy of the laser photons being shifted up or down. The shift in energy

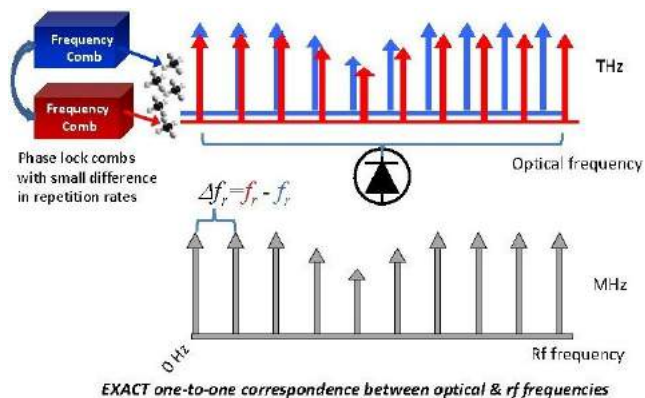


Figure 32.17: Principle of dual comb spectroscopy.

gives information about the vibrational modes in the system. Infrared spectroscopy typically yields similar, complementary, information.

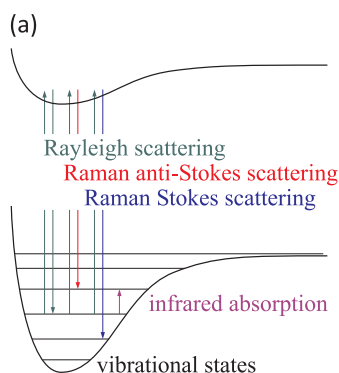


Figure 32.18: Energy-level diagram showing the states involved in Raman spectra.

Typically, a sample is illuminated with a laser beam. Electromagnetic radiation from the illuminated spot is collected with a lens and sent through a monochromator. Elastic scattered radiation at the wavelength corresponding to the laser line (Rayleigh scattering) is filtered out by either a notch filter, edge pass filter, or a band pass filter, while the rest of the collected light is dispersed onto a detector.

Spontaneous Raman scattering is typically very weak; as a result, for many years the main difficulty in collecting Raman spectra was separating the weak inelastically scattered light from the intense Rayleigh scattered laser light (referred to as 'laser rejection'). Historically, Raman spectrometers used holographic gratings and multiple dispersion stages to achieve a high degree of laser rejection. In the past, photomultipliers were the detectors of choice for dispersive Raman setups, which resulted in long acquisition times. However, modern instrumentation almost universally employs notch or edge filters for laser rejection. Dispersive single-stage spectrographs, for example Czerny-Turner (CT) monochromators (see Sec. 32.1.5), paired with CCD

detectors are common.

The name 'Raman spectroscopy' typically refers to vibrational Raman using laser wavelengths which are not absorbed by the sample. Raman spectroscopy is used in chemistry to identify molecules and study chemical bonding and intramolecular bonds. Because vibrational frequencies are specific to a molecule's chemical bonds and symmetry (the fingerprint region of organic molecules is in the wavenumber range  $500 - 1500 \text{ cm}^{-1}$ , Raman provides a fingerprint to identify molecules.

In solid-state physics, Raman spectroscopy is used to characterize materials, measure temperature, and find the crystallographic orientation of a sample. As with single molecules, a solid material can be identified by characteristic phonon modes. Information on the population of a phonon mode is given by the ratio of the Stokes and anti-Stokes intensity of the spontaneous Raman signal. Raman spectroscopy can also be used to observe other low frequency excitations of a solid, such as plasmons, magnons, and superconducting gap excitations. Distributed temperature sensing (DTS) uses the Raman-shifted backscatter from laser pulses to determine the temperature along optical fibers.

### 32.4.5 Time-resolved spectroscopy

pump-probe spectroscopy

## 32.5 Further reading

- G.C. Bjorklund, *Frequency-Modulation Spectroscopy: A new Method for Measuring Weak Absorptions and Dispersions* [DOI]
- J.L. Hall et al., *Optical Heterodyne Saturation Spectroscopy* [DOI]
- J.J. Snyder et al., [DOI]
- R.K. Kaj et al., *High-Frequency Optically Heterodyned Saturation Spectroscopy via Resonant Degenerate Four-Wave Mixing* [DOI]
- G. Camy et al., *Heterodyne Saturation Spectroscopy through Frequency Modulation of the Saturating Beam* [DOI]
- M. Ducloy et al., *Theory of Degenerate Four-Wave Mixing in Resonant Doppler-Broadened Media II* [DOI]
- J.H. Shirley, *Modulation Transfer Processes in Optical Heterodyne Saturation Spectroscopy* [DOI]
- A. Schenzle et al., *Phase Modulation Laser Spectroscopy* [DOI]
- L. Hollberg et al., *Measurement of the shift of Rydberg energy levels induced by blackbody radiation* [DOI]
- L.S. Ma et al., *Optical Heterodyne Spectroscopy Enhanced by an External Optical Cavity: Toward Improved Working Standards* [DOI]

L.S. Ma et al., *Spectroscopy of Te<sub>2</sub> with Modulation Transfer Reference Lines for Precision Spectroscopy in Yb* [\[DOI\]](#)

# Chapter 33

## Locking circuits

In a laboratory we are often confronted with the need to control the value of a physical parameter, f.ex., room temperature, currents and voltages, or the frequency and intensity of laser beams. The physical discipline dealing with the fundamental concepts of this field is called *control theory* and its application to development of automatic control systems is called *control engineering*.

In this chapter, after a brief introduction into *control theory*, we will design and construct a few automatic control systems, which are common in quantum optics labs.

### 33.1 Introduction to control theory

The minimum ingredients of a control system are 1. a *sensor* measuring the actual value of the parameter to be controlled (e.g., a thermometer), 2. an *actuator* capable of correcting the value (e.g., a heater or cooler), and 3. a suitable *controller* (*servo system*) linking sensor and actuator thus providing a feedback.

The controller comprises a *comparator* comparing the measured value with a reference and delivers the difference to a controller, which may be implemented electronically by proportional control, *PID control*, bistable hysteretic control, or programmable logic control. Older controller units have been mechanical, as in a carburetor. Finally, the value computed by the controller is delivered to an actuator, which manipulates and changes a variable in the controlled system (or *plant*).

#### 33.1.1 Open- and closed-loop control

Fundamentally, there are two types of control loop: *open loop* control, and *closed loop* (feedback) control.

In open loop control, the control action from the controller is independent of the 'process output' (or 'controlled process variable'). An example of this is a central heating boiler controlled only by a timer, so that heat is applied for a constant time, regardless of the temperature of the building. The control action is the switching on/off of the boiler. The process output is the building temperature.

In closed loop control, the control action from the controller is dependent on the process output. In the case of the boiler analogy, this would include a thermostat to monitor the building temperature, and thereby feed back a signal to ensure the controller maintains the building at the temperature set on the thermostat. A closed loop controller therefore has a feedback loop which ensures the controller exerts a

control action to give a process output the same as the 'reference input' or 'set point'. For this reason, closed loop controllers are also called feedback controllers.

The definition of a closed loop control system is *a control system capable of canceling the deviation of a system variable from a reference value by means of a feedback signal computed from a measured value of the variable and used to act on the system in a controlled way* [658]. Automatic feedback control has revolutionized all areas of human activities.

To overcome the limitations of the open-loop controller, control theory introduces *feedback*. A closed-loop controller uses feedback to control states or outputs of a dynamical system. Its name comes from the information path in the system: process inputs (e.g. voltage applied to an electric motor) have an effect on the process outputs (e.g. speed or torque of the motor), which is measured with sensors and processed by the controller; the result (the control signal) is 'fed back' as input to the process, closing the loop.

Closed-loop controllers have the following advantages over open-loop controllers:

- disturbance rejection (such as hills in the cruise control example above)
- guaranteed performance even with model uncertainties, when the model structure does not match perfectly the real process and the model parameters are not exact
- unstable processes can be stabilized
- reduced sensitivity to parameter variations
- improved reference tracking performance

In some systems, closed-loop and open-loop control are used simultaneously. In such systems, the open-loop control is termed feedforward and serves to further improve reference tracking performance.

### 33.1.1.1 Closed-loop transfer function

Due to noise the variables of the system become time-dependent. The output of the system  $y(t)$  is fed back through a sensor measurement  $F$  to a comparison with the reference value  $r(t)$ . The controller  $C$  then takes the error  $e(t)$  (difference) between the reference and the output to change the inputs  $u(t)$  to the system under control  $P$ . This is shown in the figure. This kind of controller is a closed-loop controller or feedback controller. We will restrain here to *single-input-single-output control* systems (SISO) disregarding the possibility of having multiple and interdependent inputs and outputs.

If we assume the controller  $C$ , the plant  $P$ , and the sensor  $F$  are linear and time-invariant (i.e. elements of their transfer function  $C(s)$ ,  $P(s)$ , and  $F(s)$  do not depend on time), the systems above can be analyzed using the Laplace transform on the variables,  $U(s) = \mathcal{L}u(t)$ ,  $Y(s) = \mathcal{L}y(t)$ , and  $R(s) = \mathcal{L}r(t)$ . Here,

$$s \equiv \iota f \tag{33.1}$$

is an abbreviation for the imaginary Fourier frequency component  $f$  of the noise. In the following sections we will, however, characterize the transfer functions in terms

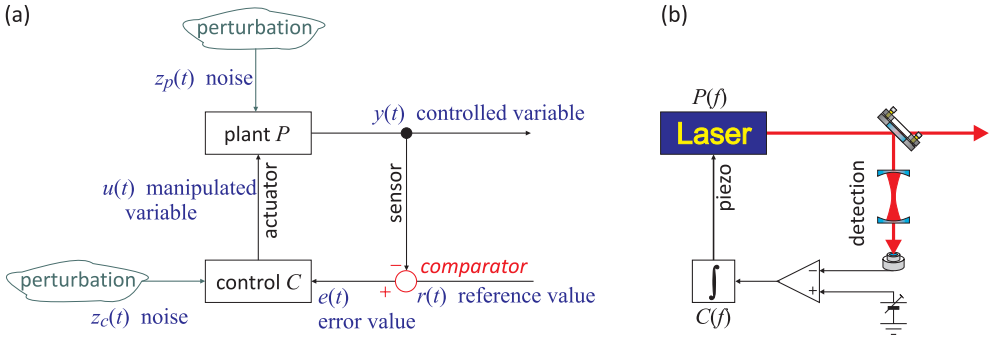


Figure 33.1: (a) General schematic diagram of a feedback loop. (b) Possible implementation for the frequency stabilization of a laser to a cavity resonance,

of real Fourier frequencies. The theoretical foundation of Linear Time-Independent (LTI) systems is outsourced to Sec. 34.2.

For a control to work, it needs to know in which direction to act and when the control point is reached. Therefore, each control needs a slope (*discriminator*) crossing zero. This can be implemented by comparing the signal  $Y(f)$  delivered by the detector (for simplicity assumed to be frequency-independent) with a reference signal  $R$ . The error signal  $E(f) = R(f) - Y(f)$  is then processed by a controller  $C$ , and the control signal  $U(f)$  is passed, via an actuator (for simplicity assumed to be frequency-independent), to the controlled device  $P$ . The controlled device (and obviously all other components of the circuit) are subject to perturbations  $Z$ . The transfer functions form a closed control circuit described by the following relations:

$$Y(f) = P(f)U(f) \quad \text{and} \quad U(f) = C(f)E(f) \quad \text{and} \quad E(f) = R(f) - Y(f). \quad (33.2)$$

Solving the system of equations (33.2) for  $Y(f)$  in terms of  $R(f)$  gives,

$$Y(f) = \frac{P(f)C(f)}{1 + P(f)C(f)} R(f) \equiv H(f)R(f). \quad (33.3)$$

$H(s)$  is referred to as the closed-loop transfer function of the system. The numerator  $V(f) \equiv P(f)C(f)$  is called the *forward gain* (*open-loop gain*) from  $R$  to  $Y$ , and the denominator is one plus the gain in going around the feedback loop, the so-called *loop gain*. If  $|P(f)C(f)| \gg 1$ , i.e. it has a large norm with each value of  $f$ , and then  $Y(f) \simeq R(f)$  and the output closely tracks the reference input.

### 33.1.1.2 Noise reduction via feedback circuits

We have seen that the idea of *locking*, whether mechanical or electronic, is to bring a given physical signal  $Y$  to a predetermined value  $R$  and lock it there, which is the role of the control circuit or *regulator*. Now, considering a possible perturbation of the plant (see Fig. 33.1) by noise  $Z_p$  and also of the regulator by noise  $Z_c$ , the result (33.3) must be generalized,

$$Y(f) = \frac{P(f)C(f)}{1 + P(f)C(f)} R(f) + \frac{P(f)C(f)}{1 + P(f)C(f)} Z_c(f) + \frac{1}{1 + P(f)C(f)} Z_p(f), \quad (33.4)$$



or,

$$Y(f) = \frac{1}{1 + V(f)^{-1}} [R(f) + Z_c(f)] + \frac{1}{1 + V(f)} Z_p(f). \quad (33.5)$$

This shows that, provided the open loop gain is high enough, perturbations affecting the plant can be efficiently be neutralized. In contrast, noise entering via the control cannot be suppressed, and this fact is independent on the chosen controller transfer function: *Perturbations entering between the measurement point and the input of the regulator are not eliminated!* Consequently, the detector (which generally works with very low signals) should not introduce or let penetrate noise, because this affects the variable to be controlled: Any variation of the steering variable at the regulator will be transmitted 1 to 1.

In the following, we will discuss the most common controller called PID-servo.

### 33.1.2 PID feedback control

A *PID controller* continuously calculates an error value  $e(t)$  as the difference between a desired setpoint and a measured process variable and applies a correction based on proportional, integral, and derivative terms. PID is an acronym for Proportional-Integral-Derivative, referring to the three terms operating on the error signal to produce a control signal.

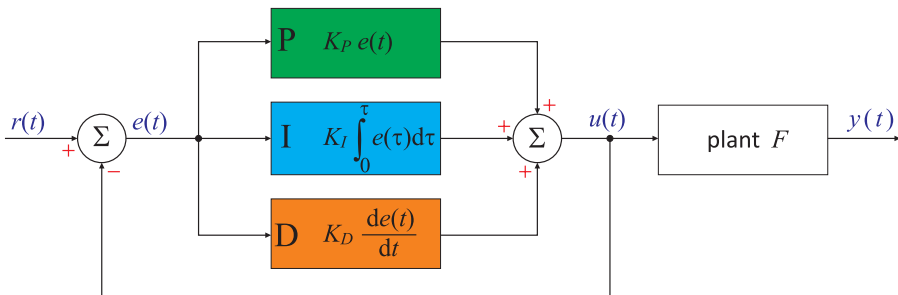


Figure 33.2: A block diagram of a PID controller in a feedback loop,  $r(t)$  is the desired process value or 'set point', and  $y(t)$  is the measured process value. A proportional-integral-derivative controller (PID controller) is a control loop feedback mechanism control technique widely used in control systems.

The theoretical understanding and application dates from the 1920s, and they are implemented in nearly all analogue control systems; originally in mechanical controllers, and then using discrete electronics and latterly in industrial process computers. The PID controller is probably the most-used feedback control design.

If  $u(t)$  is the control signal sent to the system,  $y(t)$  is the measured output and  $r(t)$  is the desired output, and tracking error  $e(t) = r(t) - y(t)$ , a PID controller has the general form,

$$u(t) = K_P e(t) + K_I \int e(\tau) d\tau + K_D \frac{de(t)}{dt}. \quad (33.6)$$

The desired closed loop dynamics is obtained by adjusting the three parameters  $K_P$ ,  $K_I$ , and  $K_D$ , often iteratively by 'tuning' and without specific knowledge of a plant model. Stability can often be ensured using only the proportional term. The integral term permits the rejection of a step disturbance (often a striking specification in process control). The derivative term is used to provide damping or shaping of the response <sup>1</sup>.

Applying Laplace transformation results in the transformed PID controller equation,

$$U(f) = \left( K_P + K_I \frac{1}{if} + K_D if \right) E(f) \equiv C(f)E(f), \quad (33.7)$$

defining the PID controller transfer function  $C(f)$ .

From equations (33.6) or (33.7) we immediately see that the PID transfer functions can readily be implement in electronic circuits using resistors (P), capacitors (I), and inductances (D).

**Example 130 (Comparing servo controllers):** We now assume a low-pass behavior for the plant,

$$P(f) = \frac{1}{1 + if/f_c},$$

and analyze the feedback circuit for four cases.

- The first one is that of a proportional servo,  $C(f) = K_P$ . Then, Eq. (33.5) reads,

$$Y = \frac{K_P}{1 + if/f_c + K_P} (R + Z_c) + \frac{1 + if/f_c}{1 + if/f_c + K_P} Z_p$$

$$\left\{ \begin{array}{l} \xrightarrow{s \rightarrow 0} \frac{K_P}{1 + K_P} (R + Z_c) + \frac{1}{1 + K_P} Z_p \\ \xrightarrow{s \rightarrow \infty} \frac{K_P f_c}{if} (R + Z_c) + Z_p \end{array} \right. .$$

We see that, for limited open-loop gain, noise affecting the plant  $Z_p$  is not eliminated at low frequencies. Additionally, at high frequencies, the gain for the error signal  $R$  drops like  $-6\text{dB/oct}$ .

- The second case is that of an integral servo  $C(f) = K_I/if$ . Then Eq. (33.5) reads,

$$Y = \frac{K_I/if}{1 + if/f_c + K_I/if} (R + Z_c) + \frac{1 + if/f_c}{1 + if/f_c + K_I/if} Z_p$$

$$\left\{ \begin{array}{l} \xrightarrow{f \rightarrow 0} R + Z_c + \frac{if}{K_I} Z_p \\ \xrightarrow{\rightarrow \infty} \frac{K_I f_c}{(if)^2} (R + Z_c) + Z_p \end{array} \right. .$$

Apparently, the noise  $Z_p$  is now eliminated at low frequencies. However, the gain for  $R$  drops even faster at high frequencies.

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<sup>1</sup>PID controllers are the most well established class of control systems: however, they cannot be used in several more complicated cases, especially if MIMO systems are considered.

- The third case is that of a PI-servo,  $C(f) = K_P + K_I/\imath f$ . Then Eq. (33.5) reads,

$$Y = \frac{K_P + K_I/\imath f}{1 + \imath f/f_c + K_P + K_I/\imath f} (R + Z_c) + \frac{1 + \imath f/f_c}{1 + \imath f/f_c + K_P + K_I/\imath f} Z_p$$

$$\left\{ \begin{array}{l} \xrightarrow{f \rightarrow 0} R + Z_c + \frac{\imath f}{K_I} Z_p \\ \xrightarrow{f \rightarrow \infty} \frac{f_c K_P}{\imath f} (R + Z_c) + Z_p \end{array} \right. ,$$

which represents a viable compromise, since it has the same low-frequency behavior as the I-servo, but at high frequencies the gain for  $R$  drops only like  $-6\text{dB/oct}$ .

- Finally, the fourth case is that of a PID-servo,  $C(f) = K_D \imath f + K_P + K_I/\imath f$ . Then Eq. (33.5) reads,

$$Y = \frac{K_D \imath f + K_P + K_I/\imath f}{1 + \imath f/f_c + K_D \imath f + K_P + K_I/\imath f} (R + Z_c) + \frac{1 + \imath f/f_c}{1 + K_D \imath f + K_P + K_I/\imath f} Z_p$$

$$\left\{ \begin{array}{l} \xrightarrow{f \rightarrow 0} R + Z_c + \frac{\imath f}{K_I} Z_p \\ \xrightarrow{f \rightarrow \infty} \frac{1}{1 + \imath f/f_c} (R + Z_c) + \frac{1}{f_c K_D} Z_p \end{array} \right. .$$

The low-frequency behavior remains still the same, but at high frequencies the gain for  $R$  stays constant.

A time domain analysis shows that  $P$  regulators have little phase lag, but the controlled variable can not be zeroed. On the other hand,  $I$  regulators have finite control bandwidth, but the controlled variable can be zeroed.  $PI$  regulators (parallel circuit of  $P$  and  $I$  regulators) have a reaction time  $T_n = K_P/K_I$ ; that is, the jump response is advanced by  $T_n$  in comparison to the regulator  $I$ .

In the time domain we can summarize that regulators

- $D$  are characterized by the absence of memory, but they are very fast,
- $P$  have no idea of the strength of their impact,
- $I$  increase their impact in time until the error disappears.

For practical PID controllers, a pure differentiator is neither physically realizable nor desirable due to amplification of noise and resonant modes in the system. Therefore, a phase-lead compensator type approach is used instead, or a differentiator with low-pass roll-off [344, 244, 245, 686]. See Excs. 33.2.3.1 and 33.2.3.2.

Like any real system, the controlled device behaves as a low-pass for manipulations or perturbations at high frequency. In other words, the device can only respond to external perturbations with finite speed. This delay of the response leads to a phase shift that can reverse the sign of the error signal  $E(f)$  and transform a negative feedback into a positive feedback. Now, in the case that there are high frequency perturbations, for which the amplification of the closed control circuit is  $> 1$ , these perturbations can be amplified to form oscillations. These oscillations, which occur at the bandwidth of the closed loop gain are called *servo oscillations*.

