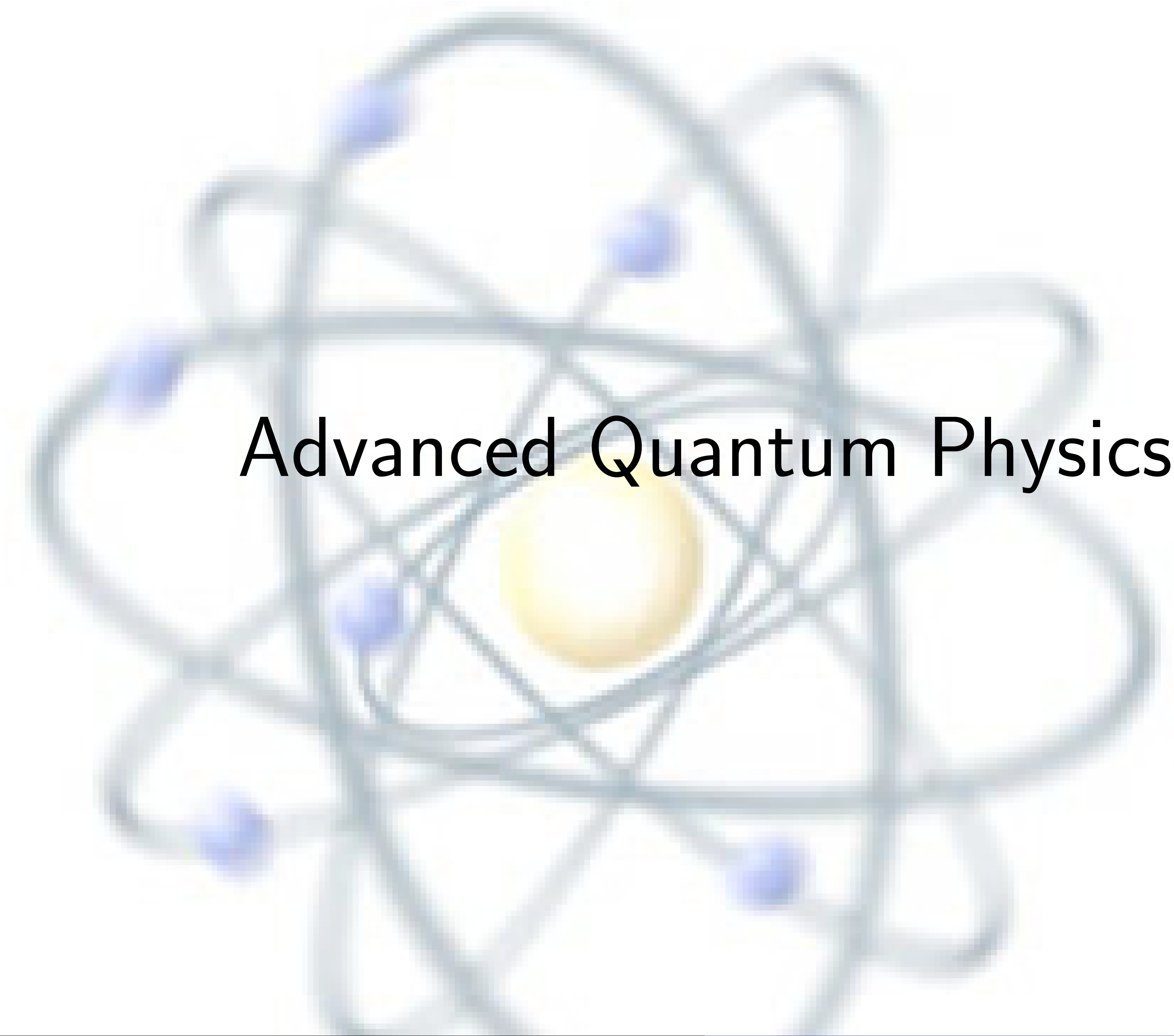
Advanced Quantum Physics



Aim of the course

Building upon the foundations of wave mechanics, this course will introduce and develop the broad field of quantum physics including:

- Quantum mechanics of point particles
- Approximation methods
- Basic foundations of atomic, molecular, and solid state physics
- Basic elements of quantum field theory
- Scattering theory
- Relativistic quantum mechanics

Although these topics underpin a variety of subject areas from high energy, quantum condensed matter, and ultracold atomic physics to quantum optics and quantum information processing, our focus is on development of **basic conceptual principles** and **technical fluency**.

