Mathematical Concepts of Quantum Mechanics

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Feb 1, 2001

Preface

These lectures (the first 16 chapters) cover a one term course taken by a mixed group of senior undergraduate and junior graduate students specializing either in mathematics or physics. The mathematics students had some background in advanced analysis, while physics students had introductory quantum mechanics. To satisfy such a disparate audience, we decided to select material which is interesting from the viewpoint of modern theoretical physics, and which illustrates an interplay of ideas from various fields of mathematics such as operator theory, probability, differential equations, and differential geometry. Given our time constraint, we have pursued mathematical content at the expense of rigor. However, wherever we have sacrificed the latter, we have tried to explain whether the result is an established fact, or, mathematically speaking, a conjecture, and in the former case, how a given argument can be made rigorous.

Moreover, even in dealing with mathematics students we found it useful, if not necessary, to review basic mathematical notions such as the spectrum of an operator, and the Fréchet or variational derivative, which we needed for the course. As a result, the text is interspersed with mathematical detours which occupy in total about half of the material. A mathematically sophisticated reader can skim through them, or skip them altogether, and concentrate on physical applications. On the other hand, a reader familiar with the physical content of quantum mechanics, and who would like to enhance his or her mathematics, could concentrate on those detours and consider the physics chapters as an application of the mathematics in a familiar setting.

Acknowledgment: The authors are grateful to V. Buslaev, J. Froehlich, W. Hunziker, and Yu. Ovchinnikov for useful discussions.

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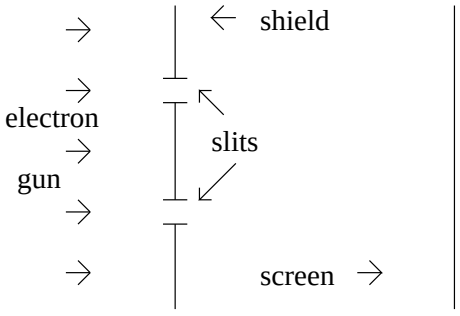
Chapter 1

Physical background

In this introductory chapter, we present a very brief overview of the basic structure of quantum mechanics, and touch on the physical motivation for the theory. A detailed mathematical discussion of quantum mechanics is the focus of the subsequent chapters of the book.

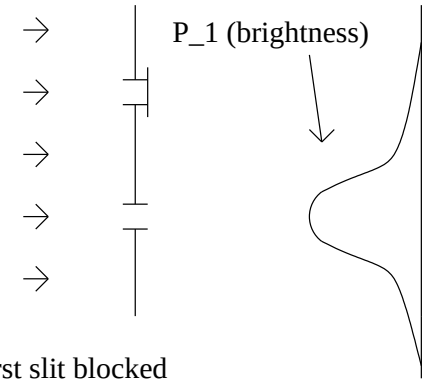
1.1 The double-slit experiment

Suppose a stream of electrons is fired at a shield in which two narrow slits have been cut (see figure 1.1). On the other side of the shield is a detector screen.

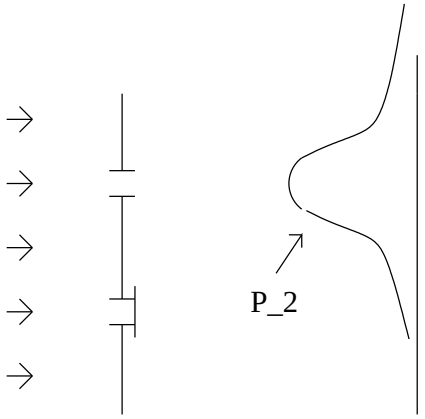


experimental set-up (1.1)

Pictured in figures 1.2-1.3 is the intensity distribution observed on the screen when either of the slits is blocked.

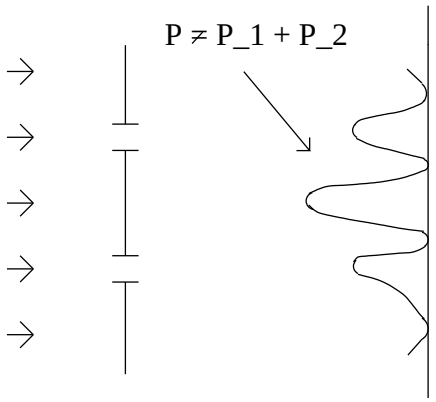


first slit blocked (1.2)



second slit blocked (1.3)

When both slits are open, the observed intensity distribution is shown in figure 1.4.

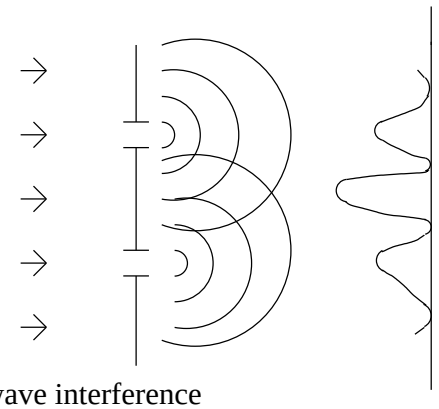


both slits open (1.4)

Remarkably, this is not the sum of the previous two distributions; ie, $P \neq P_1 + P_2$. We make some observations based on this experiment.