Fig. 33.3 illustrates the necessity of optimizing the gain and the frequency response of the servo circuit: A proportional servo simply providing a frequency-independent gain  $C(f) = K_P$  will lead to a forward gain  $R(f) \propto P(f)$  exhibiting a low-pass behavior, i.e. a phase-shift  $\phi = -\pi/2$  transforming negative to positive feedback. The gain at the frequency where this happens need to be lower than 1, otherwise the feedback servo will generate servo-oscillations, i.e. it will oscillate at the lowest Fourier frequencies where noise is amplified. A PI-servo alleviates this problem by a phase shift in opposite direction.

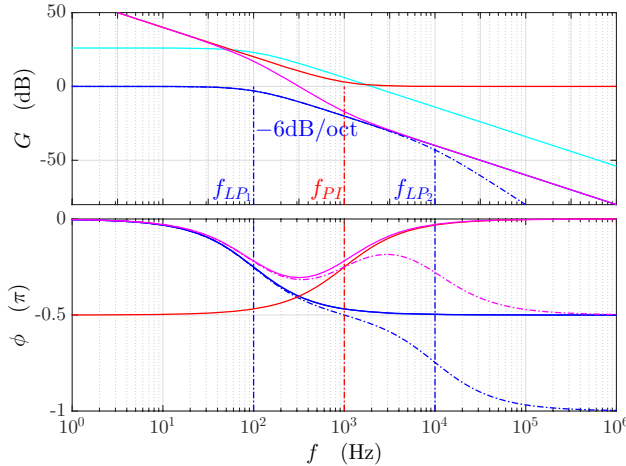


Figure 33.3: (code) Bode diagram for a plant subject to low-pass behavior and for a PI-servo. (blue solid) Low-pass filter with 100 Hz bandwidth; (blue dash-dotted) another low-pass filter at 100 kHz; (cyan) same as blue, but amplified by 20 dB; (red) PI-servo; (magenta) open-loop amplification.

### 33.1.3 Noise transfer in feedback loops

In order to develop a model for noise transfer we must understand what noise is and how it can be measured. This is not a simple task and we therefore outsourced a proper discussion to Sec. 34.3. Here, we will only use the information that noise affecting a signal  $y(t)$  is quantified by a *spectral noise density* defined as the Fourier transform of the signal's autocorrelation function (34.59),

$$S_y(f) \equiv \mathcal{F}[\overline{y^*(t)y(t+\tau)}] . \tag{33.8}$$

Now, we can see how noise is transmitted through an LTI device  $P(f)$ :

$$\boxed{Y(f) = P(f)X(f) \Rightarrow S_y(f) = |P(f)|^2 S_x(f)} . \tag{33.9}$$

This result can be applied to our formula (33.5) describing a feedback loop,

$$\boxed{S_y(f) = \left| \frac{1}{1 + V(f)^{-1}} \right|^2 S_c(f) + \left| \frac{1}{1 + V(f)} \right|^2 S_p(f)} . \tag{33.10}$$

This formula describes how a servo control shapes the noise spectrum of a feedback-controlled variable  $y(t)$ .

**Example 131 (Noise reduction by feedback):** As an example, let us study the control circuit for stabilizing a laser to a cavity mode depicted in Fig. 33.1(b) using the following additional background information: The laser frequency  $\omega$  be perturbed by  $1/f$  noise described by the power spectral density,

$$S_p(f) \equiv 2 \cdot 10^{-24} / f .$$

This noise enters the feedback loop via the fluctuations  $z_p(t)$  depicted in

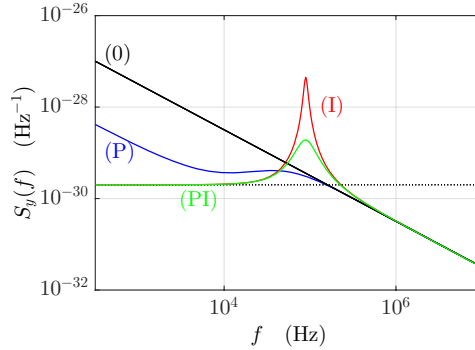


Figure 33.4: (code) Spectral density of frequency fluctuations of the servo system exhibited in Fig. 33.2. Shown is the spectral noise density  $S_y(f)$  of the laser light for 4 different feedback gain curves: (black solid) no feedback control  $C(f) = 0$ , (blue) P-regulator with  $C(f) = 4$ , (red) I-regulator with  $C(f) = 5 \cdot 10^6 / \nu f$ , and (green) PI-regulator  $C(f) = 4 + 5 \cdot 10^6 / \nu f$ .

Fig. 33.1(a). The black solid line in Fig. 33.4 traces the noise spectrum  $S_p(f)$ , which is also the noise expected for the laser without feedback loop. Furthermore the optical cavity, which constitutes the essential part of the regulator, is itself afflicted by acoustic noise and thermal drifts which, for simplicity, we describe by a white Fourier frequency spectrum given by,

$$S_c(f) \equiv 2 \cdot 10^{-30} \text{ Hz}^{-1} ,$$

and represented by the black dotted line in Fig. 33.4. As we have seen, servo systems always have a finite bandwidth beyond which noise is fully coupled to the system. For example in laser frequency locks, the weakest point of a servo chain is often the small bandwidth of a piezo transducer used to correct the length of the laser cavity. We describe this behavior by a low-pass filter for the transfer function of the laser,

$$P(f) = \frac{1}{1 + \nu f / f_c}$$

with a bandwidth of  $f_c = 10$  kHz.

Fig. 33.4 demonstrates how the  $1/f$  noise  $S_p(f)$  can be efficiently suppressed at frequencies below the low-pass filter cut-off  $f_c$  to a value limited by the white noise  $S_c(f)$  entering through the regulator. As predicted by the formula (33.10), the suppression of the noise  $S_p(f)$  becomes all the better, as the open-loop gain

$V(f)$  gets higher. However, with the amplification of the controller, also the gain of the closed control circuit increases, and this necessarily causes phase shifts, which lead to (servo-)oscillations in the circuit appearing as a strong peak of strong noise around a certain Fourier frequency  $f_{bw}$  characterizing the bandwidth of the closed loop servo system. Note that high-frequency noise, to which the cavity might be subject, is not coupled to the laser, because it is filtered by the low-pass filter  $P(f)$  to the same extent as the error signal itself.

The next example, exhibited in Fig. 33.5, shows the experimental characterization of a dye laser locked via the Pound-Drever-Hall technique (see Sec. 33.3.3) to an optical cavity.

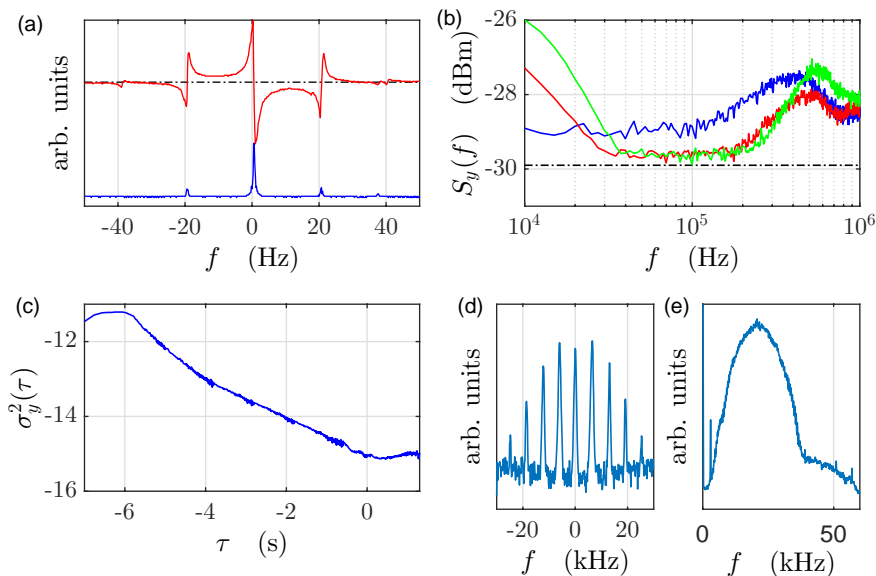


Figure 33.5: Characterization of a Pound-Drever-Hall stabilization of a dye laser. (a) PDH error signal (red) and cavity transmission signal (blue), (b) spectral density of frequency fluctuations, (c) Allan variance. (d-e) Beat signals of Mach-Zehnder interferometers. In (d) one interferometer arm is passed through an optical fiber attached to a piezo transducer to which a sinusoidal 5 kHz modulation of is applied. This demonstrates the sensitivity of optical fibers to acoustic noise. In (e) one interferometer arm is send to another optical table and back. This demonstrates how mechanical vibrations of optical components in the beam path can broaden the spectrum of a laser field.

## 33.2 Amplitude stabilization circuits

### 33.2.1 Laser intensity stabilization with an AOM

The light emitted from lasers is generally subject to *frequency fluctuations* and *intensity fluctuations*, which are unacceptable for many applications. In this section we will construct an *intensity stabilization* for a laser beam.

One way of stabilizing the light intensity of a laser beam consists in using the an acousto-optic modulator, as shown in Fig. 33.6. The first Bragg diffraction order (see Sec. 31.3.1) is focused onto a photodiode. Intensity fluctuations of the light recorded by the photodiode are converted into voltage fluctuations, processed by an electronic circuit fed back to the AOM. The intensity of light diffracted into the first order can be controlled via the power of the radiofrequency alimenting the AOM. The control circuit can now be conceived such as to neutralize the intensity fluctuations recorded by the photodiode.

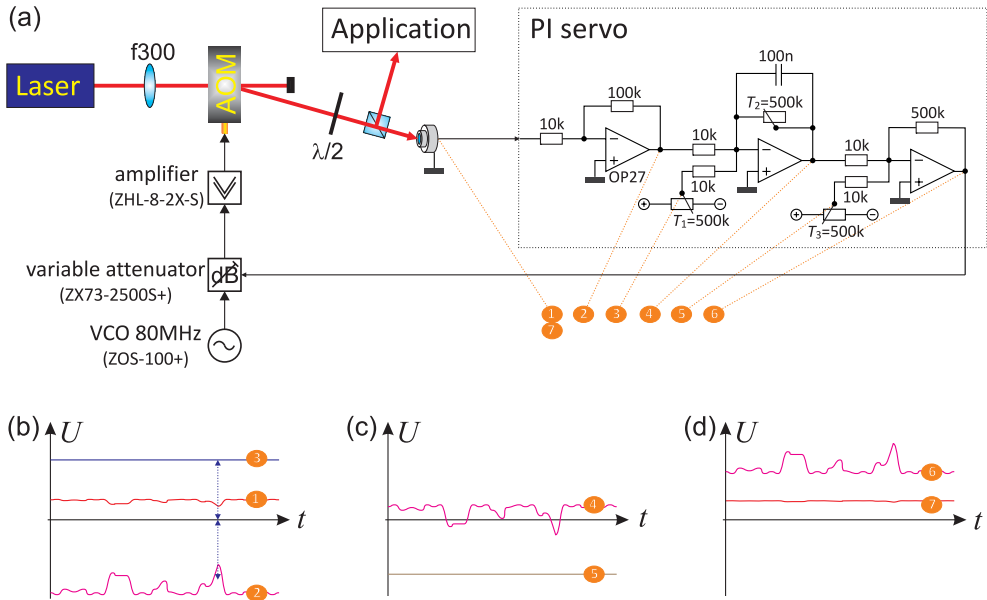


Figure 33.6: (a) Layout of the intensity control. The variable attenuator controls the amplitude of the radiofrequency driving the AOM: low voltage (0 V) increases the attenuation, high voltage (+16 V) reduces it. The sketched control circuit realizes a negative feedback, when the photodetector produces a positive signal. (b-d) Signals recorded at the test points of the circuits shown in (a). See text for explanations.

### 33.2.1.1 Operation principle and adjustment procedure

The idea of the intensity stabilization is illustrated in Fig. 33.6(b-d): The laser intensity scattered into the first diffraction order is recorded by a photodiode (test point 1 in the figure). The signal is then amplified (and inverted) by a first OpAmp (test point 2). The trimmer  $T_1$  (test point 3) is now adjusted to a positive voltage compensating the DC part of the signal (2), i.e., the sum (2+3) after being inverted and amplified by the second OpAmp (test point 4), should be around zero DC. The signal (2+3) is called *error signal*, since it is this signal which tells us in which direction the control circuits has to work to counteract the power fluctuation. In the present design, the second OpAmp also incorporates the PI servo (see Sec. 33.1), which can be adjusted via the amplification of the trimmer  $T_2$  and the capacity  $C$ .

It is now important to realize, that the variable attenuator works best around a given control voltage, which is provided by adding via the trimmer  $T_3$  (test point 5) and a third OpAmp an appropriate offset. Furthermore, we note that variable attenuator reduces its attenuation with increasing control voltage. Thus, the control signal (test point 6) works to enhance the efficiency of the AOM, when the photodiode signals a power drop, and vice versa. As a result, the light power in the first diffraction order is stabilized, however, at a level inferior to the unstabilized power [686, 245].

The trimmers of the servo circuits can be adjusted using the following procedure:

1. Observe the light intensity and its fluctuations at test point (1), set test point (4) to ground (e.g. short-circuiting the trimmer  $T_2$ ), and adjust trimmer  $T_3$  until the light intensity level is at bit lower than the lowest fluctuations.
2. Reconnect test point (4) to the circuit and adjust trimmer  $T_1$  until the voltage at test point (4) cancels to zero.

### 33.2.2 PI servo for a current stabilization

Many applications in quantum optics require very stable high currents, for instance, in coils generating magnetic field for atomic trapping potentials. Here, we will construct a *PI servo* to para realize a *current stabilization*.

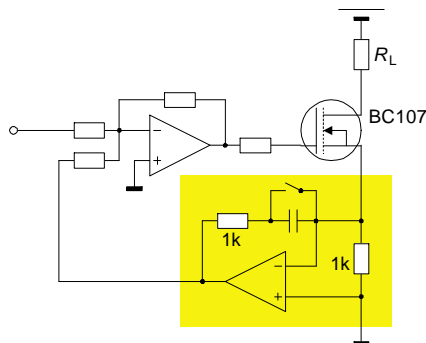


Figure 33.7: Current stabilization.

### 33.2.3 Exercises

#### 33.2.3.1 Ex: Integrator

Determine the transfer function of the circuit depicted in Fig. 33.8. What kind of control circuit is it?

#### 33.2.3.2 Ex: PID controller

Consider the PID controller transfer function in series,

$$C(f) = K \left( 1 + \frac{1}{ifT_I} \right) (1 + ifT_D) ,$$



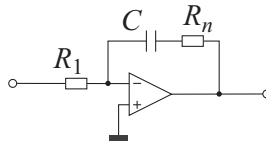


Figure 33.8:

a first-order low-pass filter in the feedback loop,

$$F(f) = \frac{1}{1 + \imath f T_F} ,$$

and a linear actuator with low-pass behavior,

$$P(f) = \frac{A}{1 + \imath f T_P} .$$

How do you have to choose the various time constants in order to let the closed-loop transfer function be  $H(f) = 1$ .

### 33.2.4 *Experiment: Development of an intensity stabilization*

We will now set up an intensity stabilization. For the realization of the project prior knowledge of 1. photodetectors (see Sec. 30.2.1), 2. acousto-optic modulators (AOM) (see Sec. 31.3.1), 3. electronic circuits (see Sec. 30.1.3), and 4. control circuits (see Sec. 33.1) is required.

1. Realize the optical setup illustrated in Fig. 33.6. Optimize the alignment of the AOM (in particular, the focus and the Bragg angle) in order to maximize the efficiency of the AOM. Take care not to saturate the photodiode, if necessary adapt the load resistance (see Sec. 30.1.). Study the data sheet of the variable attenuator.
2. Derive and plot the transfer function for ac-signals of the electronic circuit. What kind of control circuit is it?
3. Set up the electronic circuit exhibited in Fig. 33.6. Test it by observing the signals at the six test points marked in the circuit diagram. Understand and interpret the roles of the three adjustable parameters: input offset, amplification, and output offset.
4. Incorporate the servo circuit into the optical setup as shown in Fig. 33.6. How to make sure the circuit is operating properly? <sup>2</sup>.

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<sup>2</sup>Datasheet for the VCO see appendix Fig. 34.15,  
data sheet for the variable attenuator see appendix Fig. 34.16,  
data sheet for the amplifier see appendix Fig. 34.14.

### 33.2.5 *Experiment: PI servo for a current stabilization*

How to control high currents? How to dramatically increase the switching speed despite inductive loads and eddy currents?

1. Connect a resistive charge to a voltage source. Insert a *MOSFET* into the circuit and a small resistor. Control the gate of the MOSFET with a voltage and measure the current of the circuit via the voltage drop at the small resistor as a function of the gate voltage.
2. Now control the gate voltage via the voltage measured at the small resistor and measure again the dependency voltage-to-current.

## 33.3 Frequency stabilization circuits

Although lasers are often monochromatic, they generally have a poor intrinsic frequency stability, that is, the frequency of the light field  $E(t) = \sin \omega t$  drifts in time,  $\omega = \omega(t)$  on a time scale, which is slow in comparison to the oscillation period  $1/\omega$ . The reasons for these drifts are typically acoustic noise or thermal drifts to which the laser device is subject and which are difficult to avoid.

Often it is much easier to guarantee the mechanical and thermal stability of a passive device exhibiting resonances, such as an optical cavity. Furthermore, nature provides intrinsically stable resonances, such as narrow atomic transitions. These resonances can be used to actively stabilize the frequency of lasers via feedback servo circuits. In the following sections we will present a few common techniques.

### 33.3.1 Side-of-fringe stabilization to/of a Fabry-Pérot cavity

Resonances are generally characterized by peaked profiles symmetrically centered about a resonance frequency  $\omega_0$ . Excited by a laser field of frequency  $\omega$ , they respond by an oscillation whose amplitude depends on the detuning  $\omega - \omega_0$ . Unfortunately, the amplitude of the response signal does not tell us, whether the detuning is positive or negative. We have to invent techniques allowing us to extract this information from the response signal and to generate a true error signal.

One of these techniques is the *side-of-fringe stabilization* technique illustrated in Fig. 33.9. Here, the laser is tuned to one side of the optical resonance such that, when the laser frequency drifts, the response signal increases or decreases correspondingly. Technically, this is achieved by comparing (i.e. subtracting) the response signal with a stable reference signal.

### 33.3.2 Lock-in method for frequency stabilizing to/of a cavity

One method of stabilizing a laser on a resonator consists in modulating the frequency slightly and then demodulating the transmission signal of the resonator at the same frequency. This is the so-called *lock-in method*. Frequency modulation of the laser beam can be done by modulating the laser diode feed current, the piezo of the extended laser cavity or using an AOM. Fig. 33.10 shows the layout of the optical assembly.

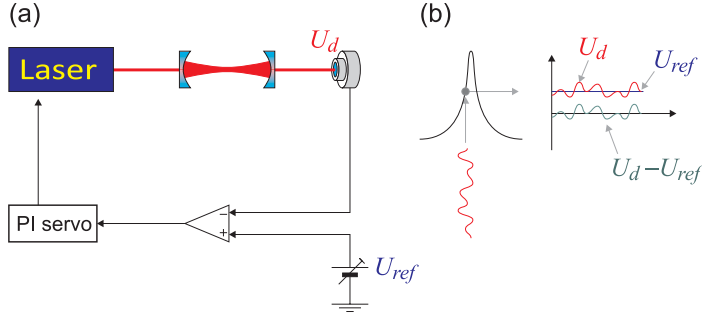


Figure 33.9: (a) Frequency stabilization to a cavity using the side-of-fringe method. (b) The laser is tuned to rising (or falling) slope of a transmission curve of a Fabry-Pérot cavity. The error signal is compared with reference voltage.

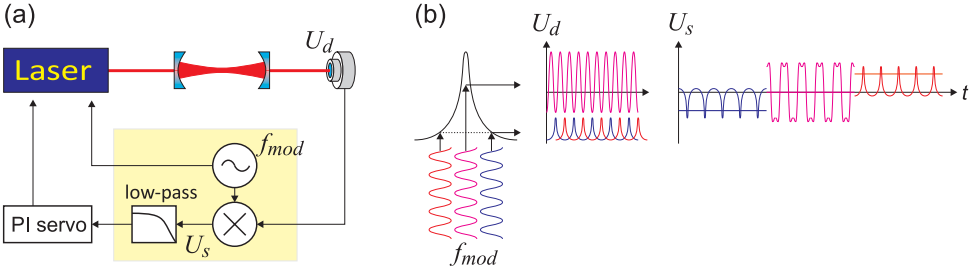


Figure 33.10: (a) Frequency stabilization to a cavity using the lock-in method. (b) Frequency-modulated signals applied to a resonance suffer a period doubling, when the signal frequency is close to resonance. By demodulating the signals discriminated at the resonance profile, we obtain, after averaging over a period, a DC voltage that is proportional to the frequency detuning. The yellow area denotes the components constituting the lock-in amplifier.