Prerequisites

This course will assume (a degree of) familiarity with course material from NST IB Quantum Physics (or equivalent):

- Failure of classical physics
- Wave-particle duality, and the uncertainty principle
- The Schrödinger equation
- Wave mechanics of unbound particles
- Wave mechanics of bound particles
- Operator methods
- Quantum mechanics in three dimensions
- Spin and identical particles

Since this material is pivotal to further developments, we will begin by revisiting some material from the Part IB course.

Further prerequisites...

Quantum physics is an inherently mathematical subject – it is therefore inevitable that the course will lean upon some challenging concepts from mathematics:

e.g. operator methods, elements of Sturm-Liouville theory (eigenfunction equations, etc,), variational methods (Euler-Lagrange equations and Lagrangian methods – a bit), Green functions (a very little bit – sorry), Fourier analysis, etc.

Fortunately/unfortunately* (*delete as appropriate) such mathematical principles remain an integral part of the subject and seem unavoidable.

Since there has been a change of lecturer, a change of style, and partially a change of material, I would welcome feedback on accessibility of the more mathematical parts of the course!

Synopsis: (mostly revision) Lectures 1-4ish

1. **Foundations of quantum physics:**

   Historical background; wave mechanics to Schrödinger equation.

2. **Quantum mechanics in one dimension:**

   Unbound particles: potential step, barriers and tunneling; bound states: rectangular well, δ-function well; Kronig-Penney model.

3. **Operator methods:**

   Uncertainty principle; time evolution operator; Ehrenfest's theorem; symmetries in quantum mechanics; Heisenberg representation; quantum harmonic oscillator; coherent states.

4. **Quantum mechanics in more than one dimension:**

   Rigid rotor; angular momentum; raising and lowering operators; representations; central potential; atomic hydrogen.

Synopsis: Lectures 5-10

5. **Charged particle in an electromagnetic field:**

   Classical and quantum mechanics of particle in a field; normal Zeeman effect; gauge invariance and the Aharonov-Bohm effect; Landau levels.

6. **Spin:**

   Stern-Gerlach experiment; spinors, spin operators and Pauli matrices; spin precession in a magnetic field; parametric resonance; addition of angular momenta.

7. **Time-independent perturbation theory:**

   Perturbation series; first and second order expansion; degenerate perturbation theory; Stark effect; nearly free electron model.

8. **Variational and WKB method:**

   Variational method: ground state energy and eigenfunctions; application to helium; Semiclassics and the WKB method.

Synopsis: Lectures 11-15

9. **Identical particles:**

   Particle indistinguishability and quantum statistics; space and spin wavefunctions; consequences of particle statistics; ideal quantum gases; degeneracy pressure in neutron stars; Bose-Einstein condensation in ultracold atomic gases.

10. **Atomic structure:**

    Relativistic corrections – spin-orbit coupling; Darwin structure; Lamb shift; hyperfine structure. Multi-electron atoms; Helium; Hartree approximation and beyond; Hund's rule; periodic table; coupling schemes LS and jj; atomic spectra; Zeeman effect.

11. **Molecular structure:**

    Born-Oppenheimer approximation; H_2^+ ion; H_2 molecule; ionic and covalent bonding; solids; molecular spectra; rotation and vibrational transitions.

Synopsis: Lectures 16-19

12. **Field theory: from phonons to photons:**

    From particles to fields: classical field theory of harmonic atomic chain; quantization of atomic chain; phonons. Classical theory of the EM field; waveguide; quantization of the EM field and photons.

13. **Time-dependent perturbation theory:**

    Rabi oscillations in two level systems; perturbation series; sudden approximation; harmonic perturbations and Fermi's Golden rule.

14. **Radiative transitions:**

    Light-matter interaction; spontaneous emission; absorption and stimulated emission; Einstein's A and B coefficents; dipole approximation; selection rules; †lasers.

Synopsis: Lectures 20-24

15. **Scattering theory**

    Elastic and inelastic scattering; method of particle waves; Born approximation; scattering of identical particles.

16. **Relativistic quantum mechanics:**

    Klein-Gordon equation; Dirac equation; relativistic covariance and spin; free relativistic particles and the Klein paradox; antiparticles; coupling to EM field: minimal coupling and the connection to non-relativistic quantum mechanics; †field quantization.

What's missing?

- "Philosophy" of quantum mechanics
  (e.g. nothing on EPR paradoxes, Bell's inequality, etc.)
- Specializations and applications (covered later in Lent and Part III)
  (e.g. nothing detailed on quantum information processing, etc.)