1. We cannot predict exactly where a given electron will hit the screen, we can only determine the distribution of locations.

2. The intensity pattern (called an *interference pattern*) we observe when both slits are open is similar to the pattern we see when a wave propagates through the slits: the intensity observed when the waves E_1 and E_2 (the waves here are represented by complex numbers encoding the amplitude and phase) originating at each slit are combined, is proportional to $|E_1 + E_2|^2 \neq |E_1|^2 + |E_2|^2$ (see figure 1.5).



wave interference (1.5)

We can draw some conclusions based on these observations.

1. Matter behaves in a random way.
2. Matter exhibits wave-like properties.

In other words, the behaviour of individual electrons is intrinsically random, and this randomness propagates according to laws of wave mechanics. These observations form a central part of the paradigm shift introduced by the theory of quantum mechanics.

1.2 Wave functions

In quantum mechanics, the state of a particle is described by a complex-valued function of position and time, $\psi(x,t)$, $x \in \mathbb{R}^3$, $t \in \mathbb{R}$. This is called a *wave function* (or *state vector*). In light of the above discussion, the wave function should have the following properties.

1. $|\psi(\cdot,t)|^2$ is the probability distribution for the particle's position. That is, the probability that a particle is in the region $\Omega \subset \mathbb{R}^3$ at time t is $\int_\Omega |\psi(x,t)|^2 dx$. Thus, we require the normalization $\int_{\mathbb{R}^3} |\psi(x,t)|^2 dx = 1$.
2. ψ satisfies some sort of wave equation.

For example, in the double-slit experiment, if ψ_1 gives the state beyond the shield with the first slit closed, and ψ_2 gives the state beyond the shield with the second slit closed, then $\psi = \psi_1 + \psi_2$ describes the state with both slits open. The interference pattern observed in the latter case reflects the fact that $|\psi|^2 \neq |\psi_1|^2 + |\psi_2|^2$.

1.3 State-space

The space of all possible states of the particle at a given time is called the *state space*. For us, the state space of a particle will usually be the square-integrable functions:

$$L^2(\mathbb{R}^3) \equiv \{\psi : \mathbb{R}^3 \to \mathbb{C} \mid \int_{\mathbb{R}^3} |\psi|^2 < \infty\}$$

(we can impose the normalization condition as needed). This is a vector space, and has an inner-product given by

$$\langle \psi, \phi \rangle \equiv \int_{\mathbb{R}^3} \bar{\psi}\phi$$

(in fact, it is a "Hilbert space"; i.e. it is complete - see section 2.1).

1.4 The Schrödinger equation

We now give a motivation for the equation which governs the evolution of a particle's wave function. This is the celebrated *Schrödinger equation.*

Our equation should satisfy certain physically sensible properties.

1. The state $\psi(\cdot, t_0)$ at time $t = t_0$ should determine the state $\psi(\cdot, t)$ for all later times $t > t_0$ (*causality*).

2. If ψ and ϕ are evolutions of states, then $\alpha\psi + \beta\phi$ (α, β constants) should also describe the evolution of a state (the *superposition principle*).

3. In "everyday situations," quantum mechanics should be close to the classical mechanics we are used to (the *correspondence principle*).

The first requirement means that ψ should satisfy an equation which is first-order in time, namely

$$\frac{\partial}{\partial t}\psi = A\psi \tag{1.6}$$

for some operator A on the state space. The second requirement implies that A must be a *linear* operator.

We use the third requirement in order to find the correct form of A. We first recall that one of the fundamental equations of classical mechanics is of the first order in time. It is the *Hamilton-Jacobi equation*,

$$\frac{\partial}{\partial t}S = -h(x, \nabla_x S) \tag{1.7}$$

where $h(x, k) = |k|^2/2m + V(x)$ is the classical *Hamiltonian function*, V is the potential,m is the mass, and $S(x, t)$ is the classical *action.* This equation, in turn, is similar to the *eikonal equation*,

$$(\partial\phi/\partial t)^2 - |\nabla_x \phi|^2 = 0$$

which is a high-frequency approximation of the wave equation for $u = ae^{i\phi}$. We make an analogy between the passage from the wave equation to the eikonal equation (that is, from *wave optics* to *geometric optics*) and the passage from quantum mechanics to classical mechanics. Thus, we seek equation (1.6), requiring that is has solutions of the form

$$\psi(x, t) = a(x, t)e^{iS(x,t)/\hbar}$$

where $\hbar$ is some very small constant, with S satisfying equation (1.7). Assuming a, S, and their derivatives are of order one in $\hbar$, then to the leading order in $\hbar$, ψ satisfies the equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\Delta_x\psi(x,t) + V(x)\psi(x,t). \tag{1.8}$$

This equation is of the desired form (1.6). In fact it is the right equation, and is called the *Schrödinger equation*. It can be written as

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi = H\psi} \tag{1.9}$$

where the linear operator H, given by

$$\boxed{H\psi \equiv -\frac{\hbar^2}{2m}\Delta\psi + V\psi}$$

is called a *Schrödinger operator*. The operator $\Delta = \sum_{j=1}^{d}\partial_j^2$ is the *Laplacian* (d = spatial dimension, usually 3), and the function (and multiplication operator) V is the *potential*. The small constant $\hbar$ is called *Planck's constant*; it is one of three fundamental constants in nature. For the record, its value is roughly

$$\hbar \approx 6.6255 \times 10^{-27} \text{ erg sec.}$$

Example 1.1 Here are just a few examples of potentials.