The principle of control through modulation is explained in Fig. 33.10(a). A laser beam passes twice (round-trip) through an *acousto-optic modulator* fed by a radiofrequency voltage with modulated frequency,  $\omega(t) = \omega_c + M \cos ft$ . Here, the modulation frequency is much lower than its amplitude (or frequency excursion),  $f \ll M$ . The laser beam is now injected into an optical cavity and the frequency of the laser tuned near a resonance of the cavity. The dependence of the transmission on the frequency is described in good approximation of the *Airy formula* by a Lorentzian,

$$I(\omega) = \frac{\gamma^2}{4(\omega - \omega_0)^2 + \gamma^2} . \tag{33.11}$$

The signal transmitted through the cavity [see Fig. 33.10(b)],

$$U_d(t) = I(\omega(t)) = \frac{\gamma^2}{4(\omega_c + M \cos ft - \omega_0)^2 + \gamma^2} , \tag{33.12}$$

is demodulated by a lock-in amplifier [see Fig. 33.10(c)],

$$U_s(t) = U_d(t) \cos(ft + \phi) , \tag{33.13}$$

integrated with a locking electronics [see Fig. 33.10(d)]

$$\bar{U}_s(t) = \frac{1}{T} \int_0^T U_s(t) dt . \quad (33.14)$$

and used to control the piezo of the laser's extended cavity.

### 33.3.3 Pound-Drever-Hall stabilization

When the frequency of a carrier wave  $\omega$  is modulated by a frequency  $\Omega$ <sup>3</sup>, the spectrum consists of sidebands the frequencies and phases of which can be calculated from an expansion of the wave in Bessel functions. Let  $N$  be the modulation excursion and  $J_k(x)$  the Bessel function of the order  $k$ . Higher-order sidebands  $k > 1$  are usually dropped in the calculation,

$$e^{i(\omega t + N \sin \Omega t)} = e^{i\omega t} [-J_1(N)e^{i\Omega t} + J_0(N) + J_1(N)e^{-i\Omega t}] . \quad (33.15)$$

From the latter expression, it can be seen that the spectrum of sidebands is formed

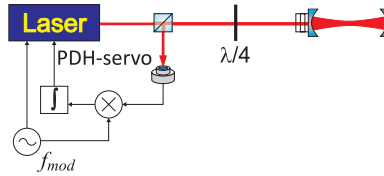


Figure 33.11: Frequency stabilization to a cavity using the Pound-Drever-Hall method.

by the frequencies  $\omega$  and  $\omega \pm \Omega$ . A resonator responds to a field of incident light  $E_0(\omega)$  oscillating with frequency  $\omega$  by reflecting the field ( $R$ : reflectivity of mirrors,  $\delta_{fsr}$ : free spectral range)

$$E_r(\omega) = E_0(\omega) \sqrt{R} \frac{1 - e^{-i\omega/\delta_{fsr}}}{1 - R e^{-i\omega/\delta_{fsr}}} , \quad (33.16)$$

where the amplitude and the phase of the reflected light field follow from the relation  $E_r(\omega) = |E_r(\omega)|e^{i\phi(\omega)}$ . Obviously the field of the reflected light is strong only, when the laser frequency is close to one mode of the resonator (when  $\omega/\delta$  is an integer number). By inserting Eq. (33.16) into Eq. (33.15), we obtain the response of the resonator to a field containing sidebands as a function of the frequency of light  $\omega$ , of the modulation frequency  $\Omega$ , and of the cavity finesse,

$$\begin{aligned} |E_{tot}|^2 &= |e^{i\omega t} [J_1(N)E_r(\omega + \Omega)e^{i\Omega t} + J_0(N)E_r(\omega) - J_1(N)E_r(\omega - \Omega)e^{-i\Omega t}]|^2 \\ &= J_0(N)J_1(N)E_r(\omega + \Omega)e^{i\Omega t} + J_0(N)J_1(N)E_r^*(\omega - \Omega)e^{i\Omega t} + \dots + c.c. . \end{aligned} \quad (33.17)$$

The contributions of the reflected field to the current in the photodetector,  $|E_r|^2$ , oscillating with frequency  $\Omega$  and extracted by the alternating current  $e^{-i\Omega t + i\theta}$  ( $\theta$  is

<sup>3</sup>Remember that we specify all frequencies except the free spectral range  $\delta_{fsr}$  in radians.

an arbitrarily chosen phase angle), are

$$\begin{aligned}
 S_{PDH} &= |E_{tot}|^2 e^{-i\Omega t + i\theta} \\
 &= J_0(N)J_1(N)\text{Re}\{e^{i\theta}[E_r^*(\omega)E_r(\omega + \Omega) - E_r(\omega)E_r^*(\omega - \Omega)]\} + \dots
 \end{aligned}
 \tag{33.18}$$

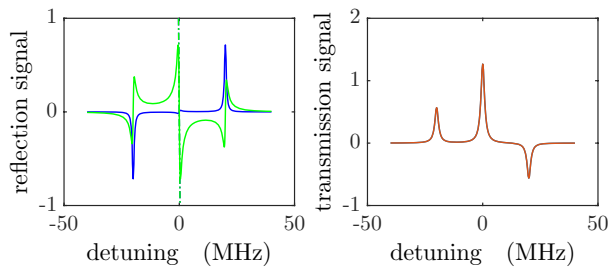


Figure 33.12: (code) (Left) Pound-Drever-Hall reflection signal for  $\theta = 0, \pi/2$ . (Right) Transmission signal.

By a suitable choice of the modulation index, the pre-factor containing Bessel functions (and therefore the signal amplitude) can be maximized. That is the case, for  $M \simeq 1.1$  (see Exc. 31.4.5.1). Each of the two parts of the summation in the above equation is the result of a beating of the carrier  $E_r(\omega)$  with one of the sidebands  $E_r(\omega \pm \Omega)$ . Only those optical sidebands being close to a mode of the resonator provide, along with the radiofrequency sidebands, contributions to the reflection signal

The dependence of the reflection signal  $S_{PDH}$  on the frequency  $\omega$  is shown in Fig. 33.12(a). The antisymmetric shape and the zero-crossing slope are ideal for use as a discriminator generating an *error signal* for a frequency stabilization. This method is called *Pound-Drever-Hall method*.

### 33.3.4 Phase stabilization of standing waves

For the stabilization of the phase of a standing wave one can use the following scheme. It is similar to the homodyne method used with the Michelson interferometer with the difference that laser beam separation and recombination are done at different beam splitters.

### 33.3.5 Frequency-offset locking with phase-locked loops

Many application in spectroscopy require two stable lasers emitting at different but well-defined and tunable frequencies. Examples are stimulated Raman transitions, or the spectroscopy of atoms interacting with optical cavities [118]. In the following we will discuss and compare different approaches to locking one laser to another laser using a phase-locked loop (PLL). See also [\(watch talk\)](#).

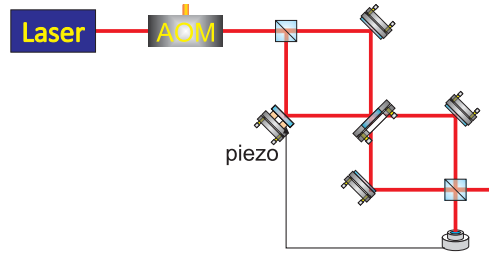


Figure 33.13: Phase stabilization.

### 33.3.5.1 VCO and mixing

In a *phase-locked loop* one tries to synchronize a self-sustained oscillator, in general realized by a VCO, with a local oscillator. The VCO generates an ac-voltage  $U_{rf}$ , whose frequency is tuned via a dc-control-voltage  $U_{ct}$  around a center frequency  $\omega_0$ , as shown in Fig. 33.14(a). It can be modeled by,

$$U_{rf}(t) = 2B \cos \phi(t) \quad \text{with} \quad \frac{d\phi}{dt} = \omega_0 + KU_{ct}(t) . \quad (33.19)$$

The local oscillator produces an ac-voltage,  $U_{lo}(t) = A \sin \phi_{lo}(t)$ . A mixer multiplies both signals,

$$U_d(t) = AB (\sin[\phi_{lo}(t) - \phi(t)] + \sin[\phi_{lo}(t) + \phi(t)]) . \quad (33.20)$$

See also Exc. 33.3.7.1.

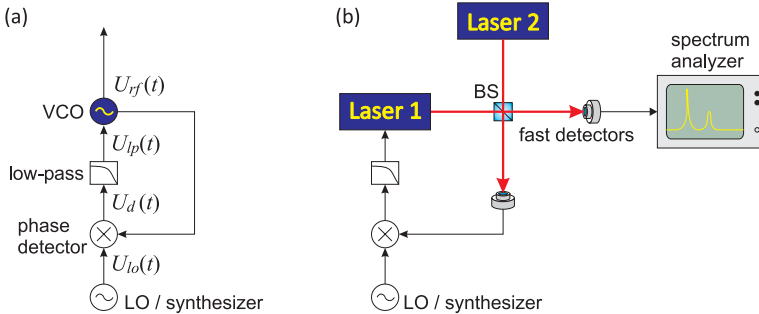


Figure 33.14: (a) PLL to lock a VCO to a reference oscillator LO. (b) PLL to lock the difference frequency of two lasers to a LO.

### 33.3.5.2 Low-pass filtering

The multiplied signal  $U_d$  contains all information about frequency deviations of the VCO from the LO. To extract them, we *low-pass filter* this signal, cutting off all high frequency components, i.e. apply the filter transfer function,

$$F(f) = (1 + sRC)^{-1} . \quad (33.21)$$

The signal of the filter is  $U_{lp}(f) \equiv F(f)U_d(f)$ . In time domain, which is obtained by a Laplace transform,  $F(t) = (RC)^{-1}\theta(t)e^{-t/RC}$ , such that

$$U_{lp}(t) = F \star U_d(t) = \int_{-\infty}^{\infty} F(t - \tau)U_d(\tau)d\tau = \frac{e^{-t/RC}}{RC} \int_{-\infty}^t e^{\tau/RC}U_d(\tau)d\tau . \quad (33.22)$$

The derivative is obviously,

$$\frac{dU_{lp}}{dt} + \frac{U_{lp}}{RC} = \frac{U_d(t)}{RC} = \frac{AB}{RC} \sin [\phi_{lo}(t) - \phi(t)] , \quad (33.23)$$

inserting the above expression for  $U_d$ . Note, that we would have obtained the same result using control theory (see Sec. 33.1).

### 33.3.5.3 Phase synchronization

The phase synchronization servo is closed by setting  $U_{ct} = U_{lp}$ . Thus we may substitute  $U_{lp}(t)$  and define  $\psi \equiv \phi - \phi_{lo}$ ,

$$\frac{d^2\psi}{dt^2} + \frac{1}{RC} \frac{d\psi}{dt} + \frac{KAB}{RC} \sin \psi = -\frac{d^2\phi_{lo}}{dt^2} - \frac{1}{RC} \left( \frac{d\phi_{lo}}{dt} - \omega_0 \right) . \quad (33.24)$$

In most cases the LO frequency varies slowly, so that we may assume  $\dot{\phi}_{lo} = \omega_{lo}$ ,

$$\frac{d^2\psi}{dt^2} + \frac{1}{RC} \frac{d\psi}{dt} + \frac{KAB}{RC} \sin \psi = -\frac{1}{RC} (\omega_{lo} - \omega_0) . \quad (33.25)$$

Hence, a PLL generates a signal  $U_{rf}(t)$  having approximately the same (time-dependent) frequency as the local oscillator  $U_{lo}(t)$ . The equation is identical to that of an overdamped rotator or a resistively shunted Josephson junction [547].

We observe that the PLL is locking to servo oscillations. The spectrum of signal produced by the VCO exhibits sidebands as soon as the loop is closed. Their amplitude depends on the gain, their frequency varies with the offset voltage controlling the VCO.

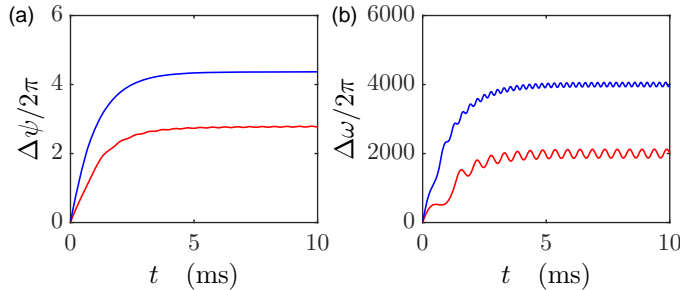


Figure 33.15: (code) Simulation of (a) the phase and (b) frequency difference in a PLL for (red)  $\omega_{lo} - \omega_0 = (2\pi) 2$  kHz and (blue) 4 kHz.

### 33.3.6 Frequency-offset locking using transfer cavities

Sometimes we want to take a ultra-high resolution spectrum in a frequency region, where there is no reference frequency available nearby. By nearby we mean frequency regimes which can be reached by PLLs based on frequency beats on fast photodetectors, as studied in Sec. 33.3.5. A possible method consists in the use of an optical *transfer cavity*.

Here, a reference laser stabilized to a known frequency  $\omega_{ref}$ , e.g. via a saturation spectroscopy to an atomic transition, is used to lock a piezo-tunable optical cavity (called transfer cavity), as shown in Fig. 33.16. The cavity in turn is used to lock the spectroscopy laser  $\omega_{blu-las}$ , e.g. via the Pound-Drever-Hall method.

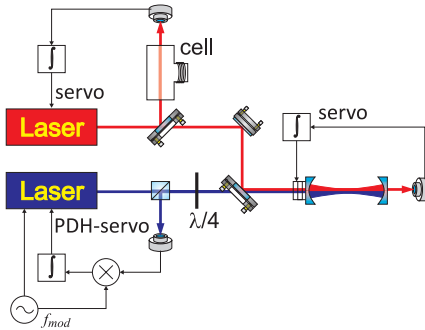


Figure 33.16: Schematic view of a transfer cavity locking system involving three cascaded servo systems for (i) the stabilization of the reference laser to a known frequency; (ii) of the transfer cavity to the reference laser, and (iii) of the spectroscopy laser to the transfer cavity.

Two issues need to be considered when using the transfer cavity scheme:

- The scheme does not permit tuning of the spectroscopy laser; this feature must be included using, e.g. AOMs (see Sec. 31.3.1) or PLL offset locks (see Sec. 33.3.5).
- The use of piezo in the transfer cavity is incompatible with its high-level thermal and mechanical stabilization. This means that special care must be taken in the design of the reference laser in order to avoid degradation of the stability of the transfer cavity via the servo lock.

The whole locking scheme consists of three cascaded servo loops (see Fig. 33.16). To model the transfer of stability from the reference to the spectroscopy laser, we write down the following relations,

$$\begin{aligned}\omega_{red-las} &= H_{sat}(f)\omega_{ref} \\ N_{red-trns}\delta_{fsr} &= H_{trns}(f)\omega_{red-las} \\ \omega_{blu-las} &= H_{pdh}(f)N_{blu-trans}\delta_{fsr} .\end{aligned}\tag{33.26}$$

In the absence of noise or for perfect servos,  $H_x \rightarrow 1$ , we get,

$$\omega_{blu-las} = \frac{N_{blu-trans}}{N_{red-trans}}\omega_{red-las} .\tag{33.27}$$



We assume specific transfer functions for the closed-loop gains of the three servos and describe the impact of noise by adding frequency deviations  $\Delta\omega$  entering at various points.

### 33.3.7 Exercises

#### 33.3.7.1 Ex: Schemes for laser tuning

Discuss the two PLL-setups shown in Fig. 33.17.

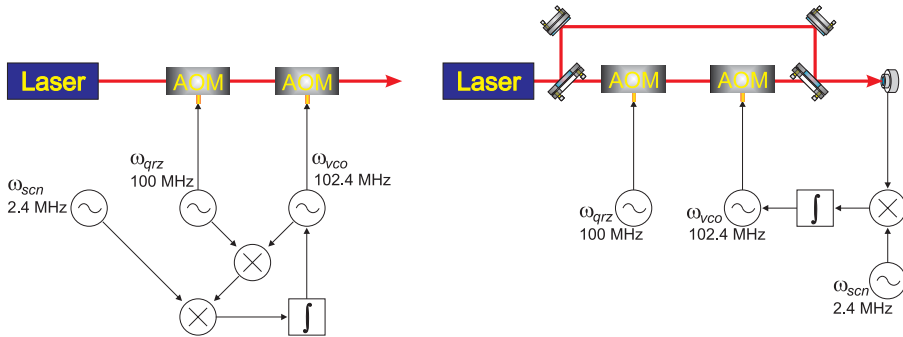


Figure 33.17: Two schemes for laser tuning.

#### 33.3.8 Experiment: Stabilizing a laser to a cavity

Here is, how we are going to stabilize a laser to a cavity:

1. Stabilize a helium-neon laser to a Fabry-Pérot cavity, generating a frequency modulation by modulating the laser diode current or the piezo of the extended cavity. Choose a modulation frequency in the range of  $f \simeq 1$  kHz and a modulation amplitude in the range of  $M \simeq 5$  MHz. Adjust the reference voltage of the control electronics until the error signal is symmetrical.
2. If you do not have a lock-in amplifier available, construct one following the project Sec. 30.4.3.
3. Now, do the opposite, stabilizing the optical cavity to the laser frequency using the resonator piezo as control element.
4. Vary the optical setup now modulating the frequency using an AOM (see Fig. 33.18).

#### 33.3.9 Experiment: Pound-Drever-Hall locking

Now we will stabilize a laser to a cavity using the Pound-Drever-Hall technique [96, 211]:

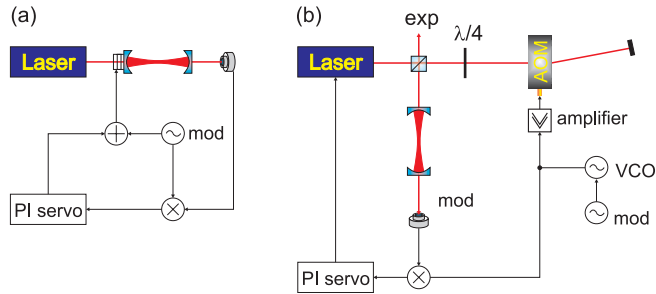


Figure 33.18: Variations on the same theme: (a) Frequency stabilization of a cavity to a laser frequency using the lock-in method. This method is often used for spectral filtering of a laser beam by a transmission etalon. (b) Frequency stabilization of a laser to a cavity using an AOM. The advantage of using an AOM compared to the scheme shown in Fig. 33.10 is, that only the beam injected into the cavity is modulated, but not the beam used for the main experiment.

1. Consider the reflected signal. To do this, separate the beam injected into the resonator from the reflected beam by means of a  $\lambda/4$  waveplate and a polarizing beam splitter.
2. Now analyze the reflected signal with a fast photodetector at a spectrum analyzer.
3. Demodulate the signal with the modulation frequency. Vary the length of the cables. Optimize the slope of the error signal by a suitable choice of frequency and modulation excursion <sup>4</sup>.

## 33.4 Further reading

### 33.4.1 on frequency noise description

D.W. Allan, *Statistics of atomic frequency standards* [DOI]

J.A. Barnes et al., *Characterization of frequency stability* [DOI]

J.L. Stewart, *The power spectrum of a carrier frequency modulated by Gaussian noise* [DOI]

D.S. Elliott et al., *Extracavity laser band-shape and bandwidth modification* [DOI]

L.S. Cutler, *Some Aspects of the Theory and Measurement of Frequency Fluctuations in Frequency Standards* [DOI]

D.B. Sullivan et al., *Characterization of Clocks and Oscillators* [ISBN]

<sup>4</sup>Datasheet for the VCO see appendix Fig. 34.15, data sheet for the power splitter see appendix Fig. 34.17, data sheet for the mixer see appendix Fig. 34.18.

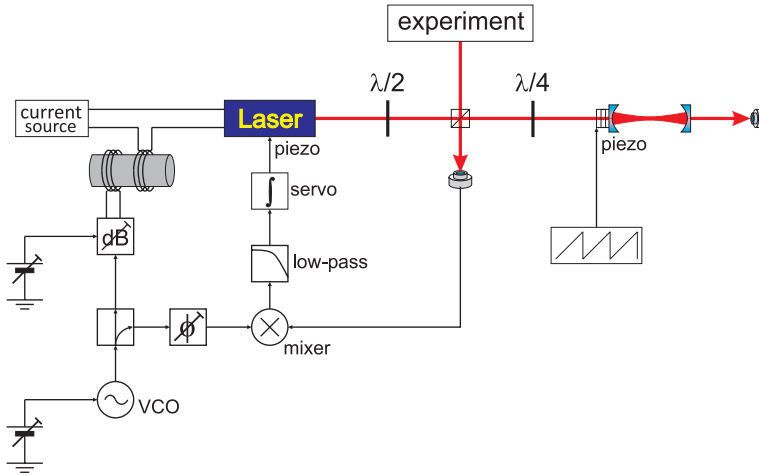


Figure 33.19: Setup of a frequency regulator following Pound-Drever-Hall. VCO: Voltage-Controlled Oscillator, LT: power splitter, dB: variable attenuator, LP: low-pass filter.