Handouts and lecture notes

- Both lecture notes and overheads will be available (in pdf format) from the course webpage:

  www.tcm.phy.cam.ac.uk/~bds10/aqp.html

  But try to take notes too.

- The lecture notes are extensive (apologies!) and, as with textbooks, include more material than will covered in lectures or **examined**.

  Unlike textbooks, the lecture notes may contain (many?) typos – corrections welcome!

- *For the most part*, non-examinable material will be listed as "INFO blocks" in lecture notes.

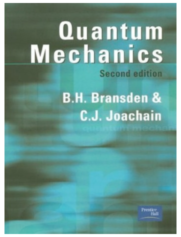
  Generally, the examinable material will be limited to what is taught in class, i.e. the overheads.

Supervisions and problem sets

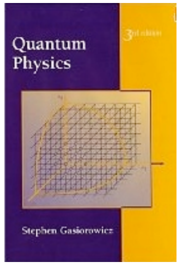
- To accompany the **four** supervisions this term, there will be four problem sets. Answers to all probems will be made available via the webpage in due course.

- If there are problems/questions with lectures or problem sets, please feel free to contact me by e-mail (`bds10@cam.ac.uk`) or in person (Rm 539, Mott building).

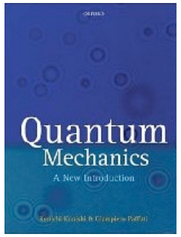
A few (random but recommended) books



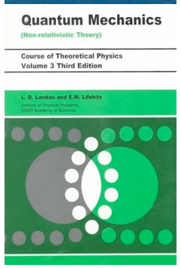
B. H. Bransden and C. J. Joachain, **Quantum Mechanics**, (2nd edition, Pearson, 2000). *Classic text covers core elements of advanced quantum mechanics; strong on atomic physics.*



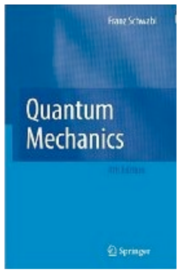
S. Gasiorowicz, **Quantum Physics**, (2nd edn. Wiley 1996, 3rd edition, Wiley, 2003). *Excellent text covers material at approximately right level; but published text omits some topics which we address.*



K. Konishi and G. Paffuti, **Quantum Mechanics: A New Introduction**, (OUP, 2009). *This is a new text which includes some entertaining new topics within an old field.*



L. D. Landau and L. M. Lifshitz, **Quantum Mechanics: Non-Relativistic Theory, Volume 3**, (Butterworth-Heinemann, 3rd edition, 1981). *Classic text which covers core topics at a level that reaches beyond the ambitions of this course.*