1. Free motion : $V \equiv 0$.
2. A wall: $V \equiv 0$ on one side, $V \equiv \infty$ on the other (meaning $\psi \equiv 0$ here).
3. The double-slit experiment: $V = \infty$ on the shield, and $V = 0$ elsewhere.
4. The Coulomb potential : $V(x) = -\alpha/|x|$ (describes a hydrogen atom).
5. The harmonic oscillator : $V(x) = \frac{m\omega^2}{2}|x|^2$.

We will analyze some of these examples, and others, in Chapter 8.

Chapter 2

Mathematical detour: operator theory

We have seen in Chapter 1 that the space of quantum-mechanical states of a system is a vector space with an inner-product (in fact a Hilbert space). We saw also that an operator (a Schrödinger operator) on this space enters the basic equation (the Schrödinger equation) governing the evolution of states. In fact, the theory of operators on a Hilbert space provides the basic mathematical framework of quantum mechanics. This chapter is devoted to an overview of those aspects of operator theory that are essential to a study of quantum mechanics.

2.1 Operators on Hilbert spaces

Let $\mathcal{H}$ be a (complex) vector space. We assume $\mathcal{H}$ is endowed with an *inner-product*, $\langle \cdot, \cdot \rangle$. Recall that this means the map

$$\langle \ , \ \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$$

satisfies the properties

1. linearity (in the second argument):

$$\langle v, \alpha w + \beta z \rangle = \alpha \langle v, w \rangle + \beta \langle v, z \rangle$$

2. conjugate symmetry: $\langle w, v \rangle = \overline{\langle v, w \rangle}$

3. positive definiteness: $\langle v, v \rangle > 0$ for $v \neq 0$

for any $v, w, z \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{C}$. It follows that the map $\|\cdot\| : \mathcal{H} \to [0, \infty)$ given by

$$\|v\|^2 = \langle v, v \rangle$$

is a *norm* on $\mathcal{H}$. Recall that this means that for any $v, w \in \mathcal{H}$ and $\alpha \in \mathbb{C}$,

1. $\|\alpha v\| = |\alpha| \|v\|$
2. $\|v + w\| \leq \|v\| + \|w\|$
3. $\|v\| > 0$ for $v \neq 0$.

If $\mathcal{H}$ is *complete* in this norm (that is, all Cauchy sequences converge), then $\mathcal{H}$ is called a *Hilbert space*.

We recall here two frequently used facts about Hilbert spaces (see, eg, [Fo] or [RSI] for proofs).

Proposition 2.1 (Cauchy-Schwarz inequality) *For $v, w \in \mathcal{H}$, a Hilbert space,*

$$|\langle v, w \rangle| \leq \|v\| \|w\|.$$

Recall that a set $\{v_n\} \subset \mathcal{H}$, $n = 1, 2, \ldots$ is called *orthonormal* if $\|v_n\| = 1$ for all n and $< v_n, v_m >= 0$ for $n \neq m$. It is a *complete orthonormal set* (or *basis*) if the collection of finite linear combinations of the v_n's is dense in $\mathcal{H}$.

Proposition 2.2 (Parseval relation) *Suppose $\{v_n\} \subset \mathcal{H}$ is a complete orthonormal set. Then for any $w \in \mathcal{H}$,*

$$\|w\|^2 = \sum_n |\langle w, v_n \rangle|^2.$$

In this chapter, the main objects of study are linear operators on $\mathcal{H}$ (that is, maps A from $\mathcal{H}$ to itself, which are linear: $A(\alpha v + \beta w) = \alpha A v + \beta A w$). Actually, we only require an operator A to be defined on a domain $D(A) \subset \mathcal{H}$ which is dense in $\mathcal{H}$ (that is, given any $v \in \mathcal{H}$ and $\epsilon > 0$, there is a $w \in D(A)$ such that $\|v - w\| < \epsilon$).

Example 2.3 Our usual example of a Hilbert space is

$$L^2(\mathbb{R}^d) \equiv \{\psi : \mathbb{R}^d \to \mathbb{C} \mid \int_{\mathbb{R}^d} |\psi|^2 < \infty\}$$

with the inner-product

$$\langle \psi, \phi \rangle \equiv \int_{\mathbb{R}^d} \bar{\psi} \phi.$$

An example of a dense subset of $L^2(\mathbb{R}^d)$ is $C_0^\infty(\mathbb{R}^d)$, the infinitely-differentiable functions with compact support (meaning they vanish outside of some ball in $\mathbb{R}^d$).