- G. Di Domenico et al., *Simple approach to the relation between laser frequency noise and laser line shape* [DOI]
- J. Appel et al., *A versatile digital GHz phase lock for external cavity diode lasers* [DOI]
- L. Ricci et al., *A compact grating-stabilized diode laser system for atomic physics* [DOI]
- G. Ritt et al., *Laser frequency offset locking using a side of filter technique* [DOI]
- A.S. Arnold et al., *A simple extended-cavity diode laser* [DOI]
- E.C. Cook et al., *High passive-stability diode-laser design for use in atomic-physics experiments* [DOI]
- C.J. Hawthorn et al., *Littrow configuration tunable external cavity diode laser with fixed direction output beam* [DOI]
- Huanqian Loh et al., *Influence of grating parameters on the linewidths of external-cavity diode lasers* [DOI]
- Y. Shimada et al., *A simplified 461-nm laser system using blue laser diodes and a hollow cathode lamp for laser cooling of Sr* [DOI]

### 33.4.2 on laser stabilization

- J. Alnis et al., *Stable diode lasers for hydrogen precision spectroscopy* [DOI]
- J. Alnis et al., *Subhertz linewidth diode lasers by stabilization to vibrationally and thermally compensated ultralow-expansion glass Fabry-Pérot cavities* [DOI]

- L. Couturier et al., *Laser frequency stabilization using a commercial wavelength meter* [\[DOI\]](#)
- K. Huang et al., *Microcontroller-based locking in optics experiments* [\[DOI\]](#)
- Shun Wu et al., *Direct fiber comb stabilization to a gas-filled hollow-core photonic crystal fiber* [\[DOI\]](#)
- Y.N. Zhao et al., *Sub-Hertz frequency stabilization of a commercial diode laser* [\[DOI\]](#)
- R.W.P. Drever et al., *Laser Phase and Frequency Stabilization Using an Optical Resonator* [\[DOI\]](#)
- D. Budker et al., *Obtaining frequency markers of variable separation with a spherical mirror Fabry-Perot interferometer* [\[DOI\]](#)

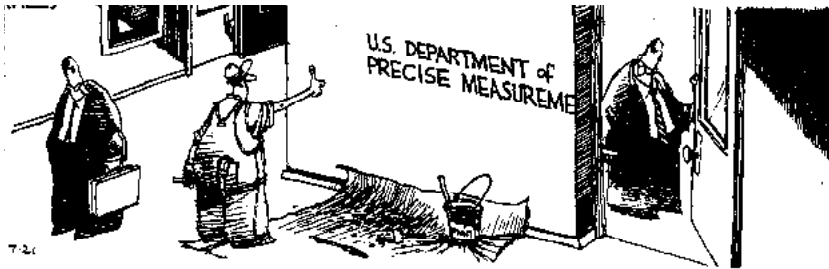
### 33.4.3 on control theory

- U. Tietze et al., *Halbleiterschaltungstechnik* [\[ISBN\]](#)
- O. Föllinger et al., *Regelungstechnik: Einführung in die Methoden und ihre Anwendung* [\[ISBN\]](#)



## Chapter 34

# Appendices to 'Instrumentation of a Quantum Optics Lab'



### 34.1 Calculating the uncertainty of measured quantities

#### 34.1.1 Mean value and standard deviation

Mean value and *standard deviation* are defined by,

$$\bar{x} \equiv \frac{1}{N} \sum_k x_k \quad \text{and} \quad \sigma_{\bar{x}} \equiv \sqrt{\frac{1}{N-1} \sum_k (x_k - \bar{x})^2}. \quad (34.1)$$

The standard deviation can be weighed by a confidence parameter,

$$\bar{x} \equiv \frac{\sum_k w_k x_k}{\sum_k w_k} \quad \text{and} \quad \sigma_{\bar{x}} \equiv \frac{1}{\sqrt{\sum_k w_k}} \quad (34.2)$$

Weighing by individual standard deviation,

$$w_k \equiv \frac{1}{\sigma_k^2} \quad \text{for} \quad \sigma_k = \sigma_0 \quad (34.3)$$

gives,

$$\bar{x} \equiv \frac{\sum_k \frac{x_k}{\sigma_k^2}}{\sum_k \frac{1}{\sigma_k^2}} = \sigma_{\bar{x}}^2 \sum_k \frac{x_k}{\sigma_k^2} \xrightarrow{\sigma_k = \sigma_0} \frac{1}{N} \sum_k x_k \quad \text{with} \quad \sigma_{\bar{x}} \equiv \frac{1}{\sqrt{\sum_k \frac{1}{\sigma_k^2}}} \xrightarrow{\sigma_k = \sigma_0} \frac{\sigma_0}{\sqrt{N}} \quad (34.4)$$

or,

$$\hat{\sigma}_{\bar{x}} \equiv \sigma_{\bar{x}} \chi_v \xrightarrow{\sigma_k = \sigma_0} \sqrt{\frac{1}{N-1} \sum_k (x_k - \bar{x})^2} \quad (34.5)$$

$$\chi_v = \sqrt{\frac{1}{N-1} \sum_k \frac{(x_k - \bar{x})^2}{\sigma_k^2}} .$$

From error propagation

$$\Delta \bar{x} \equiv \sqrt{\frac{1}{N} \sum_k \Delta x_k^2} . \quad (34.6)$$

### 34.1.1.1 $\chi^2$ -fit

The  $\chi^2$ -fit of a constant of a function  $y = f(x)$  to a measured data set  $(x_k, y_k)$  is,

$$\chi^2 = \frac{1}{N(N-1)} \sum_k [f(x_k) - y_k]^2 . \quad (34.7)$$

The above formula suggest that, increasing the number of measurements  $N \rightarrow \infty$  we could pull the error to zero. This, however, is NOT TRUE. If the standard deviation is smaller than the precision  $\Delta$  of the measurement tool, the error will be limited by  $\Delta$ ,

$$\bar{y} \pm \max(\sigma, \Delta) . \quad (34.8)$$

### 34.1.2 Error propagation

The *error propagation* for a function  $f(x_1, x_2, \dots)$  is given by,

$$\Delta f = \sqrt{\left(\frac{\partial f}{\partial x_1}\right)^2 \Delta x_1^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 \Delta x_2^2 + \dots} < \left|\frac{\partial f}{\partial x_1}\right| \Delta x_1 + \left|\frac{\partial f}{\partial x_2}\right| \Delta x_2 + \dots . \quad (34.9)$$

Calculations can often be simplified by noting that the four fundamental operations,  $f = x_1 \pm x_2$ ,  $f = x_1 x_2$ , and  $f = \frac{x_1}{x_2}$  allow us to simply add the relative errors,

$$\frac{\Delta f}{f} = \frac{\Delta x_1}{x_1} + \frac{\Delta x_2}{x_2} . \quad (34.10)$$

Alternatively, we may use the following quick rules,

$$\begin{aligned} \text{sum} : f \pm \Delta f &= (x \pm \Delta x) + (y \pm \Delta y) &= (x + y) &\pm (\Delta x + \Delta y) \\ \text{subtraction} : f \pm \Delta f &= (x \pm \Delta x) - (y \pm \Delta y) &= (x - y) &\pm (\Delta x + \Delta y) \\ \text{multiplication} : f \pm \Delta f &= (x \pm \Delta x) \cdot (y \pm \Delta y) &= (x \cdot y) &\pm (x \Delta y + y \Delta x) \\ \text{division} : f \pm \Delta f &= \frac{x \pm \Delta x}{y \pm \Delta y} &= \frac{x}{y} &\pm \frac{1}{y^2} (x \Delta y + y \Delta x) \\ \text{power} : f \pm \Delta f &= (x \pm \Delta x)^n &= x^n &\pm n x^{n-1} \Delta x \end{aligned} \quad (34.11)$$

**Example 132 (Error propagation):** Let us study the following example,

$$f = \frac{x_1}{x_2 + a}$$

$$\implies \Delta f = f \frac{\Delta x_1}{x_1} + f \frac{\Delta(x_2 + a)}{x_2 + a} = f \frac{\Delta x_1}{x_1} + f \frac{\Delta x_2}{x_2 + a} .$$

### 34.1.3 Fitting a curve

We start defining the following prescription to calculate mean values,

$$\bar{x} \equiv \frac{1}{N} \sum_{k=1}^N x_k \quad , \quad \overline{xy} \equiv \frac{1}{N} \sum_{k=1}^N x_k y_k . \quad (34.12)$$

For a *fit* of a *linear curve*  $f(x) = ax + b$  to a data set  $\{x_k, y_k\}_{k \in [1, N]}$ , we calculate,

$$f(x) = ax + b \quad , \quad a = \frac{\overline{xy} - \bar{x} \bar{y}}{\overline{x^2} - \bar{x}^2} = \frac{\overline{(x - \bar{x})y}}{(x - \bar{x})^2} \quad , \quad b = \frac{\bar{y} \overline{x^2} - \overline{xy} \bar{x}}{\overline{x^2} - \bar{x}^2} = \bar{y} - a \bar{x} . \quad (34.13)$$

The uncertainties are obtained via,

$$\Delta y = \sqrt{\frac{N}{N-2} (\overline{ax + b - y})^2} \quad , \quad \Delta a = \Delta y \sqrt{\frac{1}{N \overline{x^2} - \bar{x}^2}} = \frac{\Delta y}{\sqrt{N \overline{x^2} - \bar{x}^2}} \quad (34.14)$$

$$\quad , \quad \Delta b = \Delta y \sqrt{\frac{\overline{x^2}}{N \overline{x^2} - \bar{x}^2}} = \Delta y \sqrt{\frac{\overline{x^2}}{N \overline{x^2} - \bar{x}^2}} .$$

To fit an *exponential curve*  $f(x) = \beta e^{\alpha x}$ , we simply convert the data set  $\{x_k, v_k\} \equiv \{x_k, \lg y_k\}$ , calculate the mean values of the decadal logarithm using the recipe (34.12), and fit a linear curve  $\tilde{f}(x) = \lg f(x) = \frac{\alpha}{\ln 10} x + \lg \beta \equiv ax + b$  in a semi-logarithmic scale to the data set  $\{x_k, v_k\}$ . This gives,

$$f(x) = \beta e^{\alpha x} \quad , \quad \frac{\alpha}{\ln 10} = a = \frac{\overline{x \lg y} - \bar{x} \overline{\lg y}}{\overline{x^2} - \bar{x}^2} \quad , \quad \lg \beta = b = \frac{\overline{\lg y} \overline{x^2} - \overline{x \lg y} \bar{x}}{\overline{x^2} - \bar{x}^2} . \quad (34.15)$$

To fit a *power law curve*  $f(x) = \beta x^\alpha$ , we simply convert the data set  $\{u_k, v_k\} \equiv \{\lg x_k, \lg y_k\}$ , calculate the mean values of the decadal logarithm using the recipe (34.12), and fit the linear curve  $\tilde{f}(x) = \lg f(x) = \alpha \lg x + \lg \beta \equiv ax + b$  in a double-logarithmic scale to the data set  $\{u_k, v_k\}$ . This gives,

$$f(x) = \beta x^\alpha \quad , \quad \alpha = a = \frac{\overline{\lg x \lg y} - \overline{\lg x} \overline{\lg y}}{\overline{\lg x^2} - \overline{\lg x}^2} \quad , \quad \lg \beta = b = \frac{\overline{\lg y} \overline{\lg x^2} - \overline{\lg x \lg y} \overline{\lg x}}{\overline{\lg x^2} - \overline{\lg x}^2} . \quad (34.16)$$



### 34.1.4 Probability density

Consider a function  $P(x)$  having the meaning of a *probability* depending on a variable  $x \in [-\infty, \infty]$ . The *probability density*  $\rho(x)$  is defined as its derivative,  $\rho(x) = P'(x)$ , such that,

$$P(x) = \int_{-\infty}^{\infty} \rho(t) dt \quad \text{with} \quad P(-\infty) = 0 \quad \text{and} \quad P(\infty) = 1 . \quad (34.17)$$

Every probability must have the same likeliness, i.e.,

$$P(x) = \zeta_n , \quad (34.18)$$

where  $\zeta_n \in [0, 1]$  is a uniformly distributed *random variable*. In order to numerically generate a *stochastic distribution*, we have to invert the distribution function, i.e. when  $\zeta_n$  is generated by a computer, then

$$\boxed{x_n = P^{-1}(\zeta_n)} \quad (34.19)$$

is the distribution of the random variable  $x_n$ . In other words, a histogram of  $x_n$  reproduces the probability density  $\rho(x)$ .

Let us, for example, consider the Boltzmann distribution,

$$P(x) \equiv 1 - e^{-\beta x} . \quad (34.20)$$

Probing the probability with a random number, as in (34.18), we obtain the random variable via (34.19),

$$x_n = P^{-1}(\zeta_n) = -\frac{1}{\beta} \ln(1 - \zeta_n) . \quad (34.21)$$

The histogram of this random variable  $x_n$  can directly be compared with the probability density  $\rho(x)$  given by,

$$\rho(x) = P'(x) = \beta e^{-\beta x} . \quad (34.22)$$

This is illustrated in Fig. 34.1(a).

**Example 133 (Probability density of a Gaussian distribution):** Another example is the *error function* given by,

$$\text{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt .$$

By define the probability function,

$$P(x) \equiv \frac{1}{2} [\text{erf}(x) - \text{erf}(-\infty)] = \frac{1}{\sqrt{\pi}} \int_{-\infty}^x e^{-t^2} dt .$$

Probing the probability with a random number, as in (34.18), we obtain the random variable via (34.19),

$$x_n = P^{-1}(\zeta_n) = \text{erf}^{-1}(2\zeta_n - 1) .$$

The histogram of this random variable  $x_n$  can directly be compared with the probability density  $\rho(x)$ , which is nothing else than the Gauss function,

$$\rho(x) = P'(x) = \frac{1}{\sqrt{\pi}} e^{-x^2} = 2\text{erf}'(x) .$$

This is illustrated in Fig. 34.1(b).

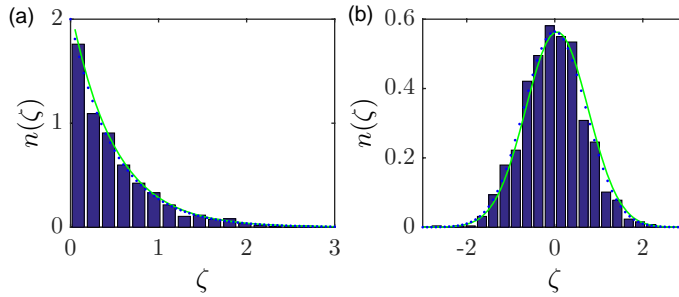


Figure 34.1: (code) (a) Boltzmann distribution simulated by random numbers (histogram). The numerical derivative of this distribution is shown as a blue dotted line, and the probability density as a green solid line. (b) Error function probability distribution simulated by random numbers (histogram). The numerical derivative of the error function is shown as a blue dotted line, and the Gauss function as a green solid line.

## 34.2 Deepening control theory

The variation of a physical quantity (e.g., a voltage or a temperature) in time is called *signal*. In a specific environment or technical device, such a variation may cause other physical quantities to change as well. For example, the rise in temperature of an optical cavity may modify its length and its resonance frequency, while the inverse is not true. This feature is illustrated by a block diagram as shown in Fig. 34.2, where  $x(t)$  denotes the variation of a physical quantity (called *input*) that causes the variation of another quantity  $y(t)$  (called *output*). The precise way how  $y(t)$  depends on  $x(t)$  depends on the particularities of the device, which is labeled by a symbol  $\mathcal{T}$  called transfer function.  $\mathcal{T}$  is in fact an operator acting on functions and transforming input signals into output signals.

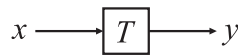


Figure 34.2: Transfer and modification of a time-dependent signal.

While we have described above the transfer of (time-varying) signals, the same feature can be treated in frequency domain via Fourier or Laplace-transforms. This script is not the right place to recapitulate the mathematics of these transforms, and we will restrict ourselves to reproducing some of the most fundamental results, as we may need them in the following.

### 34.2.1 Analysis techniques - frequency domain and time domain

Mathematical techniques for analyzing and designing control systems fall into two different categories:

**Frequency domain:** In this type the values of the state variables, the mathematical variables representing the system's input, output and feedback are represented

as functions of frequency. The input signal and the system's transfer function are converted from time functions to functions of frequency by a transform such as the Fourier transform, Laplace transform, or Z transform. The advantage of this technique is that it results in a simplification of the mathematics; the differential equations that represent the system are replaced by algebraic equations in the frequency domain which are much simpler to solve. However, frequency domain techniques can only be used with linear systems, as mentioned above.

**Time-domain state space representation:** In this type the values of the state variables are represented as functions of time. With this model the system being analyzed is represented by one or more differential equations. Since frequency domain techniques are limited to linear systems, time domain is widely used to analyze real-world nonlinear systems. Although these are more difficult to solve, modern computer simulation techniques such as simulation languages have made their analysis routine.

In contrast to the frequency domain analysis of the classical control theory, modern control theory utilizes the time-domain state space representation, a mathematical model of a physical system as a set of input, output and state variables related by first-order differential equations. To abstract from the number of inputs, outputs and states, the variables are expressed as vectors and the differential and algebraic equations are written in matrix form (the latter only being possible when the dynamical system is linear). The state space representation (also known as the 'time-domain approach') provides a convenient and compact way to model and analyze systems with multiple inputs and outputs. With inputs and outputs, we would otherwise have to write down Laplace transforms to encode all the information about a system. Unlike the frequency domain approach, the use of the state-space representation is not limited to systems with linear components and zero initial conditions. 'State space' refers to the space whose axes are the state variables. The state of the system can be represented as a point within that space.

### 34.2.1.1 Signal transfer through LTI systems without delay

For an operator  $\mathcal{T}$  transforming a temporal signal  $x(t)$  into a signal  $y(t)$ ,

$$y(t) = \mathcal{T}x(t) , \quad (34.23)$$

to be *linear* and time-independent, we require,

$$\begin{aligned} \mathcal{T}[\alpha x_1(t) + \beta x_2(t)] &= \alpha \mathcal{T}[x_1(t)] + \beta \mathcal{T}[x_2(t)] \\ \mathcal{T}[x(t - \tau)] &= \mathcal{T}[x(t)] \star \delta(t - \tau) , \end{aligned} \quad (34.24)$$

where the  $\star$  denotes a convolution,

$$(f \star g)(t) = \int_{-\infty}^{\infty} f(\tau)g(t - \tau)d\tau . \quad (34.25)$$

Such system are called *Linear Time-Independent LTI* systems <sup>1</sup>.

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<sup>1</sup>To be more general, also the derivative and integral of the output signal must be included (see later sections).

**34.2.1.2 Laplace transform**

We define the *Laplace transform*  $\mathcal{L}$  as a linear operator acting on a signal  $x(t)$  defined through,

$$\mathcal{L}... \equiv \int_{-\infty}^0 ...e^{st} d\tau . \tag{34.26}$$

The frequency variable is denoted by the imaginary quantity  $s = \iota f$ . The question is now, what is the meaning of the Laplace operator?

To answer this question, we start introducing the pulse response  $h(t)$  via

$$h(t) = \mathcal{T}[\delta(t)] \tag{34.27}$$

as the reaction of a system  $\mathcal{T}$  to a pulse  $\delta(t)$ . Now, it is easy to see, that the operator  $\mathcal{P}$  defined as,

$$\mathcal{P}... \equiv h(t) \star ... , \tag{34.28}$$

and which describes the convolution of an arbitrary input signal with the pulse response, satisfies the above linearity condition. Now calculating,

$$\mathcal{P}e^{st} = h(t) \star e^{st} = \int_{-\infty}^0 h(\tau)e^{s(t-\tau)} d\tau = \mathcal{L}[h(t)] \cdot e^{st} = (\mathcal{L}h)(s) \cdot e^{st} , \tag{34.29}$$

we find that the functions  $e^{st}$  are eigenfunctions of the operator  $\mathcal{P}$  with the eigenvalues  $\mathcal{L}[h(t)]$ , which are just the Laplace transforms of the pulse response.

We can now expand arbitrary functions  $x(t)\theta(t)$  in a Laplace series and obtain,

$$\mathcal{L}[h(t) \star x(t)] = \int_{-\infty}^0 h(t) \star e^{st} x(t)dt = (\mathcal{L}h)(s) \int_{-\infty}^0 e^{st} x(t)dt = (\mathcal{L}h)(s) \cdot (\mathcal{L}x)(s) . \tag{34.30}$$

The convolution on the left-hand side is in time domain, while the product on the right-hand side is in frequency domain.