F. Schwabl, **Quantum Mechanics**, (Springer, 4th edition, 2007). *Best text for majority of course.*

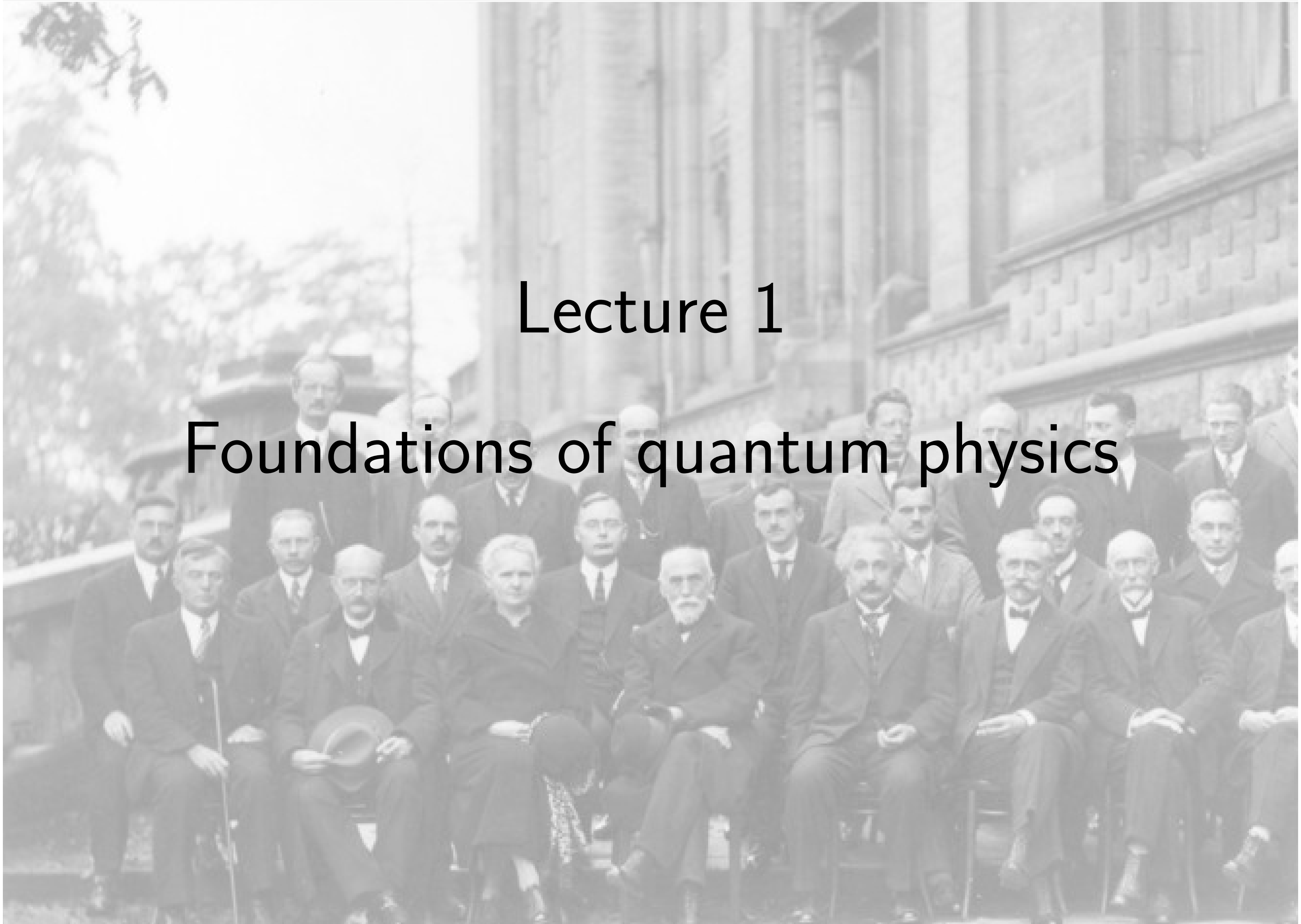
Books

- ...but, in general, there are a very large number of excellent textbooks in quantum mechanics.
- It is a good idea to spend some time in the library to find the text(s) that suit you best.
- It is also useful to look at topics from several different angles.

Wave mechanics and the Schrödinger equation

- Aim of the first several lectures is to review, consolidate, and expand upon material covered in Part IB:
  1. Foundations of quantum physics
  2. Wave mechanics of one-dimensional systems
  3. Operator methods in quantum mechanics
  4. Quantum mechanics in more than one dimension

- To begin, it is instructive to go back to the historical foundations of quantum theory.



Lecture 1

Foundations of quantum physics

Foundations of quantum physics: outline

1. Historically, origins of quantum mechanics can be traced to failures of 19th Century classical physics:
    - Black-body radiation
    - Photoelectric effect
    - Compton scattering
    - Atomic spectra: Bohr model
    - Electron diffraction: de Broglie hypothesis
2. Wave mechanics and the Schrödinger equation
3. Postulates of quantum mechanics

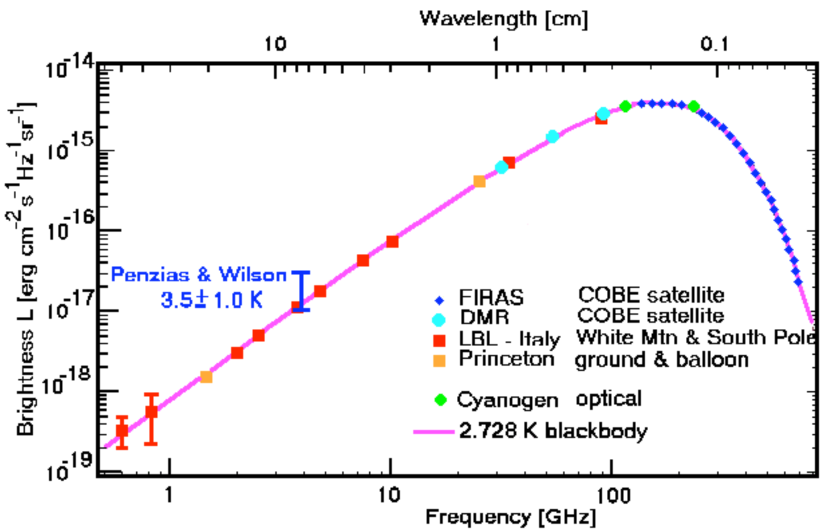
Black-body radiation

- In thermal equilibrium, radiation emitted by a cavity in frequency range $\nu = \frac{c}{\lambda}$ to $\nu + d\nu$ is proportional to mode density and fixed by equipartition theorem ($k_B T$ per mode):

Rayleigh-Jeans law $$\rho(\nu, T)\, d\nu = \frac{8\pi\nu^2}{c^3} k_B T\, d\nu$$

i.e. $\rho(\nu, T)$ increases without bound – UV catastrophe.

e.g. emission from cosmic microwave background ($T \simeq 2.728K$)



- Experimentally, distribution conforms to Rayleigh-Jeans law at low frequencies but at high frequencies, there is a departure!