Example 2.4 Here is a list of examples of linear operators, A, on $L^2(\mathbb{R}^d)$. In each case, we can simply choose $D(A)$ to be the obvious domain $D(A) \equiv \{\psi \in L^2 | A\psi \in L^2\}$.

1. The identity map
$$\mathrm{i}d : \psi \mapsto \psi$$

2. Multiplication by a coordinate
$$x_j : \psi \mapsto x_j\psi$$
(i.e. $(x_j\psi)(x) = x_j\psi(x)$)

3. Multiplication by a continuous function $V : \mathbb{R}^d \to \mathbb{C}$
$$V : \psi \mapsto V\psi$$
(again meaning $(V\psi)(x) = V(x)\psi(x)$).

4. Differentiation
$$p_j : \psi \mapsto -i\hbar\partial_j\psi$$

5. The Laplacian
$$\Delta : \psi \mapsto \sum_{j=1}^{d} \partial_j^2\psi$$

6. Schrödinger operator
$$H : \psi \mapsto -\frac{\hbar^2}{2m}\Delta\psi + V\psi$$

7. integral operator with kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$
$$\mathcal{K} : \psi \mapsto \int K(\cdot, y)\psi(y)dy$$
(i.e. $(\mathcal{K}\psi)(x) = \int K(x, y)\psi(y)dy$).

The domain of the first example is obviously the whole space L^2. The domain of the last example depends on K. The domains of the others are easily seen to be dense, as they contain C_0^∞.

Remark 2.5 *If the kernel K is allowed to be a* distribution *(a generalized function), then the last example contains all the previous ones as special cases.*

It is useful in operator theory to single out those operators with the property of boundedness (which is equivalent to continuity).

Definition 2.6 *An operator A is* bounded *if*

$$\|A\| \equiv \sup_{\{\psi \mid \|\psi\|=1\}} \|A\psi\| < \infty. \tag{2.1}$$

In fact, the expression (2.1) defines a norm which makes the subspace $B(\mathcal{H})$ of bounded operators on $\mathcal{H}$ into a complete normed vector space (a *Banach space*) As we will see, the bounded operators are, in some respects, much easier to deal with than the unbounded operators. However, since some of the most important operators in quantum mechanics are unbounded, we will need to study both.

2.2 Adjoints

In quantum mechanics, operators which are *self-adjoint* play a central role. The present section is devoted to a discussion of this class of operators, and to the broader class of *symmetric* operators. All operators A are assumed to be defined on a dense domain $D(A)$.

Definition 2.7 *The* adjoint *of an operator, A, on $\mathcal{H}$, is the operator A^* defined by*

$$\langle A^*\psi, \phi\rangle = \langle \psi, A\phi\rangle \tag{2.2}$$

for all $\phi \in D(A)$, for ψ in the natural domain

$$D(A^*) \equiv \{\psi \in \mathcal{H} \mid \phi \mapsto \langle \psi, A\phi\rangle \text{ extends to a bounded functional on all of } \mathcal{H}\}.$$

It is left as an exercise to show this definition makes sense.

Problem 2.8 Show that equation (2.2) defines a unique linear operator A^* on $D(A^*)$.

Definition 2.9 *A is* symmetric *if*

$$\langle A\psi, \phi\rangle = \langle \psi, A\phi\rangle$$

for all ψ, ϕ in $D(A)$.

Definition 2.10 *A is* self-adjoint *if $A = A^*$ (that is, A is symmetric and $D(A) = D(A^*)$).*

It is usually much easier to show that a given operator is symmetric than to show that it is self-adjoint, as the latter question involves additional domain considerations.

Problem 2.11 Referring to our list of examples of operators on L^2 (example 2.4), show that the following operators are symmetric.

1. The multiplication operator V (if $V(x)$ is real-valued).
2. The differentiation operator, p_j (hint: integrate by parts).
3. The Laplacian, Δ.
4. The Schrödinger operator, H (again if V is real).
5. The integral operator $\mathcal{K}$ (if $K(y,x) = \overline{K(x,y)}$).

In fact, p_j and Δ are actually self-adjoint on L^2, as is V if it is a "nice enough" function (we will be more specific in section 7.2).

The subtleties surrounding domains and the question of self-adjointness are absent for bounded operators, as the following lemma demonstrates.

Lemma 2.12 *If A is bounded, then we can assume $D(A) = \mathcal{H}$.*

Proof: For any $u \in \mathcal{H}$, there is a sequence $\{u_n\} \subset D(A)$ such that $u_n \to u$ as $n \to \infty$ (by the density of $D(A)$). Then the relation

$$\|Au_n - Au_m\| \leq \|A\|\|u_n - u_m\|$$

(by definition of $\|A\|$) shows that $\{Au_n\}$ is a Cauchy sequence, so $Au_n \to v$, some $v \in \mathcal{H}$ (by completeness of H), and we set $Au \equiv v$. This extends A to a bounded operator on all of $\mathcal{H}$. □

Corollary 2.13 *If A is bounded and symmetric, it is self-adjoint.*

Proof: Since A is bounded, we may assume $D(A) = \mathcal{H}$. Thus $D(A^*) = \mathcal{H}$ (check this), and so $D(A) = D(A^*)$. Hence A is self-adjoint. □

We will, however, have to deal with unbounded operators. As an example, consider the following:

Problem 2.14 Show $p_j \equiv -i\hbar\partial_j$ is unbounded on $L^2(\mathbb{R}^d)$.