**34.2.1.3 Pulse and jump response from a transfer function**

The transmission of a signal by an element of a control loop can be described in the temporal or spectral domain [245, 260, 452], and we can switch from one representation to another via Laplace transformation. Operators of LTI systems  $\mathcal{T}$  are represented by products with spectral functions in frequency-domain,  $\tilde{F}(s) \dots = (\mathcal{L}F)(s) \dots$  or convolutions with time-varying functions in time-domain,  $F(t) \star \dots$ ,

$$\begin{aligned} y(t) &= \mathcal{T}x(t) & (34.31) \\ \xrightarrow{\text{Laplace}} \tilde{y}(s) &= \tilde{F}(s) \cdot \tilde{x}(s) \\ \xrightarrow{\text{inverse Laplace}} y(t) &= F(t) \star x(t) . \end{aligned}$$

In practice, the function  $\tilde{F}(f)$  can be determined by feeding a sinusoidal signal with amplitude  $x(s)$  into the system, measuring  $y(s)$  (which is a complex number) <sup>2</sup>,

---

<sup>2</sup>From now on, we will drop the tilde  $\sim$  on transfer functions and amplitudes, when it is clear that we are in frequency-domain.

and calculating

$$F(s) = \frac{y(s)}{x(s)} . \quad (34.32)$$

The transitory behavior  $F(t)$  can in practice be extracted via an adequate choice of the test function, f.ex., the response to a pulse:

$$\begin{aligned} x(t) &= \delta(t) & (34.33) \\ \xrightarrow{\text{Laplace}} y(s) &= F(s) \\ \xrightarrow{\text{inverse Laplace}} y(t) &= F(t) , \end{aligned}$$

or to a sudden jump:

$$\begin{aligned} x(t) &= \theta(t) & (34.34) \\ \xrightarrow{\text{Laplace}} y(s) &= F(s)/s \\ \xrightarrow{\text{inverse Laplace}} y(t) &= \int_0^t F(\tau) d\tau . \end{aligned}$$

Here,  $\theta(t)$  denotes the Heavyside function, which is 1 for  $t > 0$  and 0 else. The time-dependent function, which describes the pulse response is often used as a symbol for a specific control loop element.

The pulse response works in a similar way as the Green's function procedure: Wanting to know how a loop control element  $F$  transforms a given input signal  $x(t)$  into an output signal  $y(t)$ , i.e.,  $y(t) = F(t) \star x(t)$ , we produce a rapid pulse leading to the output,

$$y_\delta(t) = F(t) \star \delta(t) = F(t) . \quad (34.35)$$

Now, once we know  $F(t)$ , the response to arbitrary input signals can be computed via,

$$y(t) = y_\delta(t) \star x(t) . \quad (34.36)$$

#### 34.2.1.4 Bode diagram and polar diagram

The *Bode diagram* illustrates the transfer function in the spectral domain on a bilogarithmic scale separating the amplitude spectrum from the phase spectrum [see Fig. 34.3(a-b)]. Frequency regions, where  $|F(s)|$  or  $\varphi(s)$  vary particularly strongly are nicely emphasized in the polar representation [see Fig. 34.3(c-d)].

For LTI systems  $F(s)$  is always a rational function and can, hence, be represented by its poles and zeros in the complex plane,

$$F(s) = A \frac{(s - a_1)(s - a_2) \dots (s - a_n)}{(s - b_1)(s - b_2) \dots (s - b_n)} . \quad (34.37)$$

With this,  $F(s)$  is analytical and conform, i.e., multiple curves in the  $s$ -plane are represented in an isogonal way in the  $F(s)$ -plane. In order to avoid that the eigenfunctions  $e^{st}$  oscillate and diverge, it is necessary that all the poles and zeros are in the left halfplane.

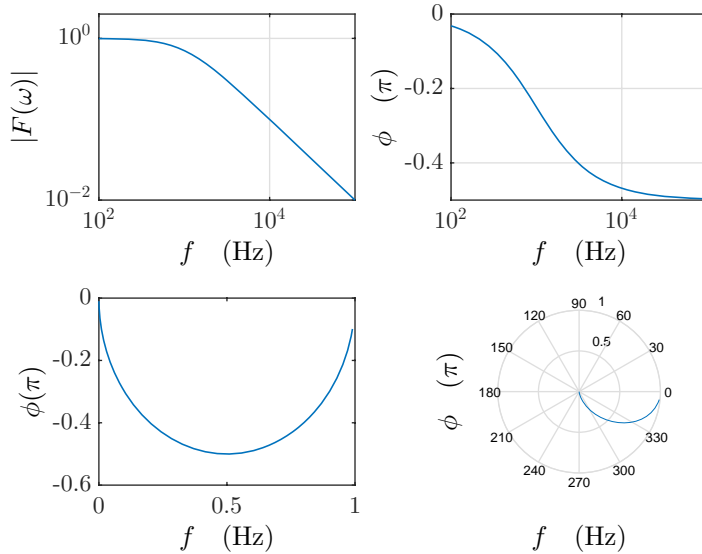


Figure 34.3: (code) Bode diagram.

### 34.2.2 Algebra of transfer circuits

A technical realization of a signal transfer circuit is illustrated by a signal flux diagram, which itself corresponds to the formalism of linear operators. As shown in Fig. 34.4, signals can be

- (a) added  $(f_1 + f_2)(t) \equiv f_1(t) + f_2(t)$ ,
- (b) multiplied  $(f_1 \cdot f_2)(t) \equiv f_1(t) \cdot f_2(t)$ ,
- (c) combined  $f_1(t) = f_2(t)$ ,
- (d) transformed  $f_2(t) = F[f_1](t) \equiv F(f_1(t))$ ,
- (e) connected in parallel  $(F_1 + F_2)[f(t)] \equiv F_1[f(t)] + F_2[f(t)]$ ,
- (f) connected in series  $(F_1 \circ F_2)[f(t)] \equiv F_1[F_2[f(t)]]$ ,

Mathematically, the functions  $f(t)$  form a *vector space* and the operators  $F[f]$  a *ring*. The linear operators generally are defined implicitly by a system of differential equations. The particular case of linear systems is considerably simpler. The general circuit shown in Fig. 34.4(g) corresponds to the differential equation,

$$0 = F[x_1, \dots, x_k, \partial_t x_1, \dots, \partial_t x_k, y_1, \dots, y_j] . \tag{34.38}$$

The linearity  $F[\lambda f_1 + \mu f_2] = \lambda F[f_1] + \mu F[f_2]$  warrants that this equation becomes,

$$0 = [1 + \partial_t + \dots + \int dt + \dots]y_k = [1 + \partial_t + \dots + \int dt + \dots]x_j . \tag{34.39}$$

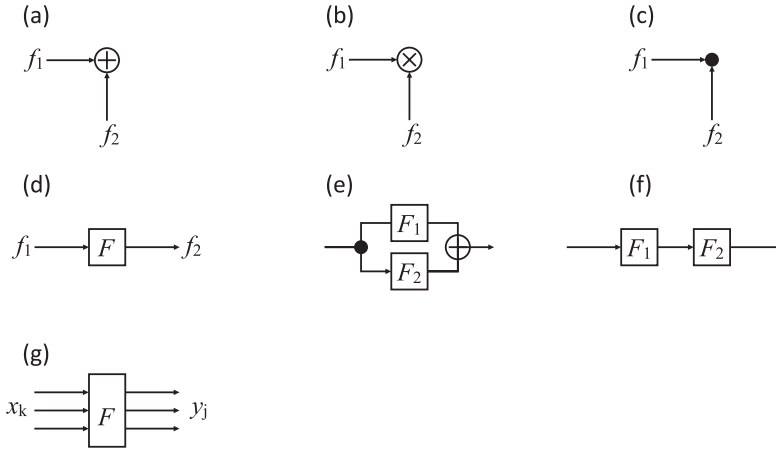


Figure 34.4: LTI circuits.

Note that the multiplication, the derivation, and the integration are linear operators in the same sense as the Fourier and the Laplace transformation.

Linear differential equations can be Laplace transformed. The corresponding transfer function is,

$$F(s) = \mathcal{L}\{F(-\delta + \omega)\} \equiv \frac{\mathcal{L}y(t)}{\mathcal{L}x(t)} . \tag{34.40}$$

In the Laplace-transformed space the operations multiplication, derivation, and integration are all replaced by multiplications:

$$\mathcal{L}[\lambda + \partial_t + \dots + \int dt + \dots] = \lambda + s + \dots + \frac{1}{s} . \tag{34.41}$$

With this, the control loop elements and the additive nodes can be used to completely represent a control circuit.

The characteristic responses of components are frequently non-linear (e.g. transistor). For small signal amplitudes, these response functions, and also multiplication points (e.g. mixers) can be linearized by Taylor expansion up to first order,

$$\begin{aligned} y_0 + \Delta y &= F[x_{01} + \Delta x_1, \dots, x_{0k} + \Delta x_k] \\ &= F[x_{01}, \dots, x_{0k}] + \left(\frac{\partial F}{\partial x_1}\right)_0 \Delta x_1 + \dots + \left(\frac{\partial F}{\partial x_k}\right)_0 \Delta x_k , \end{aligned} \tag{34.42}$$

with  $y_0 = 0 = F[x_{01}, \dots, x_{0k}]$  giving,

$$\Delta y = \left(\frac{\partial F}{\partial x_1}\right)_0 \Delta x_1 + \dots + \left(\frac{\partial F}{\partial x_k}\right)_0 \Delta x_k . \tag{34.43}$$

For example for a multiplication point,

$$\Delta y = K_1 \Delta x_1 + K_2 \Delta x_2 . \tag{34.44}$$

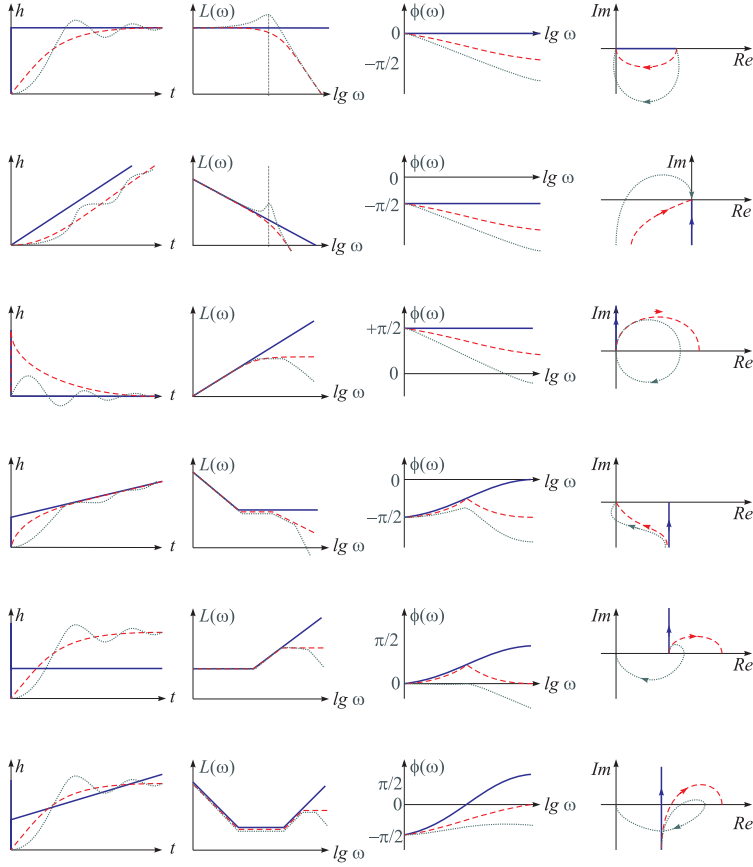


Figure 34.5: Transfer function  $h(t) = \frac{y(t)}{x_w}$ , Bode diagram amplitude  $L(\omega) = 20 \lg |F_R|$  and phase  $\varphi = \arctan \frac{\text{Im } F_R}{\text{Re } F_R}$ , and polar representation  $F(i\omega) = \text{Re } F_R + i\text{Im } F_R$  of the most common regulators. With delay time (—),  $T_2 = T_1 = 0$ , first order with delay time (- - -),  $T_2 = 0 \neq T_1$ , and second order ( $\cdot \cdot \cdot$ ),  $T_2 \neq 0 \neq T_1$ . From top to bottom, the diagrams show the regulators  $P$ ,  $I$ ,  $D$ ,  $PI$ ,  $PD$ , and  $PID$ , described by the equations (34.45) and (34.46).

### 34.2.2.1 Regulators

For many circuits, it is sufficient to restrict to combinations of resistive (proportional), capacitive (integral), and inductive (differential) circuits. Then, the general case of a control regulator is that of a  $PID - T_1 \dots T_n$ -element, meaning that:

$$T_2^2 \ddot{y} + T_1 \dot{y} + y = K_D \dot{x} + K_P x + K_I \int dt x = K_P \left( x + T_v \dot{x} + \frac{1}{T_n} \int dt x \right), \quad (34.45)$$

corresponding to the transfer function,

$$F(s) = \frac{K_D s + K_P + K_I/s}{1 + T_1 s + T_2^2 s^2} = \frac{(1 + T_v s + 1/T_n s)}{1 + T_1 s + T_2^2 s^2}. \quad (34.46)$$

In literature, two notations are used for the constants. They are linked via:  $K_D \equiv K_P T_v$  and  $K_I \equiv K_P / T_n$ . The stationary behavior is obtained setting the delays to



zero:  $T_n \equiv 0$ .

**Example 134 (PID regulators):** For example, for a *proportional regulator*, we have,

$$y = K_P x_w \quad \text{and} \quad F_R = K_P, \quad (34.47)$$

for an *integral regulator* with time delay  $T_1$ , we have,

$$T_1 \dot{y} + y = K_I \int x_w dt \quad \text{and} \quad F_R = \frac{K_I}{s(1 + sT_1)}, \quad (34.48)$$

or for a *PID regulator* without delay, we have,

$$y = K_P x_w + K_D \dot{x}_w + K_I \int x_w dt \quad \text{and} \quad F_R = K_P + \frac{K_I}{s} + K_D s. \quad (34.49)$$

Since there are three basic operations (multiplication with 1,  $s$  and  $1/s$ ), in the end, all rational circuit elements can be reduced to an addition and concatenation of proportional  $F(s) = K_P$ , integral  $F(s) = K_I/s$ , and differentials elements,  $F(s) = K_D s$ . In particular,  $PID - T_1 \dots T_n$  circuits can be constructed by putting in parallel  $P$ ,  $I$ , and  $D$  regulators concatenated with delay elements  $T_1$ . The possibility of feedback opens other possibilities [see Fig. 34.6(a)].

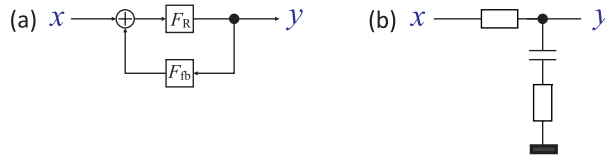


Figure 34.6: (a) Circuit with feedback, (b) low-pass filter circuit.

**Example 135 (Low-pass filter and time delays):** We consider the example of a low-pass filter exhibited in Fig. 34.6(b) and described by the equation,

$$F(\omega) = \frac{R + \omega L + 1/\omega C}{R_i + R + \omega L + 1/\omega C}. \quad (34.50)$$

I.e., we have a  $PID - T_1 T_2$  circuit.

Another example, is the dead time circuit,

$$y(t) = x(t - T_t) \quad \text{and} \quad F(s) = e^{-sT_t}. \quad (34.51)$$

We have,

$$F(\omega) = e^{-i\omega T_t} F_0 \quad \text{and} \quad |F(\omega)| = F_0 \quad \text{and} \quad \varphi(\omega) = -\omega T_t. \quad (34.52)$$

Hence, dead time circuits produce phase shifts, which are proportional to the dead time interval  $T_t$ .

### 34.2.2.2 Heuristic rules for the Bode diagram

Any deviation of the amplitude spectrum from  $n \cdot 6\text{dB}/\text{octave}$  to  $(n + 1) \cdot 6\text{dB}/\text{octave}$  causes a retardation in the phase spectrum of  $90^\circ$ . At the cut-off frequency, where the inclination changes its behavior, the phase shift is just  $45^\circ$ . A deviation to higher/lower inclinations shifts the phase by  $\pm 90^\circ$ . (This does not hold for some phase-shifting circuits).

### 34.2.2.3 Transfer function of feedback circuits

Fig. 34.6 shows the idea underlying the feedback,

$$F(s) = \frac{1}{1/F_R - F_{fb}} . \quad (34.53)$$

For example, for  $F_R = 1/T_1s$  and  $F_{fb} = -1$  we have,

$$F(s) = \frac{1}{1 + T_1s} , \quad (34.54)$$

which corresponds to a delay element (or high-pass filter).

For  $F_r$  being a proportional element, we say that the feedback rigid, for  $F_r$  being differential, the feedback is anticipating, and for  $F_r$  being integral, the feedback is delaying.

### 34.2.3 Stability of feedback circuits

As discussed above, the transfer function of the feedback circuit is,

$$H(s) = \frac{F(s)}{1 + F(s)F_{fb}(s)} . \quad (34.55)$$

The *open loop gain* is  $V(s) = F(s)F_{fb}(s)$ . The circuit is stable, when for all the eigenfunctions  $e^{st}$ , that do not decay with  $Re\ s \geq 0$ , the transfer function of the feedback circuit is finite,  $H(s) < \infty$ .

An equivalent criterion is the *Nyquist criterion*: *The curve  $V(\omega)$  to  $\omega \in [0; \infty[$  must always bypass the point of instability at  $Re\ s = -1$  leaving it on the left side. That is, considering negative frequencies, the curve should not circle this point.* Fig. 34.8 shows an example.

### 34.2.4 Further topics in control theory

#### 34.2.4.1 Nonlinear control theory

Linear control theory applies to systems made of devices which obey the superposition principle, which means roughly that the output is proportional to the input. They are governed by linear differential equations. A major subclass is systems which in addition have parameters which do not change with time, called linear time invariant (LTI) systems. These systems are amenable to powerful frequency domain mathematical techniques of great generality, such as the Laplace transform, Fourier transform,  $Z$  transform, Bode plot, root locus, and Nyquist stability criterion. These lead to a description of the system using terms like bandwidth, frequency response, eigenvalues, gain, resonant frequencies, poles, and zeros, which give solutions for system response and design techniques for most systems of interest.

Nonlinear control theory covers a wider class of systems that do not obey the superposition principle, and applies to more real-world systems, because all real control systems are nonlinear. These systems are often governed by nonlinear differential equations. If only solutions near a stable point are of interest, nonlinear systems can often be linearized by approximating them by a linear system using perturbation theory, and linear techniques can be used.

<p><i>P</i>-servo with rigid feedback</p>		<p><i>P</i></p>	$K_p = \frac{K_R}{1+K_r K_R} \xrightarrow{K_R \rightarrow \infty} \frac{1}{K_r}$
<p><i>P</i>-servo with yielding feedback</p>		<p><i>P-T<sub>1</sub></i> <i>I</i></p>	$K_p = K_R, \quad T_1 = K_R K_r \text{ for } K_R \ll \infty$ $K_1 = K_r^{-1} \text{ for } K_R \rightarrow \infty$
<p><i>P</i>-servo with yielding feedback</p>		<p><i>PD-T<sub>1</sub></i> <i>PI</i></p>	$K_p = K_R, \quad T_v = T_r, \quad T_1 = T_r + K_r K_R \text{ for } K_R \ll \infty$ $K_p = T_r / K_r, \quad T_n = T_r \text{ for } K_R \rightarrow \infty$
<p><i>P</i>-servo with delayed feedback</p>		<p><i>PD-T<sub>1</sub></i> <i>PD</i></p>	$K_p = \frac{K_R}{1+K_r K_R}, \quad T_v = T_r, \quad T_1 = \frac{T_r}{1+K_r K_R} \text{ for } K_R \ll \infty$ $K_p = 1/K_r, \quad T_v = T_r \text{ for } K_R \rightarrow \infty$
<p><i>P</i>-servo with delayed yielding feedback</p>		<p><i>PID</i></p>	$K_p = \frac{T_{r1} + T_{r2}}{K_{r1} K_{r2}}, \quad T_v = \frac{T_{r1} T_{r2}}{T_{r1} + T_{r2}}, \quad T_n = T_{r1} + T_{r2}$ <p style="text-align: right;">for <math>K_R \rightarrow \infty</math></p>
<p><i>P</i>-servo with two delay circuits in the feedback</p>		<p><i>PID</i></p>	$K_p = \frac{T_{r1} + T_{r2}}{K_r (T_{r1} - T_{r2})}, \quad T_v = \frac{T_{r1} T_{r2}}{T_{r1} + T_{r2}}, \quad T_n = T_{r1} + T_{r2}$ <p style="text-align: right;">for <math>K_R \rightarrow \infty</math> and <math>T_{r1} &gt; T_{r2}</math></p>
<p><i>I</i>-servo with rigid feedback</p>		<p><i>P-T<sub>1</sub></i></p>	$K_p = \frac{1}{K_r}, \quad T_1 = \frac{1}{K_r K_r}$
<p><i>I</i>-servo with yielding feedback</p>		<p><i>PI-T<sub>1</sub></i></p>	$K_p = \frac{K_r T_r}{1+K_r K_r}, \quad T_n = T_r, \quad T_1 = \frac{T_r}{1+K_r K_r}$

Figure 34.7: Some examples for feedback regulators. The columns show from left to right: the nomenclature, the circuit diagram, the behavior, and the constants of the LTI system.