Black-body radiation: Planck's resolution

- Planck: for each mode, ν, energy is quantized in units of $h\nu$, where h denotes the Planck constant. Energy of each mode, ν,

$$\langle\varepsilon(\nu)\rangle = \frac{\sum_{n=0}^{\infty} n\, h\nu\, e^{-nh\nu/k_{\rm B}T}}{\sum_{n=0}^{\infty} e^{-nh\nu/k_{\rm B}T}} = \frac{h\nu}{e^{h\nu/k_{\rm B}T} - 1}$$

- Leads to Planck distribution:

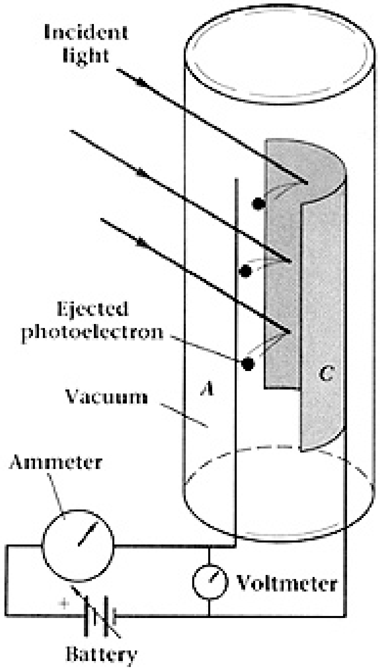
$$\boxed{\rho(\nu, T) = \frac{8\pi\nu^2}{c^3}\langle\varepsilon(\nu)\rangle = \frac{8\pi h\nu^3}{c^3}\frac{1}{e^{h\nu/k_{\rm B}T} - 1}}$$

  recovers Rayleigh-Jeans law as $h \to 0$ and resolves UV catastrophe.

- Parallel theory developed to explain low-temperature specific heat of solids by Debye and Einstein.

Photoelectric effect

- When metal exposed to EM radiation, above a certain threshold frequency, light is absorbed and electrons emitted.
- von Lenard (1902) observed that energy of electrons increased with light frequency (as opposed to intensity).
- Einstein (1905) proposed that light composed of discrete quanta (photons): $\mathrm{k.e.}_{\mathrm{max}} = h\nu - W$



- Einstein's hypothesis famously confirmed by Millikan in 1916

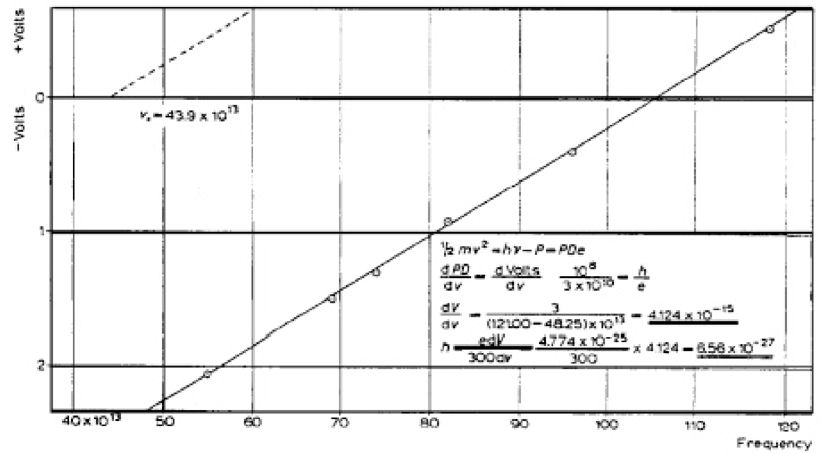


Fig. 4.