2.3 Exponentials and unitary operators

For a bounded operator, A, we can define the operator e^A through the power series

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}$$

which converges absolutely as

$$\sum \frac{\|A^n\|}{n!} \leq \sum \frac{\|A\|^n}{n!} = e^{\|A\|}.$$

Problem 2.15 Find e^{-itH} for

$$H = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad H = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

For an unbounded self-adjoint operator A, it is still possible to define the bounded operator e^{iA} using the so-called *functional calculus* (see, eg, [RSI]) which is beyond the scope of this book. We will, however, see how to define operators like e^{ip_j}, $e^{i\Delta}$ and e^{Δ} using the Fourier transform in Chapter 4.

Definition 2.16 *An operator U is* unitary *if $UU^* = U^*U = 1$ (ie $U^* = U^{-1}$).*

Using the power series definition of e^{iA} for bounded A, we can check the following relationship between unitary and self-adjoint operators:

Theorem 2.17 (Stone's Theorem) *e^{iA} is unitary iff A is self-adjoint*

Formal check:

$$e^{iA}(e^{iA})^* = e^{iA}e^{-iA^*} = e^{i(A-A^*)}$$

which is the identity iff $A = A^*$.

Problem 2.18 Prove this theorem properly for the case of bounded A.

In fact, the theorem holds even if A is unbounded and self-adjoint. The following simple example illustrates.

Example 2.19 If $\phi : \mathbb{R}^d \to \mathbb{R}$ is continuous, then the bounded operator

$$U : \psi \mapsto e^{i\phi}\psi$$

is easily checked to be unitary on L^2 (just note that U^* is multiplication by $e^{-i\phi}$). Now ϕ is bounded as a multiplication operator iff it is a bounded function. Note, however, that U is well-defined (and unitary) even if ϕ is unbounded.

We conclude this section with a couple of useful definitions.

Definition 2.20 *A self-adjoint operator A is called* positive *(denoted $A > 0$) if*

$$\langle \psi, A\psi \rangle > 0$$

for all $\psi \in D(A)$, $\psi \neq 0$. Similarly, we may define non-negative, negative, and non-positive operators.

Problem 2.21 Show that $-\Delta > 0$ on L^2 (hint: integrate by parts, or, equivalently, use the divergence theorem).

Definition 2.22 *The* commutator*, $[A, B]$, of two bounded operators A and B is the operator defined by*

$$[A, B] = AB - BA.$$

Defining the commutator of two operators when one of them is unbounded requires caution, due to domain considerations. Given this warning, we will deal with commutators of unbounded operators formally without giving them a second thought.

Chapter 3

Dynamics

We recall that the evolution of the wave function, ψ, for a particle in a potential, V, is determined by the Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{3.1}$$

where

$$H = -\frac{\hbar^2}{2m}\Delta + V$$

is the appropriate Schrödinger operator. We supplement equation (3.1) with the initial condition

$$\psi|_{t=0} = \psi_0 \tag{3.2}$$

where $\psi_0 \in L^2$. The purpose of this chapter is to investigate the existence, and basic properties, of solutions of the Schrödinger equation, and the establish the connection between these issues and the self-adjointness of H.

3.1 Conservation of probability

Since we interpret the wave function at a given instant in time as a probability distribution, we require

$$\int_{\mathbb{R}^3} |\psi(x,t)|^2 dx \equiv 1 \tag{3.3}$$

at all times. If (3.3) holds, we say that *probability is conserved.*

Theorem 3.1 *Under the evolution given by (3.1), probability is conserved iff H is symmetric.*

Proof: For ψ solving the Cauchy problem (3.1-3.2), we compute

$$\begin{aligned} d/dt\langle\psi,\psi\rangle &= \langle\dot{\psi},\psi\rangle + \langle\psi,\dot{\psi}\rangle \\ &= \langle\frac{1}{i\hbar}H\psi,\psi\rangle + \langle\psi,\frac{1}{i\hbar}H\psi\rangle \\ &= \frac{1}{i\hbar}[\langle\psi,H\psi\rangle - \langle H\psi,\psi\rangle] \end{aligned}$$

which is zero for all times iff $\langle H\phi,\phi\rangle = \langle\phi,H\phi\rangle$ for all $\phi \in D(H)$ (for the "only if" part, take $\psi_0 = \phi$). This, in turn, holds iff H is a symmetric operator (this follows from a version of the *polarization identity* - see, eg, [RSI]). □

3.2 Existence of dynamics

Definition 3.2 *We say the* dynamics exist *if the Cauchy problem (3.1-3.2) has a unique solution which conserves probability.*

Theorem 3.3 *The dynamics exist iff $H = H^*$.*

Sketch of proof: $\Rightarrow$: as we have seen, conservation of probability implies that H must be symmetric. The self-adjointness part is difficult, and we omit it.