### 34.2.4.2 MIMO control systems

In this script we restrict to *single-input single-output control systems (SISO)*, which is the simplest and most common type, in which one output is controlled by one control signal. Examples are the temperature control or an audio system, in which the control input is the input audio signal and the output is the sound waves from the speaker.

In contrast, *multiple-input multiple-output control systems (MIMO)* are found in more complicated systems. For example, modern large telescopes such as the Keck and MMT have mirrors composed of many separate segments each controlled by an actuator. The shape of the entire mirror is constantly adjusted by a MIMO active optics control system using input from multiple sensors at the focal plane, to compensate for changes in the mirror shape due to thermal expansion, contraction, stresses as it is rotated and distortion of the wavefront due to turbulence in the atmosphere.

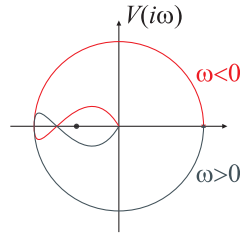


Figure 34.8: Illustration of the Nyquist criterion.

Another example are ultra-stable laser systems stabilized by combinations of fast actuators with low dynamic range and slow actuators with large dynamic range.

### 34.2.5 Exercises

#### 34.2.5.1 Ex: Step response

Calculate the step response of a low-pass filter using the Laplace transform formalism.

## 34.3 Characterization of stability

The quality factor of a resonance measured with an oscillator in its function as a measuring apparatus for the resonance frequency is named *precision*. The precision also includes the perturbations to which the controlled oscillator is exposed and can be understood as the standard deviation of the frequency realized by the standard. The temporal or spectral behavior of precision, i.e. the stability can e.g. measured directly by comparing similar but independent standards. The reciprocal of the spread of the frequency realizations of an ensemble of similar standards is called *reproducibility*. The term reproducibility is also used to compare the frequencies of an individual standard before and after readjustment of all its technical parameters.

The *accuracy* is defined as the degree of agreement between the frequency realized by the standard and the defined standard frequency, i.e. the frequency that would be displayed in the fault-free ideal case<sup>3</sup>. The accuracy is always less than the quality of the resonance and the certainty of its center frequency. It includes the precision and limits the reproducibility [11]. The fact that the accuracy is related to the ideal case of absent errors implies that it cannot be measured directly. It must be inferred indirectly through model assumptions regarding the measuring apparatus estimating the probability for presumed or possible errors. We then speak of the *uncertainty* of the measured value [140].

The temporal or spectral behavior of *accuracy* is called *stability*. It is measurable and is quantified in the frequency domain by the *spectral density of fluctuations* and in the time domain best by the *Allan variance*. The noise is now the physical phenomenon that manifests itself as a deviation from the optimal stability.

<sup>3</sup>For example, when a measurement apparatus for the constant  $\pi$  provided the value  $x = 3.141\ 59\ (12)$ , then the accuracy is  $x - \pi$  and the precision 0.000 12.

The stability that an ideal frequency standard can achieve in principle is proportional to quality factor of the resonance  $\omega/(\Delta\omega_{nat} + \Delta\omega_{broaden})$  and the signal-to-noise ratio of the control signal  $S/N$ . Hence, the stability can be optimized by choosing atomic transitions with small spontaneous decay rates  $\Delta\omega_{nat}$ . Appropriate techniques for the experimental preparation of the resonance limit the influence of line broadening mechanisms  $\Delta\omega$ . According to the Fourier theorem, the resolution of narrow lines requires long observation times. Now, the control signal of a feedback regulator can only be determined after a whole observation period. This means that the apparatus already must have an intrinsic stability good enough that the frequency does not leave the control range during a period of observation. Furthermore, a better signal-to-noise ratio can improve the precision with which the line center of the resonance can be determined.

Ultimately, the most promising way to increase the accuracy of a frequency standard seems to be to choose the highest possible transition frequencies  $\omega$ , provided that the oscillations can still be counted electronically, or be linked in a phase-coherent way to oscillators generating countable oscillations, e.g. using frequency combs. The requirement of phase coherence at optical frequencies puts the laser in the focus of interest in metrology.

### 34.3.1 Quantifying frequency fluctuations

The following sections deal with perturbation-induced fluctuations of the laser frequency, i.e. frequency noise. To characterize the behavior of an oscillator (especially when used as a frequency standard), it is necessary to introduce some concepts that allow the quantitative description of the noise. The most important are reproducibility, stability, spectral density of fluctuations, Allan variance, and emission bandwidth. The basic work on this has been carried out at the National Bureau of Standards (NBS) in Boulder, Co, USA [10, 11, 48, 162].

#### 34.3.1.1 Stability in the frequency domain, spectral fluctuation density

The instantaneous amplitude of an oscillator, e.g. the electric field of a laser radiation, can be written,

$$\mathcal{E}(t) = \mathcal{E}_0(t)e^{i\phi(t)}. \quad (34.56)$$

noise afflicts phase and amplitude. In the following we will neglect amplitude noise,  $\mathcal{E}_0(t) = \mathcal{E}_0$ , and if the frequency fluctuations only deviate slightly from a mean value,  $\omega_0 \gg |\dot{\phi}(t)|$ , we may write,

$$\phi(t) \equiv \omega_0 t + \varphi(t). \quad (34.57)$$

In the following, we will often consider normalized frequency fluctuations,

$$y(t) = \dot{\varphi}(t)/\omega_0. \quad (34.58)$$

When measuring stability, one must differentiate between *deterministic fluctuations* and *stochastic noise*. Deterministic fluctuations are usually due to inadequate control of equipment parameters. They generate systematic errors and slow drifts  $y_{sys}(t)$  which, if one recognizes them as such in time domain measurements (measure for sufficiently long times!), can be subtracted and disregarded. Stochastic noise,

however, is stationary:

$$\overline{y_{sto}(t)} = \overline{y(t) - y_{sys}(t)} = 0 \quad \text{defining} \quad \overline{y(t)} \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T y(t) dt \quad (34.59)$$

as the time average. In the following only stationary stochastic fluctuations are considered.

Let us take a look at the *autocorrelation function* of the phase defined as,

$$R_y(\tau) \equiv \overline{y^*(t)y(t+\tau)} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T y^*(t)y(t+\tau) d\tau \quad (34.60)$$

and the *spectral density of phase fluctuations* which, according to the *Wiener-Khinchine theorem*, can be obtained as the Fourier transform of the autocorrelation function,

$$S_y(f) \equiv \mathcal{F}R_y(\tau) = \int_{-\infty}^{\infty} R_y(\tau)e^{-2\pi i f \tau} d\tau . \quad (34.61)$$

The normalized density of frequency fluctuations  $S_y(f)$  is a spectral quantity with the unit 1/Hz. Frequency and phase fluctuations are linked by:

$$S_{\dot{x}}(f) = f^2 S_x(f) , \quad (34.62)$$

as will be shown in Exc. 34.3.3.1. Also,

$$S_{ax}(f) = a^2 S_x(f) , \quad (34.63)$$

If the integral of the spectral fluctuation density is finite it corresponds, according to the definition (34.62), to the noise power or the mean square deviation of a measured variable:

$$\int_0^{\infty} S_y(f) df = R_y(0) = \overline{|y(t)|^2} < \infty . \quad (34.64)$$

### 34.3.1.2 Model of noise

Measurements seem to confirm today that stochastic fluctuations in frequency standards can be traced back to a few additive noise processes with different physical origins and different frequency responses [10]:

$$S_y(f) = \sum_{\beta=-2}^2 h_{\beta} f^{\beta} . \quad (34.65)$$

The table below lists the most common ones.

This noise model is based on the assumption that the noise processes it describes operate in all Fourier frequency ranges, which violates the requirement (34.64). The dilemma does not arise in experiment, since the integration over an unlimited Fourier frequency range is not a realistic concept in that each measurement only takes a finite time  $\tau$ , so that very low frequencies below a cut-off frequency  $f_{min} = 2\pi/\tau$  are not

noise type	$S_y(f)$	$\sigma_y^2(\tau)$
white phase noise	$h_2 f^2$	$\propto \frac{h_2}{\tau^2}$
flicker phase noise	$h_1 f^1$	$\propto \frac{h_1}{\tau^2}$
white frequency noise	$h_0 f^0$	$\frac{h_0}{2\tau}$
flicker frequency noise	$h_{-1} f^{-1}$	$h_{-1} 2 \ln 2$
random walk frequency drifts	$h_{-2} f^{-2}$	$h_{-2} \frac{(2\pi)^2}{6} \tau$

Table 34.1: Spectral fluctuation density and Allan-variance for common noise processes [48].

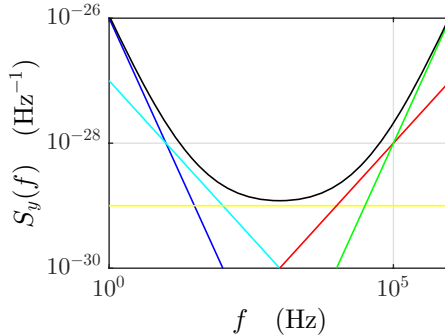


Figure 34.9: Noise model according to (34.65).

perceived. In addition, every real data acquisition system has a low-pass behavior with a cut-off frequency  $f_{max}$ , so that high frequencies also do not contribute to the integral. These bandwidth constraints enforce the condition (34.64) for the five noise processes assumed by (34.65) [431]. The measure for the noise power in any case has the form:  $\int_{f_{min}}^{f_{max}} S_y(f) df$ .

### 34.3.1.3 Description of stability in the time domain, Allan variance

Temporal frequency fluctuations of an oscillator can be measured by *discriminating the frequency fluctuations at the dispersive profile of a resonance* (or error signal) and convert it into voltage fluctuations. It is just the curve exhibited by a spectrum analyzer to which the error signal is fed, as illustrated by the left setup of Fig. 34.11.

Like any physical quantity, frequency fluctuations can only be measured as an average over an *integration time interval*  $\tau$  imposed by the measuring apparatus. The  $k$ -th measurement of the quantity  $y$  at the time  $t_k$  results in the measured value:

$$y_k(\tau) = \frac{1}{\tau} \int_{t_k}^{t_k+\tau} y(t) dt . \tag{34.66}$$

Assuming that the dead time of the measuring apparatus is negligible (if necessary, technical precautions must be taken to meet this requirement approximately), the

variance of stochastic noise can be expressed as follows:

$$\sigma_y^2(\tau) = \frac{1}{N-1} \sum_{k=1}^N y_k^2 \quad \text{where} \quad \bar{y}_k = 0. \quad (34.67)$$

The variance is a direct measure of the stability of an oscillator in time domain. It is measured from a discrimination of the error signal in a similar way as the fluctuation density  $S_y(f)$ . However, as illustrated by the left setup of Fig. 34.11, the discriminated signal is recorded in time domain, e.g. by an oscilloscope.

The variance can be linked to the spectral density of frequency fluctuations in frequency domain by Fourier transformation. With the Heaviside step function  $\Theta$  the following relationship can be given [162, 10, 29],

$$\sigma_y^2(\tau) = \int_0^\infty S_y(f) |\mathcal{F}\zeta_1(f)|^2 df \quad \text{where} \quad \zeta_1(t) = \frac{1}{\tau} \Theta_{[-\tau, 0]}(t), \quad (34.68)$$

is the area-normalized jump function, which models the duration of the integration time  $\tau$ . Its Fourier-transform is the transfer function of the equivalent filter.

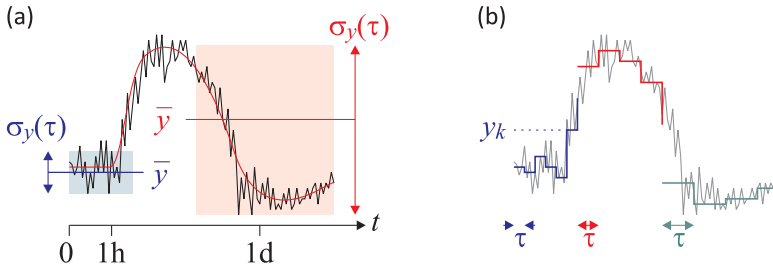


Figure 34.10: (a) Noise can exhibit very different short and long time behavior. (b) Any measurement needs a minimum integration time.

It turns out that the variance for  $1/f$  noise and for stochastic drifts ( $1/f^2$  noise) diverges at the lower limit, i.e. this variance is not useful for practical applications. The divergence comes from the fact that for longer and longer measurements ( $N \rightarrow \infty$ ), respectively, smaller and smaller Fourier frequencies ( $f \rightarrow 0$ ), longer and longer periodic fluctuations can be identified as such, while for shorter measurements they appear as linear drifts. One way out is to calculate the variance for a limited number  $k$  of measurement data and to average the variances of  $M$  of such data sets of length  $k$ . This variance converges for a larger number of noise processes. This so-called pair variance ( $k = 2$ ) or *Allan variance* is widely used:

$$\sigma_y^2(\tau) = \frac{1}{2M} \sum_{j=1}^M (y_{2j} - y_{2j-1})^2. \quad (34.69)$$

Like the normal variance, the Allan variance can also be related to the spectral density of frequency fluctuations:

$$\sigma_y^2(\tau) = \int_0^\infty S_y(f) |\mathcal{F}\zeta_2(f)|^2 df \quad \text{where} \quad \zeta_2(t) \equiv \frac{1}{\sqrt{2}} [\zeta_1(t) - \zeta_1(-t)]. \quad (34.70)$$



The Fourier transforms of the step functions  $\zeta_1(t)$  and  $\zeta_2(t)$  will be calculated in Exc. 34.3.3.2, as well as the variances for white noise.

### 34.3.2 Power spectral density

It is important not to confuse the spectral density of frequency fluctuations with the power spectral density of the oscillator defined via the *autocorrelation function of the field amplitude*<sup>4</sup>,

$$R_{\mathcal{E}}(\tau) \equiv \langle \mathcal{E}^*(t)\mathcal{E}(t+\tau) \rangle = \mathcal{E}_0^2 \langle e^{i[\phi(t+\tau)-\phi(t)]} \rangle = \mathcal{E}_0^2 e^{i\omega_0\tau} \langle e^{i[\varphi(t+\tau)-\varphi(t)]} \rangle, \quad (34.71)$$

as its Fourier transform,

$$S_{\mathcal{E}}(\omega) = \mathcal{F}R_{\mathcal{E}}(\tau). \quad (34.72)$$

The power spectral density is typically measured as the beat frequency of two independent oscillators. It is just the curve exhibited by a spectrum analyzer to which the beat signal is fed, as illustrated in the right setup of Fig. 34.11.

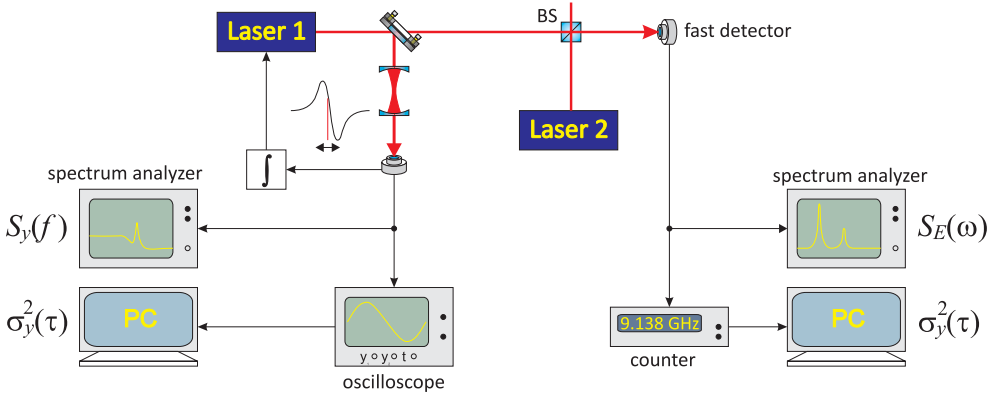


Figure 34.11: (left) Setup for measuring the spectral density of frequency fluctuations  $S_y(f)$  and the Allan variance  $\sigma_y^2(\tau)$  of laser 1 discriminating it at the slope of transmission signal of an optical cavity. (right) The power spectral density  $S_{\mathcal{E}}(\omega)$  can be found as the beat signal between two lasers and either be exhibited on a spectrum analyzer  $S_{\mathcal{E}}(\omega)$  or counted and processed to an Allan variance  $\sigma_y^2(\tau)$ .

The beat spectrum is the convolution of the emission bandwidth of the two oscillators,

$$S_{\mathcal{E}}(\omega) = S_{\mathcal{E},laser1}(\omega) * S_{\mathcal{E},laser2}(\omega). \quad (34.73)$$

In particular, for the case that we have good reasons to believe that one laser is much narrower than the other, the power spectral density  $S_{\mathcal{E}}(\omega)$  will reflect the emission spectrum of just the broader laser. Note that the power spectral density derived

<sup>4</sup>Note that the *first-order coherence* is just the normalized autocorrelation,

$$g^{(1)}(\tau) \equiv \frac{\langle \mathcal{E}^*(t)\mathcal{E}(t+\tau) \rangle}{\langle \mathcal{E}^*(t)\mathcal{E}(t) \rangle} = \frac{R_{\mathcal{E}}(\tau)}{R_{\mathcal{E}}(0)}.$$

from a beat of two independent (uncorrelated) oscillators gives us information on their true emission bandwidths, which is relevant e.g. for resolving narrow atomic transitions. On the other hand, the stability measures  $S_y(f)$  and  $\sigma_y^2(\tau)$  derived from a discriminated error signal (left setup in Fig. 34.11) only tell us the stability of an oscillator with respect to the reference from which the error signal was derived, e.g. the transmission slope of an optical cavity.

### 34.3.2.1 Spectral noise power density in the case of white noise

The spectral noise power density  $S_{\mathcal{E}}(\omega)$  of the field  $\mathcal{E}(t)$  of an oscillator can, in the case of white frequency noise, be related to the spectral density of its frequency fluctuations. In the case of a laser oscillator, the half-width half maximum of the spectral noise power density, i.e. the emission bandwidth, is often specified. We will, in the following, derive the emission spectrum for the case of white Gaussian noise [664, 225, 207].

In Exc. 34.3.3.3 we show that for a *Gaussian noise process* holds [171, 225],

$$\left\langle e^{-i[\varphi(t) - \varphi(t+\tau)]} \right\rangle = e^{-\langle [\varphi(t) - \varphi(t+\tau)]^2 \rangle / 2}. \quad (34.74)$$

Now we set  $\varphi(t) = \omega_0 \int_0^t y(t') dt'$  using (34.58) and obtain,

$$\begin{aligned} \langle [\varphi(t) - \varphi(t+\tau)]^2 \rangle &= \left\langle \omega_0^2 \left[ \int_0^\tau y(t') dt' \right]^2 \right\rangle = \omega_0^2 \int_0^\tau \int_0^\tau \langle y(t') y(t'') \rangle dt' dt'' \quad (34.75) \\ &= \omega_0^2 \int_0^\tau \int_0^\tau R_y(t' - t'') dt' dt'' = 2\omega_0^2 \int_0^\tau (\tau - t) R_y(t) dt. \end{aligned}$$

Using (34.61), we now substitute the autocorrelation function by its Fourier transform, the spectral fluctuation density,  $R_y(t) = \int_0^\infty S_y(f) e^{2\pi i f t} df$ :

$$\begin{aligned} \langle [\varphi(t) - \varphi(t+\tau)]^2 \rangle &= 2\omega_0^2 \int_0^\infty S_y(f) \int_0^\tau (\tau - t) e^{2\pi i f t} dt df \quad (34.76) \\ &= 2\omega_0^2 \int_0^\infty S_y(f) \left( \frac{\sin \pi f \tau}{2\pi f} \right)^2 df + \text{imaginary part}. \end{aligned}$$

We neglect the imaginary part.