Compton scattering

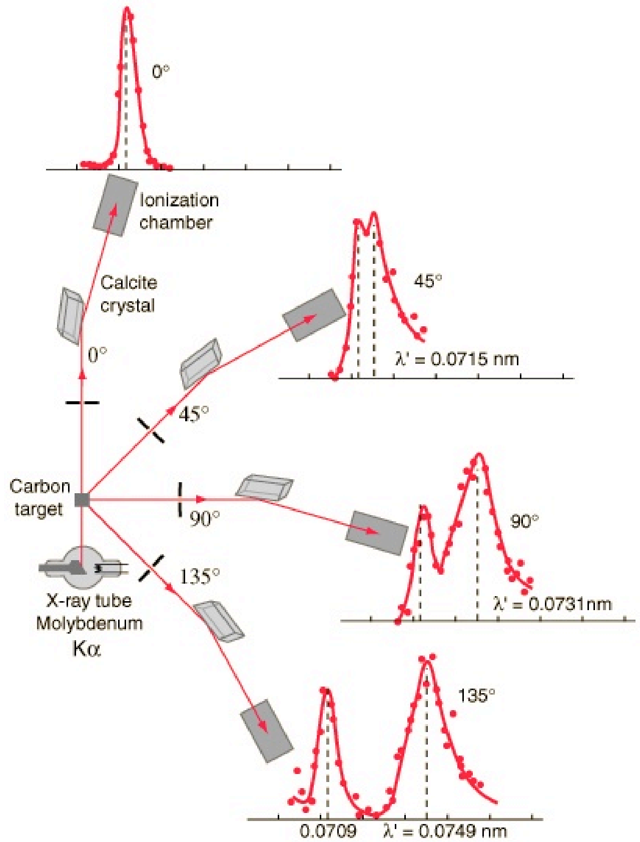
- In 1923, Compton studied **scattering of X-rays from carbon target**.
- Two peaks observed: first at wavelength of incident beam; second varied with angle.
- If photons carry momentum,

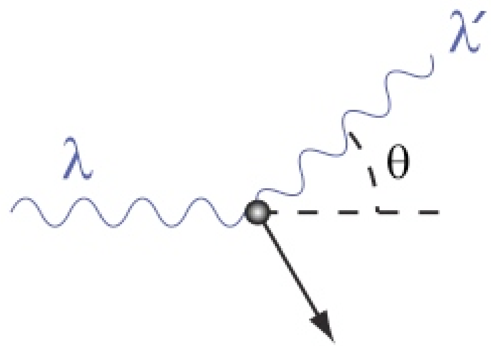
$$p = \frac{h\nu}{c} = \frac{h}{\lambda}$$

  electron can recoil and be ejected.

- Energy/momentum conservation:

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

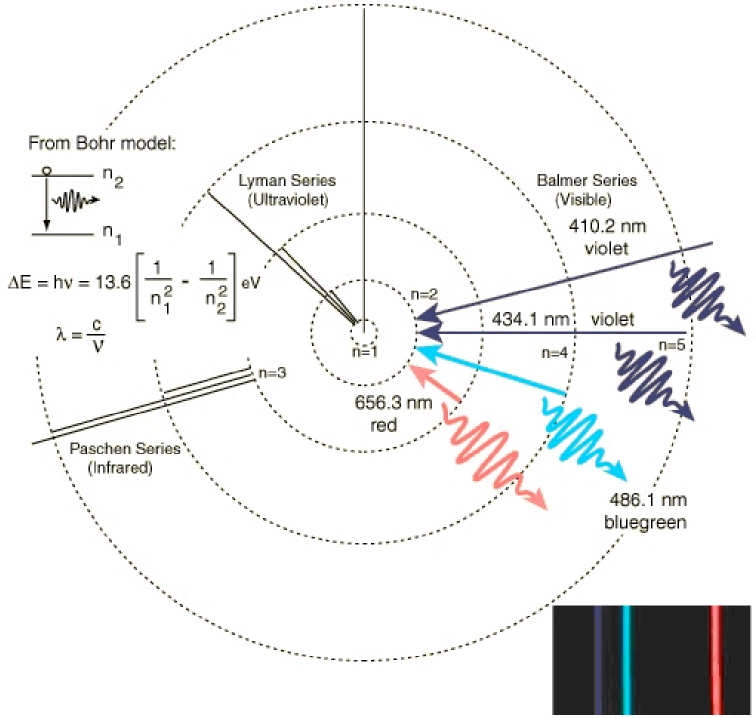




Atomic spectra: Bohr model

- Studies of electric discharge in low-pressure gases reveals that atoms emit light at discrete frequencies.
- For hydrogen, wavelength follows Balmer series (1885),