$\Leftarrow$: On the domain

$$D \equiv \{\psi \in D(H) | \|H^n\psi\| \leq M^n, \text{ some } M\}$$

we can define $U(t) \equiv e^{\frac{-iHt}{\hbar}}$ by a convergent power series. Set $\psi \equiv U(t)\psi_0$. Then ψ satisfies (3.1-3.2). The hard part is to extend this to all of L^2. It is here that the self-adjointness of H is used (as was remarked earlier, we may define $U(t)$ on L^2 via the functional calculus). We have seen already that a solution conserves probability (by symmetry of H). Finally, we note that solutions are unique by the following argument. Given any two solutions, their difference, $\tilde{\psi}$, solves (3.1) with $\tilde{\psi}|_{t=0} = 0$. By symmetry of H, $\|\tilde{\psi}(\cdot,t)\| = \|\tilde{\psi}(\cdot,0)\| = 0$ for all t, hence $\tilde{\psi} \equiv 0$. □

Problem 3.4 Check formally that

1. $U(t)\psi_0$ solves the Schrödinger equation.
2. $U(t+s) = U(t)U(s)$ (group property).

We conclude this section by emphasizing that for our Schrödinger equation formulation of quantum mechanics to make sense, the Schrödinger operator must be self-adjoint. We will address the important question of which potential functions, V, give rise to self-adjoint operators $H = -\frac{\hbar^2}{2m}\Delta + V$ in Chapter 7.

Chapter 4

Mathematical detour: the Fourier transform

The Fourier transform is a useful tool in many areas of mathematics and physics. The purpose of the present chapter is to review the properties of the Fourier transform, and to discuss the important role it plays in quantum mechanics.

4.1 Definition of the Fourier transform

The *Fourier transform* is a map, $\mathcal{F}$, which sends a function $\psi : \mathbb{R}^d \to \mathbb{C}$ into another function $\hat{\psi} : \mathbb{R}^d \to \mathbb{C}$ where for $k \in \mathbb{R}^d$,

$$\hat{\psi}(k) \equiv (2\pi\hbar)^{-d/2} \int_{\mathbb{R}^d} e^{-ik\cdot x/\hbar} \psi(x) dx$$

(it is convenient to introduce the Planck constant, $\hbar$, into our Fourier transform). It is clear that $\mathcal{F}$ is a linear operator.

In the following exercise, the reader is asked to compute a few basic Fourier transforms.

Problem 4.1 Show that under $\mathcal{F}$

1. $e^{-\frac{a}{2\hbar}|x|^2} \mapsto a^{-d/2} e^{-\frac{|k|^2}{2\hbar a}}$ $(Re(a) > 0)$ (hint: complete the square in the exponent and move the contour of integration in the complex plane)

2. $e^{-\frac{1}{2\hbar}x\cdot Ax} \mapsto (\det A)^{-1/2} e^{-\frac{1}{2\hbar}k\cdot A^{-1}k}$ (A is a positive $d \times d$ matrix) (hint: diagonalize and use the previous result)

3. $\delta(x) \mapsto (2\pi\hbar)^{-d/2}$ (here δ is the *Dirac delta function* (not really a function, but a distribution), characterized by the property $\int f(x)\delta(x)dx = f(0)$).

4.2 Properties of the Fourier transform

The great utility of the Fourier transform derives from the following properties.

1. The Plancherel theorem: $\mathcal{F}$ is a unitary map from $L^2(\mathbb{R}^d)$ to itself (note that initially the FT is defined only for integrable (L^1) functions - the statement here is that the FT extends from $L^1 \cap L^2$ to a unitary map on L^2).

2. The inversion formula: the adjoint $\mathcal{F}^*$ of $\mathcal{F}$ is given by the map $\psi \mapsto \check{\psi}$ where

$$\check{\psi}(x) \equiv (2\pi\hbar)^{-d/2} \int_{\mathbb{R}^d} e^{ix\cdot k/\hbar}\psi(k)dk$$

   (and by the Plancherel theorem, this is also the inverse).

3. $-i\hbar\widehat{\nabla_x\psi}(k) = k\hat{\psi}(k)$.

4. $\widehat{x\psi}(k) = i\hbar\nabla_k\hat{\psi}(k)$.

5. $\widehat{\phi\psi} = (2\pi\hbar)^{-d/2}\hat{\phi} * \hat{\psi}$

6. $\widehat{\phi * \psi} = (2\pi\hbar)^{d/2}\hat{\phi}\hat{\psi}$.

Here

$$(f * g)(x) \equiv \int f(y)g(x-y)dy$$

is the *convolution* of f and g. The last four properties can be loosely summarized by saying that the Fourier transform exchanges differentiation and coordinate multiplication, and products and convolutions.