For Markovian white noise the phase fluctuations are  $\delta$ -distributed, which means,

$$R_y \equiv \langle y^*(t) y(t+\tau) \rangle = h_0 \delta(\tau) \quad \text{and} \quad S_y(f) = h_0 = \text{const}. \quad (34.77)$$

I.e. the so-called *white noise* is characterized by a constant spectral density of phase fluctuations. Carrying on the calculation (34.76) for the case of white frequency noise we get,

$$\langle [\varphi(t) - \varphi(t+\tau)]^2 \rangle = \frac{h_0 \omega_0^2 |\tau|}{\pi} \int_0^\infty \left( \frac{\sin x}{x} \right)^2 dx = \frac{h_0 \omega_0^2 |\tau|}{2}. \quad (34.78)$$

With this result, we can undertake to calculate the autocorrelation function of the field amplitude (34.71),

$$R_{\mathcal{E}}(\tau) = \mathcal{E}_0^2 e^{\omega_0 \tau} e^{-h_0 \omega_0^2 |\tau| / 2}. \quad (34.79)$$

The resulting *power spectral density* (34.72) is <sup>5</sup>:

$$S_{\mathcal{E}}(\omega) = \mathcal{E}_0^2 \int_{-\infty}^{\infty} R_{\mathcal{E}}(\tau) e^{-i(\omega - \omega_0)\tau} d\tau = \frac{2h_0\omega_0^2}{4\Delta^2 + (h_0\omega_0^2/2)^2}, \quad (34.80)$$

where  $\Delta \equiv \omega - \omega_0$  is the deviation of the oscillator frequency from the center frequency  $\omega_0$ . Thus, the the emission spectrum for the case of white Gaussian noise is a Lorentzian profile with the *laser emission bandwidth*,

$$\beta = \frac{1}{2}h_0\omega_0^2. \quad (34.81)$$

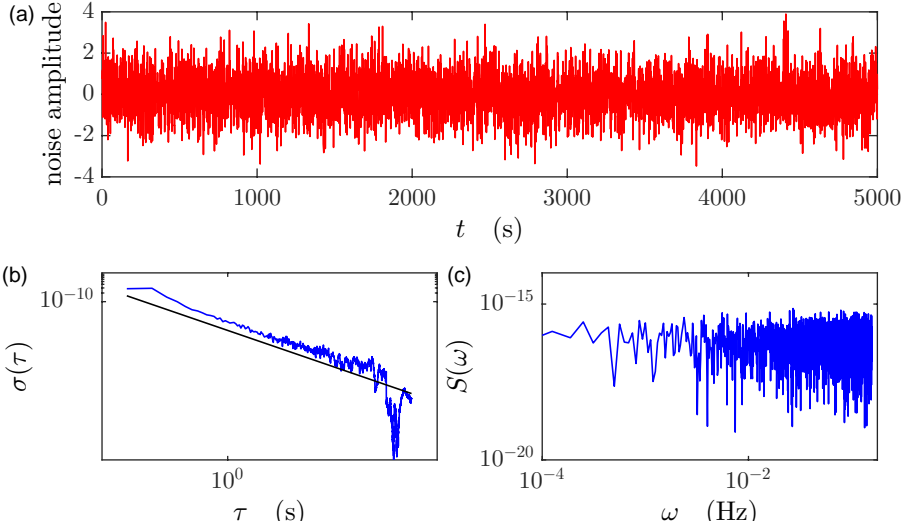


Figure 34.12: (code) Allan variance (b) and spectral density of frequency fluctuations (c) calculated from a randomly generated data set (a).

The Lorentz shape of the emission profile of an oscillator or a resonance always indicates white noise of the underlying frequency fluctuation density. In this sense, the Lorentz form of the natural broadening of an atomic resonance can also be traced back to the white noise of the vacuum fluctuations. Here, the emission bandwidth has to be replaced by the natural linewidth. The Allan variance in this case is:

$$\sigma_y^2(\tau) = \frac{h_0}{2\tau} = \frac{1}{Q^2} \frac{1}{\Gamma} \frac{1}{\tau}. \quad (34.82)$$

with the linewidth (FWHM)  $\Gamma = h_0\omega_0^2/2$  and  $Q = \omega_0/\Gamma$  and indicates the maximum achievable stability for a frequency standard that is coupled to the resonance  $\omega_0$ .

<sup>5</sup>Using  $\mathcal{F}[e^{-a|x|}] = \int_{-\infty}^{\infty} e^{-a|t|} e^{-i\omega t} dt = \frac{2a}{a^2 + \omega^2}$ .

### 34.3.2.2 Spectral noise power density in case of periodic phase perturbation

The momentary deflection of the oscillator can be described in the case of a harmonic phase disturbance by equation (34.60) with the additional condition:  $\phi(t) = N \sin \Omega t$ . The frequency fluctuation density and the Allan variance are obtained in this case:

$$S_y(f) = \left( \frac{fN}{2\omega_0} \right)^2 \delta(f - \Omega) \quad \text{resp.} \quad \sigma_y^2(\tau) = \left( \frac{\Omega N}{2\omega_0} \right)^2 \frac{\sin^2 \Omega\tau/2}{\Omega\tau/2}. \quad (34.83)$$

The spectral noise power density consists of a discrete spectrum of sidebands, the number and height of which is given by the modulation index  $N$ :

$$S_{\mathcal{E}}(\omega) = \sum_{n=-\infty}^{\infty} |J_n(N)|^2 \delta(\omega - \omega_0 - \Omega). \quad (34.84)$$

A full width at half maximum of the spectral noise power density cannot be specified. However, as a measure of the emission bandwidth of the oscillator, the frequency spacing of the sideband of the highest order can be understood, the height of which corresponds to at least half the height of the carrier frequency  $\omega_0$ .

### 34.3.3 Exercises

#### 34.3.3.1 Ex: Spectral density of frequency fluctuations

Prove the relationship  $S_{\dot{x}}(f) = f^2 S_x(f)$ .

#### 34.3.3.2 Ex: Allan variance for white noise

- Calculate the Fourier transform of step function  $\zeta_1(t)$  and the one-point variance for white noise from its definition (34.68).
- Repeat the calculation for the step function  $\zeta_2(t)$  and the Allan variance as defined in (34.70).

#### 34.3.3.3 Ex: Gaussian noise process

Prove the relationship (34.75) for a *Gaussian noise process* characterized by,

$$\frac{\langle A^{2n} \rangle}{(2n)!} = \frac{\langle A^2 \rangle^n}{2^n n!} \quad \text{and} \quad \langle A^{2n-1} \rangle = 0.$$

## 34.4 Data sheets

The following pages contain the data sheets of the main components used in this course.

# HL6722G

AlGaInP Laser Diode



ODE-208-220E (Z)

Rev.5  
Mar. 2005

## Description

The HL6722G is a 0.67  $\mu\text{m}$  band AlGaInP index-guided laser diode with a multi-quantum well (MQW) structure. It is suitable as a light source for barcode scanner, and various other types of optical equipment. Hermetic sealing of the package assures high reliability.

## Features

- Visible light output at wavelengths up to 680 nm
- Single longitudinal mode
- Continuous operating output: 5 mW CW
- Low voltage operation: 2.7 V Max
- Low current operation: 32 mA Typ
- Built-in monitor photodiode

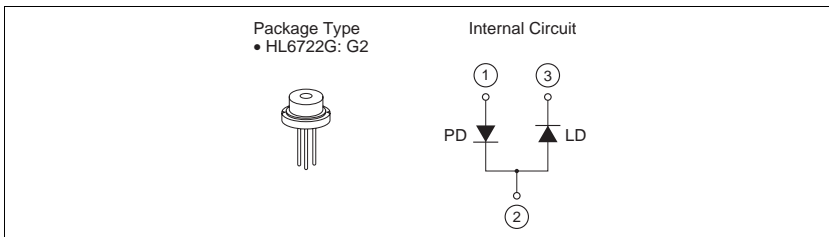


Figure 34.13: Data sheet for the diode laser from Thorlabs, model Hitachi HL6722G.

# Coaxial Amplifier

## ZHL-2-8

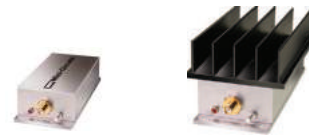
50Ω Medium High Power 10 to 1000 MHz

### Features

- wideband, 10 to 1000 MHz
- high IP3, +38 dBm typ.
- medium high power, 29 dBm min.

### Applications

- VHF/UHF
- test equipment
- cellular
- instrumentation
- laboratory



ZHL-2-8X

SMA version shown

ZHL-2-8

CASE STYLE: T34			
Connectors	Model	Price	Qty.
BNC	ZHL-2-8	\$525.00 ea.	(1-9)
BNC	ZHL-2-8X	\$515.00 ea.	(1-9)
SMA	ZHL-2-8-S	\$535.00 ea.	(1-9)
SMA	ZHL-2-8X-S	\$525.00 ea.	(1-9)

### Electrical Specifications

MODEL NO.	FREQ. (MHz)	GAIN (dB)			MAXIMUM POWER OUTPUT (dBm)		DYNAMIC RANGE		VSWR (∶1) Max.		DC POWER	
		Min.	Typ.	Max.	(1 dB Compr.)	Input (no damage)	NF (dB) Typ.	IP3 (dBm) Typ.	In	Out	Volt (V) Nom.	Current (A) Max.
ZHL-2-8	10 1000	31	35	±1.0	+29	+5	10.0	+38	2.0	2.0	24	0.6
ZHL-2-8X*	10 1000	31	35	±1.0	+29	+5	10.0	+38	2.0	2.0	24	0.6

\* Heat sink not included  
Open load is not recommended, potentially can cause damage.  
With no load derate max input power by 20 dB

To order without heat sink, add suffix X to model number. Alternative heat sinking and heat removal must be provided by the user to limit maximum temperature to 65°C, in order to ensure proper performance. For reference, this requires thermal resistance of user's external heat sink to be 1.35°C/W Max.

### Maximum Ratings

Operating Temperature -20°C to 65°C  
Storage Temperature -55°C to 100°C  
DC Voltage +25V Max.  
Permanent damage may occur if any of these limits are exceeded.

### Outline Drawing

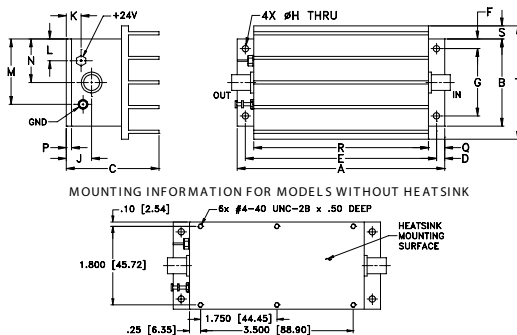


Figure 34.14: Data sheet for the rf-amplifier from MiniCircuits, model ZHL-2-8.

# Coaxial Voltage Controlled Oscillator

## ZOS-100+

Dual Output 50 to 100 MHz



### Features

- octave bandwidth
- linear tuning, 4.5 MHz/V typ.
- excellent harmonic suppression, -29 dBc typ.
- rugged shielded case
- protected by US Patent, 6,943,629

### Applications

- auxiliary output freq. monitoring
- load insensitive source

CASE STYLE: BR386			
Connectors	Model	Price	Qty.
SMA	ZOS-100+	\$119.95	(1-9)

+ RoHS compliant in accordance with EU Directive (2002/95/EC)

The +Suffix has been added in order to identify RoHS Compliance. See our web site for RoHS Compliance methodologies and qualifications.

### Electrical Specifications

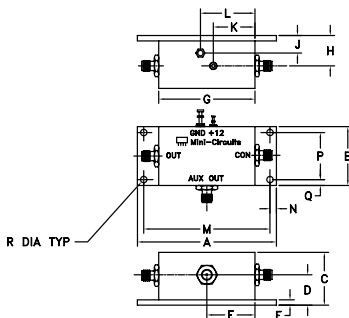
FREQUENCY (MHz)		POWER OUTPUT (dBm) Typ.		TUNING VOLTAGE (V)		PHASE NOISE (dBc/Hz) SSB at offset frequencies: Typ.			PULLING (MHz) pk-pk (open/short)	PUSHING (MHz/V)	TUNING SENSITIVITY (MHz/V)	HARMONICS (dBc)	3 dB MODULATION BANDWIDTH (MHz)	DC OPERATING POWER		
Min.	Max.	Main	Aux.	Min.	Max.	10 kHz	100 kHz	1 MHz	Typ.	Typ.	Typ.	Typ.	Max.	Typ.	Vcc (volts)	Current (mA) Max.
50	100	+9	-12	1	16	-111	-131	-143	0.026	0.25	4.5	-29	-20	0.1	12	140

### Maximum Ratings

Operating Temperature	-55°C to 85°C
Storage Temperature	-55°C to 100°C
Absolute Max. Supply Voltage (Vcc)	+16V
Absolute Max. Tuning Voltage (Vtune)	+18V

all specifications: 50 ohm system  
Permanent damage may occur if any of these limits are exceeded.

### Outline Drawing



### Outline Dimensions (inch/mm)

A	B	C	D	E	F	G	H	J	K	L	M	N	P	Q	R	wt
3.25	1.38	1.25	.71	1.13	.125	2.25	.71	.41	.98	1.28	2.950	.15	1.100	.14	.150	grams
82.65	35.05	31.75	18.03	28.70	3.18	57.15	18.03	10.41	24.89	32.51	74.93	3.81	27.94	3.56	3.81	180

### electrical schematic

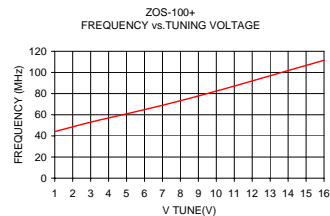
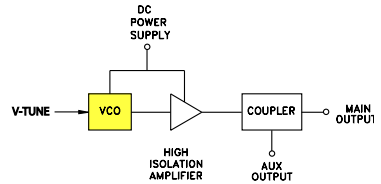


Figure 34.15: Data sheet for the Voltage-Controlled Oscillator (VCO) from Minicircuits, model ZOS-100+.

# Coaxial Voltage Variable Attenuator

## ZX73-2500+

50Ω 10 to 2500 MHz



FEMALE SMA shown  
CASE STYLE: GD958

### Maximum Ratings

Operating Temperature	-55°C to 85°C
Storage Temperature	-55°C to 85°C
Absolute Max. Supply Voltage (V+)	12V
Absolute Max. Control Voltage (Vctrl)	20V
Absolute Max. RF Input Level	+20 dBm

Permanent damage may occur if any of these limits are exceeded.

### Features

- Broadband, 10-2500 MHz
- IP3, +43 dBm typ.
- 40 dB attenuation @ 1500 MHz
- Good VSWR at in /out ports over attenuation range
- No external bias and RF matching network required
- Shielded case
- Protected by US Patent 6,790,049

### Applications

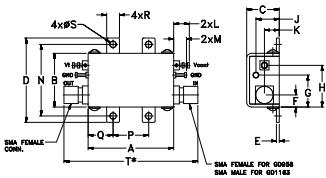
- Variable gain amplifier
- Power level control
- Feed-forward amplifiers
- ALC circuits

SMA	Connectors	Model	Price	Qty.	Case
INPUT	OUTPUT				
FEMALE	FEMALE	ZX73-2500-S+	\$49.95	(1-9)	GD958
MALE	FEMALE	ZX73-2500M-S+	\$49.95	(1-9)	GD1163

+ RoHS compliant in accordance with EU Directive (2002/95/EC)

The +Suffix has been added in order to identify RoHS Compliance. See our web site for RoHS Compliance methodologies and qualifications.

### Outline Drawing (GD958)



### Electrical Specifications (T<sub>AMB</sub> = 25°C)

FREQ. (MHz)	MIN. INSERTION LOSS, dB (+15V)		MAX. ATTENUATION dB (0V)		INPUT POWER (dBm)	CONTROL Voltage Current (V) (mA)		IP3 (dBm)	RETURN LOSS <sup>1</sup> (dB)	POWER SUPPLY Voltage Current (V) (mA)		
	Min.	Max.	Typ.	Max.		Max.	Max.			Typ.	Typ.	Max.
10	500	3.0	4.6	55	41	+20	0 - 17	30	43	20	+3 to +5	5
500	1500	3.3	5.0	40	30	+20	0 - 17	30	43	20	+3 to +5	5
1500	2500	4.0	6.2	37	25	+20	0 - 17	30	44	20	+3 to +5	5

Notes:  
 Rise/Fall time: 14µSec/25µSec Typ.  
 Switching Time, turn on/off: 14µSec/25µSec Typ.  
<sup>1</sup> Improved R. Loss in/out performance can be achieved at certain frequencies by choosing a V+ between +3V to +5V

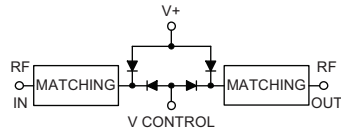
### Outline Dimensions (inch/mm)

A	B	C	D	E	F	G	H	J	
1.20	.75	.46	1.18	.04	.17	.45	.59	.33	
30.48	19.05	11.68	29.97	1.02	4.32	11.43	14.99	8.38	
K	L	M	N	P	Q	R	S	T	wt.
.21	.22	.18	1.00	.50	.35	.18	.106	1.88	grams
5.33	5.59	4.57	25.40	12.70	8.89	4.57	2.69	47.75	35.0

Note:

\* T dimension is 2.05 inch (52.07 mm) for GD1163 Case Style.

### Equivalent Schematic



ZX73-2500+ TYPICAL ATTENUATION AT 1000MHz

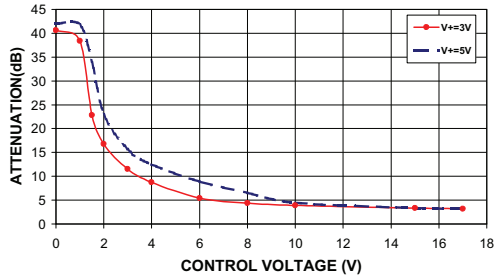


Figure 34.16: Data sheet for the voltage-controlled variable attenuator from Minicircuits, model ZX73-2500+.



# Plug-In Power Splitter/Combiner

2 Way-0° 50Ω 0.1 to 400 MHz

PSC-2-1+  
PSC-2-1



CASE STYLE: A01  
PRICE: \$14.20 ea. QTY. (1-9)

+ RoHS compliant in accordance with EU Directive (2002/95/EC)

The +Suffix identifies RoHS Compliance. See our web site for RoHS Compliance methodologies and qualifications.

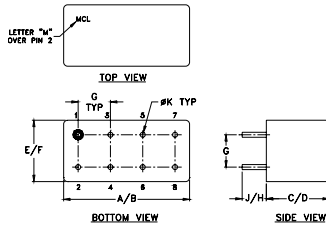
### Maximum Ratings

Operating Temperature	-55°C to 100°C
Storage Temperature	-55°C to 100°C
Power Input (as a splitter)	1W max.
Internal Dissipation	0.125W max.

### Pin Connections

SUM PORT	1
PORT 1	5
PORT 2	6
GROUND	2,3,4,7,8
CASE GROUND	2,3,4,7,8

### Outline Drawing



### Outline Dimensions (inch/mm)

	A	B	C	D	E	F
	.770	.800	.385	.400	.370	.400
	19.56	20.32	9.78	10.16	9.40	10.16
	G	H	J	K		wt
	.200	.20	.14	.031		grams
	5.08	5.08	3.56	0.79		5.2

### Features

- wideband, 0.1 to 400 MHz
- low insertion loss, 0.4 dB typ.
- rugged welded construction

### Applications

- VHF/UHF
- federal & defense communications

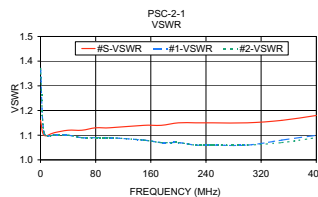
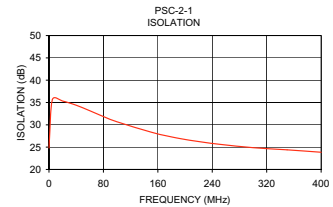
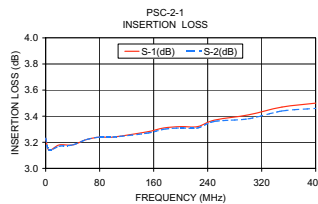
### Electrical Specifications

FREQ. RANGE (MHz)	ISOLATION (dB)						INSERTION LOSS (dB) ABOVE 3.0 dB						PHASE UNBALANCE (Degrees)			AMPLITUDE UNBALANCE (dB)		
	L		M		U		L		M		U		L	M	U	L	M	U
	Typ.	Min.	Typ.	Min.	Typ.	Min.	Typ.	Max.	Typ.	Max.	Typ.	Max.	Max.	Max.	Max.	Max.	Max.	Max.
0.1-400	20	15	25	20	25	20	0.2	0.6	0.4	0.75	0.6	1.0	2.0	3.0	4.0	0.15	0.2	0.3

L = low range [ $f_L$  to  $10 f_L$ ] M = mid range [ $10 f_L$  to  $f_U/2$ ] U = upper range [ $f_U/2$  to  $f_U$ ]

### Typical Performance Data

Frequency (MHz)	Insertion Loss (dB)		Amplitude Unbalance (dB)	Isolation (dB)	Phase Unbalance (deg.)	VSWR S	VSWR 1	VSWR 2
	S-1	S-2						
0.10	3.23	3.23	0.00	24.82	0.01	1.16	1.37	1.37
5.00	3.14	3.14	0.00	35.64	0.01	1.10	1.11	1.11
20.00	3.18	3.17	0.00	35.33	0.03	1.11	1.10	1.10
40.00	3.18	3.18	0.00	34.39	0.02	1.12	1.10	1.10
60.00	3.22	3.22	0.00	33.16	0.02	1.12	1.09	1.09
80.00	3.24	3.24	0.00	31.85	0.04	1.13	1.09	1.09
100.00	3.24	3.24	0.00	30.68	0.05	1.13	1.09	1.09
150.00	3.28	3.27	0.00	28.37	0.04	1.14	1.08	1.08
175.00	3.31	3.30	0.01	27.46	0.07	1.14	1.07	1.07
200.00	3.32	3.31	0.01	26.72	0.05	1.15	1.07	1.07
225.00	3.32	3.31	0.01	26.14	0.02	1.15	1.06	1.06
250.00	3.37	3.36	0.01	25.65	0.05	1.15	1.06	1.06
300.00	3.41	3.38	0.03	24.88	0.10	1.15	1.06	1.06
350.00	3.47	3.44	0.03	24.40	0.06	1.16	1.08	1.07
400.00	3.50	3.46	0.04	23.86	0.05	1.18	1.10	1.09



### electrical schematic



P.O. Box 350166, Brooklyn, New York 11235-0003 (718) 934-4500 Fax (718) 332-4661 For detailed performance specs & shopping online see Mini-Circuits web site



The Design Engineers Search Engine Provides ACTUAL Data Instantly From MINI-CIRCUITS At: [www.minicircuits.com](http://www.minicircuits.com)

RF/IF MICROWAVE COMPONENTS

REV. A  
M98988  
PSC-2-1  
HY/DT/CP  
07/02/02

Figure 34.17: Data sheet for the power divider from Minicircuits, model PSC-2-1.