$$\lambda = \lambda_0 \left(\frac{1}{4} - \frac{1}{n^2} \right)$$



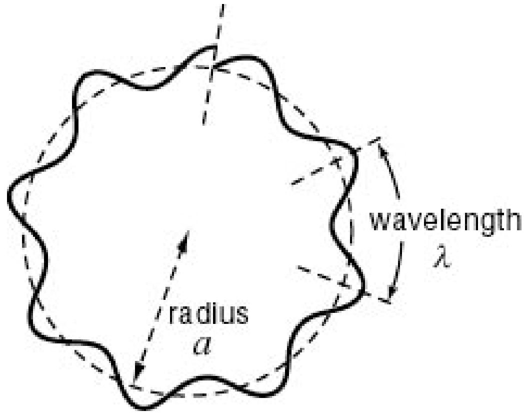
- Bohr (1913): discrete values reflect emission of photons with energy $E_n - E_m = h\nu$ equal to difference between allowed electron orbits,

$$\boxed{E_n = -\frac{\mathrm{Ry}}{n^2}}$$

- Angular momenta quantized in units of Planck's constant, $L = n\hbar$.

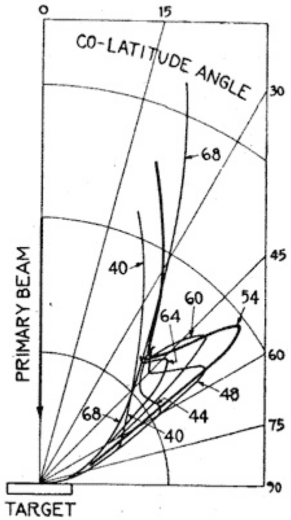
de Broglie hypothesis

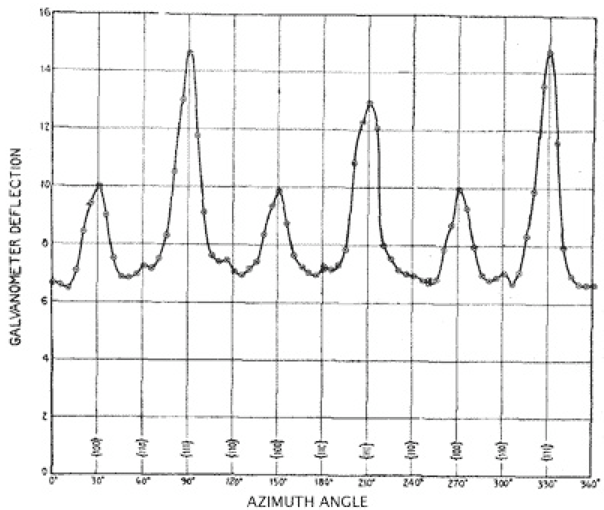
- But why only certain angular momenta? Just as light waves (photons) can act as particles, electrons exhibit wave-like properties.



$$\lambda = \frac{h}{p}, \qquad \text{i.e. } \mathbf{p} = \hbar \mathbf{k}$$

- First direct evidence from electron scattering from Ni, Davisson and Germer (1927).





Wave mechanics

Although no rigorous derivation, Schrödinger's equation can be motivated by developing connection between light waves and photons, and constructing analogous structure for de Broglie waves and electrons.

- For a monochromatic wave in vacuo, Maxwell's wave equation,

$$\boxed{\nabla^2 \mathbf{E} - \frac{1}{c^2}\partial_t^2 \mathbf{E} = 0}$$

admits the plane wave solution, $\mathbf{E} = \mathbf{E}_0 e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$, with linear dispersion, $\omega = c|\mathbf{k}|$.

- From photoelectric effect and Compton scattering, photon energy and momentum related to frequency and wavelength:

$$\boxed{E = h\nu = \hbar\omega, \qquad p = \frac{h}{\lambda} = \hbar k}$$

Wave mechanics

- If we think of wave $e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$ as describing a particle (photon), more natural to recast it in terms of energy/momentum, $\mathbf{E_0}e^{i(\mathbf{p}\cdot\mathbf{x}-Et)/\hbar}$.

  i.e. applied to plane wave, wave equation $\nabla^2\mathbf{E}-\frac{1}{c^2}\partial_t^2\mathbf{E}=0$ translates to energy-momentum relation, $E^2=(c\mathbf{p})^2$ for massless relativistic particle.