Proof: The proof of property 1 is somewhat technical and we just sketch it here (see, eg, [Fo]) for details). In particular, we will show that $\|f\| = \|\hat{f}\|$. Suppose $f \in C_0^\infty$, and let C_ϵ be the cube of side length $2/\epsilon$ centred at the origin. Choose ϵ small enough so that the support of f is contained in C_ϵ. One can show that

$$\{E_k \equiv (\epsilon/2)^{d/2}e^{ik\cdot x/\hbar} \mid k \in \epsilon\hbar\pi\mathbb{Z}^d\}$$

is an orthonormal basis of the Hilbert space $L^2(C_\epsilon)$. Thus by the Parseval equation (proposition 2.2),

$$\int |f|^2 = \int_{C_\epsilon} |f|^2 = \sum_k | < E_k, f > |^2$$

$$= (\pi\epsilon\hbar)^d \sum_{k \in \epsilon\hbar\pi\mathbb{Z}^d} |\hat{f}(k)|^2 \to \int |\hat{f}|^2$$

as $\epsilon \to 0$. $\square$

Problem 4.2 Show that $\{E_k\}$ is an orthonormal set.

Now we will prove property 3, and we leave the proofs of the other properties as exercises. Integrating by parts, we have

$$(-i\hbar\nabla\psi)\hat{}(k) = (2\pi\hbar)^{-d/2} \int e^{-ix\cdot k/\hbar} \cdot (-i\hbar\nabla)\psi(x)dx$$

$$= k \cdot (2\pi\hbar)^{-d/2} \int e^{-ix\cdot k/\hbar}\psi(x)dx = k\hat{\psi}(k).$$

To justify these manipulations we can take $\psi \in C_0^\infty$ and use the density of C_0^∞ in L^2, and the continuity of $\mathcal{F}$, in an approximation argument. $\square$

4.3 Functions of the derivative

As an application, we now show how the FT can be used to define functions of the derivative operator. We recall our notation $p \equiv -i\hbar\nabla$. Motivated by property 3 of the FT, we define an operator $g(p)$ (for sufficiently nice functions g) on L^2 as follows.

Definition 4.3 $(g(p)\psi)\hat{}(k) \equiv g(k)\hat{\psi}(k)$ *or, equivalently,* $g(p)\psi \equiv (2\pi\hbar)^{-n/2}\check{g} * \psi$.

Let us look at a few examples.

Example 4.4

1. If $g(k) = k$, then by property 3 of the FT, the above definition gives us back $g(p) = p$ (so at least our definition makes some sense).

2. Now suppose $g(k) = |k|^2$. Then $\widehat{g(p)\psi}(k) = |k|^2\hat{\psi}$.

Problem 4.5 Show that $-\hbar^2\widehat{\Delta\psi} = |k|^2\hat{\psi}$.

Thus we have $|p|^2 = -\hbar^2\Delta$. In fact, extending this example, we can define $g(p)$ when g is a polynomial "with our bare hands". It is easily seen that this definition coincides with the one above.

3. Let $g(k) = e^{-\frac{|k|^2}{2\hbar}}$ (a Gaussian). Then using the result of problem 4.1, we have $g(p)\psi(x) = (2\pi\hbar)^{-d/2}\int e^{-|x-y|^2/2\hbar}\psi(y)dy$. In light of the previous example, we can write this as (setting $\hbar = 1$ for tidiness)

$$(e^{\Delta}\psi)(x) = (4\pi)^{-d/2}\int e^{-|x-y|^2/4}\psi(y)dy.$$

Chapter 5

Observables

In any physical theory, the quantities that can be experimentally measured - the *observables* - are of obvious importance. In this chapter, we discuss the observables of quantum mechanics, as well as the notion of "quantizing" a classical theory.

5.1 Mean values and the momentum operator

We recall that in quantum mechanics, the state of a particle at time t is described by a wave function $\psi(x,t)$. The probability distribution for the position, x, of the particle, is $|\psi(\cdot,t)|^2$. Thus the mean value of the position at time t is given by $\int x|\psi(x,t)|^2dx$ (note that this is a vector in $\mathbb{R}^d$). If we define the coordinate multiplication operator

$$x_j : \psi(x) \mapsto x_j\psi(x)$$

then the mean value of the j^{th} component of the coordinate x in the state ψ is $\langle\psi, x_j\psi\rangle$.

Now compute

$$\begin{aligned} d/dt\langle\psi, x_j\psi\rangle &= \langle\dot{\psi}, x_j\psi\rangle + \langle\psi, x_j\dot{\psi}\rangle \\ &= \langle\frac{1}{i\hbar}H\psi, x_j\psi\rangle + \langle\psi, x_j\frac{1}{i\hbar}H\psi\rangle \\ &= \langle\psi, \frac{i}{\hbar}Hx_j\psi\rangle - \langle\psi, x_j\frac{i}{\hbar}H\psi\rangle \\ &= \langle\psi, \frac{i}{\hbar}[H, x_j]\psi\rangle \end{aligned}$$

(where recall $[A,B] \equiv AB - BA$ is the *commutator* of A and B).