# Plug-In Frequency Mixer

## SRA-2CM+

Level 7 (LO Power +7 dBm) 5 to 1000 MHz



### Maximum Ratings

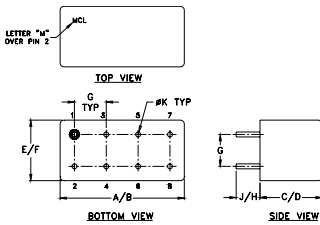
Operating Temperature	-55°C to 100°C
Storage Temperature	-55°C to 100°C
RF Power	50mW
IF Current	40mA

### Pin Connections

LO	8
RF	1
IF	3,4 <sup>A</sup>
GROUND	2,5,6,7
CASE GROUND	2,5,6,7

<sup>A</sup> pins must be connected together externally

### Outline Drawing



### Outline Dimensions (inch)

A	B	C	D	E	F
.770	.800	.385	.400	.370	.400
19.56	20.32	9.78	10.16	9.40	10.16
G	H	J	K	wt	
.200	.20	.14	.031	grams	
5.08	5.08	3.56	0.79		5.2

### Features

- excellent conversion loss, 5.27 dB typ.
- good L-R isolation, 35 dB typ. L-I isolation, 30 dB typ.
- rugged welded construction
- hermetic

### Applications

- VHF/UHF
- cellular
- defense & federal communications
- ISM/GSM

CASE STYLE: A01  
PRICE: \$18.20 ea. QTY (1-9)

**+ RoHS compliant in accordance with EU Directive (2002/95/EC)**

The +Suffix has been added in order to identify RoHS Compliance. See our web site for RoHS Compliance methodologies and qualifications.

### Electrical Specifications

FREQUENCY (MHz)	CONVERSION LOSS (dB)	LO-RF ISOLATION (dB)			LO-IF ISOLATION (dB)				
		L	M	U	L	M	U		
5-1000	DC-1000	60	50	35	30	30	25	25	20

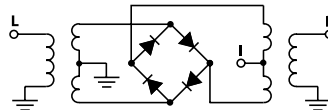
1 dB COMP.: +1 dBm typ.

L = low range [ $f_1$  to  $10 f_1$ ]  
M = mid range [ $10 f_1$  to  $f_2/2$ ]  
U = upper range [ $f_2/2$  to  $f_2$ ]

### Typical Performance Data

Frequency (MHz)		Conversion Loss (dB)	Isolation L-R (dB)	Isolation L-I (dB)	VSWR RF Port (:1)	VSWR LO Port (:1)
RF	LO	LO +7dBm	LO +7dBm	LO +7dBm	LO +7dBm	LO +7dBm
5.00	35.00	7.36	67.00	67.00	5.03	4.09
38.13	68.13	5.59	54.82	53.34	1.40	3.04
71.27	41.27	5.30	49.15	48.13	1.31	2.99
137.53	107.53	5.33	46.10	45.22	1.27	2.83
200.00	170.00	5.35	42.68	41.91	1.24	2.82
236.93	206.93	5.27	41.09	40.29	1.24	2.72
303.20	273.20	5.28	39.42	38.94	1.24	2.76
336.33	306.33	5.42	39.72	36.88	1.26	2.77
402.60	372.60	5.63	38.13	35.49	1.30	2.85
468.86	438.86	5.62	37.15	35.09	1.37	2.84
535.13	505.13	5.87	35.49	32.57	1.45	2.97
568.26	538.26	6.01	35.26	31.27	1.50	2.96
634.53	604.53	6.17	36.03	29.46	1.61	3.10
700.79	670.79	6.68	38.00	30.29	1.70	3.21
767.06	737.06	6.49	38.00	29.92	1.85	3.09
800.19	770.19	6.11	39.26	28.34	2.01	3.03
833.33	803.33	6.37	39.87	27.52	2.08	3.08
899.59	869.59	6.80	40.23	26.99	2.32	3.39
965.86	935.86	6.86	42.61	25.65	2.53	3.58
1000.00	969.00	7.10	44.90	24.17	2.76	3.76

### Electrical Schematic



P.O. Box 350166, Brooklyn, New York 11235-0003 (718) 934-4500 Fax (718) 332-4661 For detailed performance specs & shopping online see Mini-Circuits web site



The Design Engineers Search Engine Provides ACTUAL Data Instantly From MINI-CIRCUITS At: [www.minicircuits.com](http://www.minicircuits.com)

RF/IF MICROWAVE COMPONENTS

REV. A  
M86888  
SRA-2CM+  
DJR/DC/PIAM  
061211  
Page 1 of 2

Figure 34.18: Data sheet for the mixer from Minicircuits, model SRA-2CM+.

SPECIFICATIONS				
AO Medium				TeO2
Acoustic Velocity				4.2 mm/μs
Active Aperture*	2.5 mm 'L' X			1 mm 'H'
Center Frequency (Fc)				80 MHz
RF Bandwidth	20 MHz @	-10 dB		Return Loss
Input Impedance				50 Ohms Nominal
VSWR @ Fc				1.3 :1 Max
Wavelength				442-633 nm
Insertion Loss				4 % Max
Reflectivity per Surface				1 % Max
Anti-Reflection Coating				MIL-C-48497
Optical Power Density				250 W/mm <sup>2</sup>
Contrast Ratio				1000 :1 Min
Polarization				90 ° To Mounting Plane
PERFORMANCE VS WAVELENGTH				
<b>Wavelength (nm)</b>	<b>442</b>	<b>488</b>	<b>515</b>	<b>633</b>
Saturation RF Power (W)	0.27	0.33	0.36	0.55
Bragg Angle (mr)	4.2	4.6	4.9	6
Beam Separation (mr)	8.4	9.2	9.8	12
PERFORMANCE VS BEAM DIAMETER				
<b>Beam Diameter (μm)</b>	<b>200</b>	<b>300</b>	<b>500</b>	
at Wavelength (nm)	633	633	633	
Diffraction Efficiency (%)	80	83	85	
Rise Time (nsec)	34	49	80	
	15.9	10.6	6.3	
	10	5	1	

Figure 34.19: Data sheet for the acousto-optic modulator (AOM) from Crystal Technologies, model AOMO 3080-120.

**Silicon PIN Photodiodes - Large Area, Fast Response Time – 400 nm to 1100 nm**

The FFD series devices are high-quality, large-area, high-speed, N-type Si PIN photodiodes in hermetically sealed TO packages designed for the 400 nm to 1100 nm wavelength range. The FND-100Q has a quartz window to enhance UV responsivity.

**Preamplifiers**

Preamplifier modules incorporating these photodiodes are available on a custom basis.

**Si PINs – Large Area, Fast Response**

Typical Characteristics @ T = 22° C

Part #	Standard Package	Photo Sens. Diam. (mm)	Resp. @ 900 nm (A/W)	Dark Current Id (nA)	Spect. Noise Curr. Dens. In (fW/√Hz)	Cap. @ 100 kHz Cd (pF)	Response Time tr (ns)	NEP @ 900 nm (fW/√Hz)	Bias Volt (V)
FFD-040B	Y	1	0.58	1	18	1.8	2	31	15
FFD-100	B	2.5	0.58	2	25	8.5	3.5	44	15
FFD-200	C3	5.1	0.58	4	36	30	5	62	15
FND-100Q	B	2.5	0.58	10	60	8.5	2	100	90

**Typical Applications**

Laser detection systems, fast pulse detection, instrumentation, and high-speed switching.

Figure 34.20: Data sheet for the photo diode from Perkin Elmers FDD100.

## Detectors

### Silicon Epitaxial PIN Photodiodes - High Speed – 400 nm to 1100 nm

The C30736 series of high-speed epitaxial silicon PIN photodetectors provide fast response and good quantum efficiency in the spectral range between 400 nm and 1100 nm. These devices are optimized for high-speed, high volume and low cost applications. Standard sizes include 0.25 mm, 0.5 mm, 1.0 mm, 1.5 x 1.5 mm, and custom sizes can be accommodated depending on volume required. Available in plastic surface mount packages and in chip form.

#### Silicon Epitaxial PIN Photodiodes

Typical Characteristics @ T = 22° C

Part #	Standard Package	Photo Sens. Diam. (mm)	Resp. @ 870 nm (A/W)	Dark Current @2V Id (nA)	Spect. Noise Curr. Dens. In (fW/√Hz)	Cap. @ 100 kHz Cd (pF)	Response Time tr (ns)	NEP @ 870 nm (fW/√Hz)	Bias Volt (V)
C30736-1	Chip form	0.20	0.55	0.05	6	0.75	0.3	11	2
C30736-2	Chip form	0.50	0.55	0.10	10	1.5	0.5	18	2
C30736-3	Chip form	1.5 x 1.5	0.55	0.50	50	14	0.3	91	2

### Silicon PIN Photodiodes - Standard N-Type – 400 nm to 1100 nm

The C308XX series devices are high-quality N-type Si PIN photodiodes in hermetically sealed TO packages designed for the 400 nm to 1100 nm wavelength region.

#### Si PINs – Standard N-Type

Typical Characteristics @ T = 22° C

Part #	Standard Package	Photo Sens. Diam. (mm)	Resp. @ 900 nm (A/W)	Dark Current Id (nA)	Spect. Noise Curr. Dens. (fA/√Hz)	Cap. @ 100 kHz Cd (pF)	Response Time tr (ns)	NEP @ 900 nm (fW/√Hz)	Bias Volt (V)
C30807E	A	1	0.6	1	18	2.5	3	30	45
C30808E	B	2.5	0.6	3	31	6	5	52	45
C30822E	C	5	0.6	5	40	17	7	67	45
C30809E	C3	8	0.6	7	47	35	10	79	45
C30810E	D	11.4	0.6	30	98	70	12	163	45

#### Typical Applications

Laser detection systems, photometry, data transmission, instrumentation, and high-speed switching.

### Silicon PIN Photodiodes - Large Area, Fast Response Time – 400 nm to 1100 nm

The FFD series devices are high-quality, large-area, high-speed, N-type Si PIN photodiodes in hermetically sealed TO packages designed for the 400 nm to 1100 nm wavelength range. The FND-100Q has a quartz window to enhance UV responsivity.

#### Preamplifiers

Preamp module incorporating these photodiodes are available on a custom basis.

#### Si PINs – Large Area, Fast Response

Typical Characteristics @ T = 22° C

Part #	Standard Package	Photo Sens. Diam. (mm)	Resp. @ 900 nm (A/W)	Dark Current Id (nA)	Spect. Noise Curr. Dens. In (fW/√Hz)	Cap. @ 100 kHz Cd (pF)	Response Time tr (ns)	NEP @ 900 nm (fW/√Hz)	Bias Volt (V)
FFD-040B	Y	1	0.58	1	18	1.8	2	31	15
FFD-100	B	2.5	0.58	2	25	8.5	3.5	44	15
FFD-200	C3	5.1	0.58	4	36	30	5	62	15
FND-100Q	B	2.5	0.58	10	60	8.5	2	100	90

#### Typical Applications

Laser detection systems, fast pulse detection, instrumentation, and high-speed switching.

19-0350, Rev 0, 12/94



## Precision, Dual-Supply, SPST Analog Switches

MAX320/MAX321/MAX322

### General Description

The MAX320/MAX321/MAX322 are precision, dual, SPST analog switches designed to operate from  $\pm 3V$  to  $\pm 8V$  dual supplies. The MAX320 has two normally open (NO) switches and the MAX321 has two normally closed (NC) switches. The MAX322 has one NO and one NC switch. Low power consumption (1.25mW) makes these parts ideal for battery-powered equipment. They offer low leakage currents (100pA max) and fast switching speeds ( $t_{ON} = 150ns$  max,  $t_{OFF} = 100ns$  max).

The MAX320 series, powered from  $\pm 5V$  supplies, offers 35 $\Omega$  max on-resistance ( $R_{ON}$ ), 2 $\Omega$  max matching between channels, and 4 $\Omega$  max  $R_{ON}$  flatness.

These switches also offer 5pC max charge injection and a minimum of 2000V ESD protection per Method 3015.7.

For equivalent devices specified for single-supply operation, see the MAX323/MAX324/MAX325 data sheet. For quad versions of these switches, see the MAX391/MAX392/MAX393 data sheet.

### Applications

Battery-Operated Systems	Sample-and-Hold Circuits
Heads-Up Displays	Guidance and Control Systems
Audio and Video Switching	Military Radios
Test Equipment	Communications Systems
$\pm 5V$ DACs and ADCs	PBX, PABX

### Features

- ♦ Low On-Resistance, 35 $\Omega$  max (16 $\Omega$  typical)
- ♦  $R_{ON}$  Matching Between Channels <2 $\Omega$
- ♦  $R_{ON}$  Flatness <4 $\Omega$
- ♦ Guaranteed Charge Injection <5pC
- ♦ Bipolar Supply Operation ( $\pm 3V$  to  $\pm 8V$ )
- ♦ Low Power Consumption, <1.25mW
- ♦ Low Leakage Current Over Temperature, <2.5nA at +85°C
- ♦ Fast Switching,  $t_{ON}$  <150ns,  $t_{OFF}$  <100ns
- ♦ Guaranteed Break-Before-Make (MAX322 only)

### Ordering Information

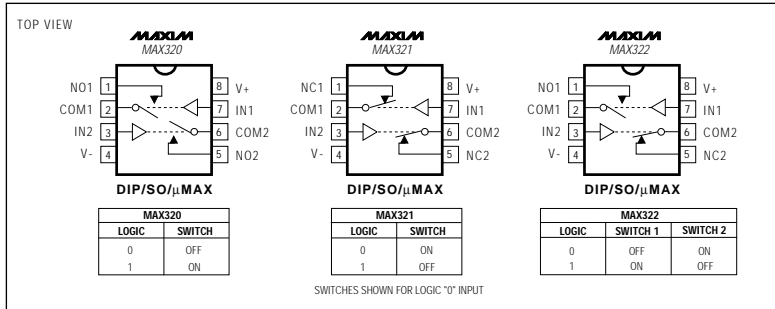
PART	TEMP. RANGE	PIN-PACKAGE
MAX320CPA	0°C to +70°C	8 Plastic DIP
MAX320CSA	0°C to +70°C	8 SO
MAX320CUA	0°C to +70°C	8 $\mu$ MAX
MAX320C/D	0°C to +70°C	Dice*
MAX320EPA	-40°C to +85°C	8 Plastic DIP
MAX320ESA	-40°C to +85°C	8 SO
MAX320EJA	-40°C to +85°C	8 CERDIP**
MAX320MJA	-55°C to +125°C	8 CERDIP**

Ordering Information continued at end of data sheet.

\* Contact factory for dice specifications.

\*\* Contact factory for availability.


### Pin Configurations/Functional Diagrams/Truth Tables



Maxim Integrated Products 1

Call toll free 1-800-998-8800 for free samples or literature.

Figure 34.22: Data sheet for the digital switch MAX322 from Maxim.


August 2000

## LM741 Operational Amplifier

### General Description

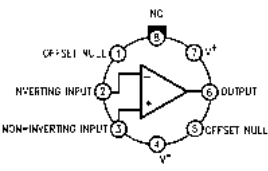
The LM741 series are general purpose operational amplifiers which feature improved performance over industry standards like the LM709. They are direct, plug-in replacements for the 709C, LM201, MC1439 and 748 in most applications. The amplifiers offer many features which make their application nearly foolproof: overload protection on the input and output, no latch-up when the common mode range is exceeded, as well as freedom from oscillations.

The LM741C is identical to the LM741/LM741A except that the LM741C has their performance guaranteed over a 0°C to +70°C temperature range, instead of -55°C to +125°C.

### Features

### Connection Diagrams

**Metal Can Package**

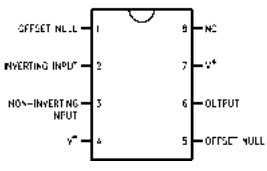


00934102

Note 1: LM741H is available per JM38510/10101

**Order Number LM741H, LM741H/883 (Note 1),  
LM741AH/883 or LM741CH**  
See NS Package Number H08C

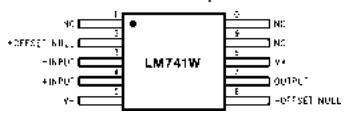
**Dual-In-Line or S.O. Package**



00934103

**Order Number LM741J, LM741J/883, LM741CN**  
See NS Package Number J08A, M08A or N08E

**Ceramic Flatpak**

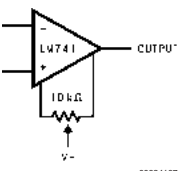


00934106

**Order Number LM741W/883**  
See NS Package Number W10A

### Typical Application

**Offset Nulling Circuit**



00934107

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www.national.com

LM741 Operational Amplifier

Figure 34.23: Data sheet for the operational amplifier LM741 from National Semiconductor.



# Low-Noise, Precision Operational Amplifier

## OP27

### FEATURES

- Low Noise:** 80 nV p-p (0.1 Hz to 10 Hz),  $3 \text{ nV}/\sqrt{\text{Hz}}$
- Low Drift:**  $0.2 \mu\text{V}/^\circ\text{C}$
- High Speed:** 2.8 V/ $\mu\text{s}$  Slew Rate, 8 MHz Gain Bandwidth
- Low  $V_{OS}$ :** 10  $\mu\text{V}$
- Excellent CMRR:** 126 dB at  $V_{CM}$  of  $\pm 11 \text{ V}$
- High Open-Loop Gain:** 1.8 Million
- Fits 725, OP07, 5534A Sockets**
- Available in Die Form**

### GENERAL DESCRIPTION

The OP27 precision operational amplifier combines the low offset and drift of the OP07 with both high speed and low noise. Offsets down to 25  $\mu\text{V}$  and drift of 0.6  $\mu\text{V}/^\circ\text{C}$  maximum make the OP27 ideal for precision instrumentation applications. Exceptionally low noise,  $e_n = 3.5 \text{ nV}/\sqrt{\text{Hz}}$ , at 10 Hz, a low 1/f noise corner frequency of 2.7 Hz, and high gain (1.8 million), allow accurate high-gain amplification of low-level signals. A gain-bandwidth product of 8 MHz and a 2.8 V/ $\mu\text{sec}$  slew rate provides excellent dynamic accuracy in high-speed, data-acquisition systems.

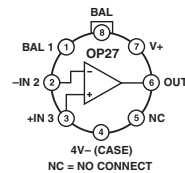
A low input bias current of  $\pm 10 \text{ nA}$  is achieved by use of a bias-current-cancellation circuit. Over the military temperature range, this circuit typically holds  $I_B$  and  $I_{OS}$  to  $\pm 20 \text{ nA}$  and 15 nA, respectively.

The output stage has good load driving capability. A guaranteed swing of  $\pm 10 \text{ V}$  into 600  $\Omega$  and low output distortion make the OP27 an excellent choice for professional audio applications.

(Continued on page 7)

### PIN CONNECTIONS

TO-99  
(J-Suffix)



8-Pin Hermetic DIP  
(Z-Suffix)

Epoxy Mini-DIP  
(P-Suffix)  
8-Pin SO  
(S-Suffix)

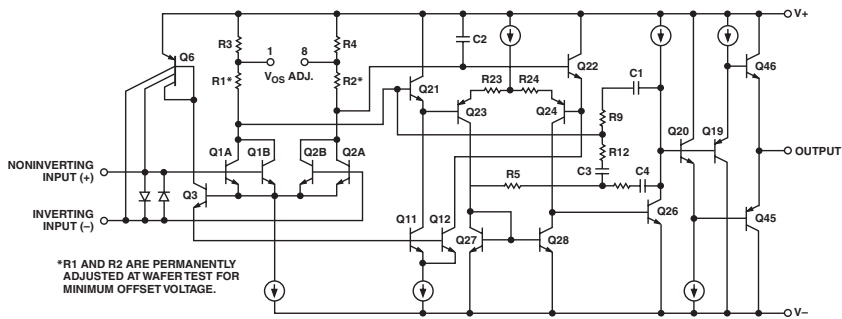
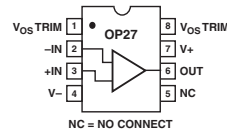


Figure 1. Simplified Schematic

Figure 34.24: Data sheet for the operational amplifier OP27 from Analog Devices.

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