- For a particle with rest mass m_0, require wave equation to yield energy-momentum invariant, $E^2=(c\mathbf{p})^2+m_0^2c^4$.
- With plane "wavefunction" $\phi(x,t)=Ae^{i(\mathbf{p}\cdot\mathbf{x}-Et)/\hbar}$, recover energy-momentum invariant by adding a constant mass term,

$$\left(\nabla^2-\frac{1}{c^2}\partial_t^2-\frac{m_0^2c^2}{\hbar^2}\right)Ae^{i(\mathbf{p}\cdot\mathbf{x}-Et)/\hbar}$$

$$=-\frac{1}{(\hbar c)^2}\left((c\mathbf{p})^2-E^2+m_0^2c^4\right)Ae^{i(\mathbf{p}\cdot\mathbf{x}-Et)/\hbar}=0$$

Schrödinger's equation

- In fact, we will see that the **Klein-Gordon equation**,

$$\left(\nabla^2 - \frac{1}{c^2}\partial_t^2 - \frac{m_0^2 c^2}{\hbar^2}\right)\phi(\mathbf{x}, t) = 0$$

  can describe quantum mechanics of massive relativistic particles, but it is a bit inconvenient for non-relativistic particles...

- If a non-relativistic particle is also described by a plane wave, $\Psi(x, t) = Ae^{i(\mathbf{p}\cdot\mathbf{x} - Et)/\hbar}$, require wave equation consistent with the energy-momentum relation, $E = \frac{\mathbf{p}^2}{2m}$.
- Although $\mathbf{p}^2$ can be recovered from action of two gradient operators, E can only be generated by single time-derivative,

$$i\hbar\partial_t\Psi(\mathbf{x}, t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{x}, t)$$

- i.e. **Schrödinger's equation** implies that wavefunction is complex!

Schrödinger's equation

How does spatially varying potential influence de Broglie wave?

- In a potential $V(\mathbf{x})$, we expect the wave equation to be consistent with (classical) energy conservation, $E = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) = H(p, x)$,

$$i\hbar\partial_t \Psi(\mathbf{x}, t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{x}, t) + V(\mathbf{x})\Psi(\mathbf{x}, t)$$

  i.e. wavelength $\lambda \sim h/p$ varies with potential.

- From the solution of the stationary wave equation for the Coulomb potential, Schrödinger deduced allowed values of angular momentum and energy for **atomic hydrogen**.
- These values were the same as those obtained by Bohr (except that the lowest allowed state had zero angular momentum).

Postulates of quantum mechanics

1. The state of a quantum mechanical system is completely specified by the complex wavefunction $\Psi(\mathbf{r}, t)$.

- $\Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)\, d\mathbf{r}$ represents probability that particle lies in volume element $d\mathbf{r} \equiv d^d r$ located at position $\mathbf{r}$ at time t. For single particle,

$$\int_{-\infty}^{\infty} \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)\, d\mathbf{r} = 1$$

- The wavefunction must also be single-valued, continuous, and finite.

2. To every observable in classical mechanics there corresponds a linear, Hermitian operator, $\hat{A}$, in quantum mechanics.

- If the result of a measurement of an operator $\hat{A}$ is the number a, then a must be one of the eigenvalues,

$$\hat{A}\Psi = a\Psi$$

Postulates of quantum mechanics

3. If system is in a state described by Ψ, average value of observable corresponding to $\hat{A}$ given by $\langle A \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi \, d\mathbf{r}$.

- Arbitrary state can be expanded in eigenvectors of $\hat{A}$ ($\hat{A}\Psi_i = a_i \Psi_i$)

$$\Psi = \sum_i^n c_i \Psi_i, \qquad \text{i.e. } P(a_i) = |c_i|^2, \quad \langle A \rangle = \sum_i a_i |c_i|^2$$

4. A measurement of Ψ that leads to eigenvalue a_i causes wavefunction to "collapse" into corresponding eigenstate Ψ_i, i.e. measurement effects the state of the system.

5. The wavefunction according to the time-dependent Schrödinger equation, $i\hbar\partial_t \Psi = \hat{H}\Psi$.

Postulates in hand, is it now just a matter of application and detail?

- How can we understand how light quanta (photons) emerge from such a Hamiltonian formulation?
- How do charged particles interact with an EM field?
- How do we read and interpret spectra of multielectron atoms?
- How do we address many-body interactions between quantum particles in an atom, molecule, or solid?
- How do we elevate quantum mechanics to a relativistic theory?
- How can we identify and characterize instrinsic (non-classical) degrees of freedom such as spin?
- How to incorporate non-classical phenomena such as particle production into such a consistent quantum mechanical formulation?

These are some of the conceptual challenges that we will address in this course.

Next lecture

1. Foundations of quantum physics
2. Wave mechanics of one-dimensional systems
3. Operator methods in quantum mechanics
4. Quantum mechanics in more than one dimension