We compute

$$\Delta(x\psi) = x\Delta\psi + 2\nabla\psi$$

and use this to get

$$\frac{i}{\hbar}[H, x_j] = -\frac{i\hbar}{m}\nabla_j$$

giving finally

$$d/dt\langle\psi, x_j\psi\rangle = \frac{1}{m}\langle\psi, -i\hbar\nabla_j\psi\rangle.$$

As before, we denote the operator $-i\hbar\nabla_j$ by p_j. As well, we denote the mean value $\langle\psi, A\psi\rangle$ of an operator A by $< A >_\psi$. Then the above becomes

$$\boxed{m\frac{d}{dt} < x_j >_\psi = < p_j >_\psi} \tag{5.1}$$

which is reminiscent of the definition of the classical momentum. We call the operator p the *momentum operator*. In fact, p_j is a self-adjoint operator on $L^2(\mathbb{R}^d)$.

Using the FT, we compute the mean value of the momentum operator

$$\langle\psi, p_j\psi\rangle = \langle\hat{\psi}, \widehat{p_j\psi}\rangle$$

$$= \langle\hat{\psi}, k\hat{\psi}\rangle = \int k|\hat{\psi}(k)|^2 dk.$$

This, and similar computations, show that $|\hat{\psi}(k)|^2$ is the probability distribution for the particle momentum.

5.2 Observables

Definition 5.1 *An* observable *is a self-adjoint operator on the state space* $L^2(\mathbb{R}^3)$.

We have already seen a few examples of observables, including the position operators, x_j, the momentum operators, p_j and the *Hamiltonian operator*,

$$H = -\frac{\hbar^2}{2m}\Delta + V = \frac{1}{2m}|p|^2 + V.$$

Another example (with an obvious classical analogue) is furnished by the *angular momentum operators*, $L_j = (x \times p)_j$.

The reader is invited to derive the following equation for the evolution of the mean value of an observable.

Problem 5.2 Check that for any observable, A, we have

$$d/dt < A >_\psi = \langle \psi, \frac{i}{\hbar}[H, A]\psi \rangle.$$

We would like to use this result on the momentum operator. Simple computations give $[\Delta, p] = 0$ and $[V, p] = i\hbar \nabla V$, so that

$$\frac{i}{\hbar}[H, p] = -\nabla V$$

and hence

$$\boxed{d/dt < p_j >_\psi = < -\nabla_j V >_\psi .} \tag{5.2}$$

This is a quantum mechanical mean-value version of Newton's equation of classical mechanics. Or if we include equation (5.1), we have the analogue of Hamilton's equations.

Since obviously $[H, H] = 0$, we also have $d/dt < H >= 0$, which is the mean-value version of the conservation of energy.

5.3 Heisenberg representation

The framework outlined up to this point is called the *Schrödinger representation* of quantum mechanics. Chronologically, quantum mechanics was first formulated in the Heisenberg representation, which we now describe. For an observable A, define

$$A(t) \equiv e^{itH/\hbar} A e^{-itH/\hbar}.$$

Since $\psi = e^{-itH/\hbar}\psi_0$ (the solution of Schrödinger's equation), and $e^{-itH/\hbar}$ is unitary, we have (by a simple computation which is left as an exercise) that

$$< A >_\psi = < A(t) >_{\psi_0} . \tag{5.3}$$

Problem 5.3

1. Prove equation (5.3).

2. Prove that

$$\frac{d}{dt}A(t) = \frac{i}{\hbar}[H, A(t)].$$

This last equation is called the *Heisenberg equation* for the time evolution of the observable A. In particular, taking x and p for A, we obtain the quantum analogue of the Hamilton equations of classical mechanics:

$$m\dot{x}(t) = p(t) \tag{5.4}$$

and

$$\dot{p}(t) = -\nabla V(x(t)). \tag{5.5}$$

In the Heisenberg representation, then, the state is fixed (at ψ_0), and the observables evolve according to the Heisenberg equation. Of course, the Schrödinger and Heisenberg representations are completely equivalent (by a unitary transformation).

5.4 Quantization

We now describe a procedure for passing from classical mechanics to quantum mechanics, called *quantization*.

We start with the Hamiltonian formulation of classical mechanics, where the basic objects are as follows.

1. The *phase space* (or state space) $\mathbb{R}^3_x \times \mathbb{R}^3_k$ equipped with the *Poisson bracket*, $\{\cdot,\cdot\}$. The latter is defined on pairs of functions on $\mathbb{R}^3_x \times \mathbb{R}^3_k$ by

$$\{f,g\} = \sum_{j=1}^{n} \left(\frac{\partial f}{\partial k_j}\frac{\partial g}{\partial x_j} - \frac{\partial f}{\partial x_j}\frac{\partial g}{\partial k_j}\right).$$

2. The Hamiltonian, $h(x,k)$, a real function on $\mathbb{R}^3_x \times \mathbb{R}^3_k$ (which gives the energy of the classical system).

Then the classical dynamics of the system are given by *Hamilton's equations*:

$$\dot{x} = \{H, x\} \qquad \dot{k} = \{H, k\}.$$

The corresponding fundamental objects in quantum mechanics are the following.

1. The state space $L^2(\mathbb{R}^3_x)$, and the commutator, $\frac{i}{\hbar}[\cdot\cdot]$, of two operators acting on $L^2(\mathbb{R}^3_x)$

2. A Schrödinger operator, $H = h(x,p)$ (the Hamiltonian) acting on the state space.

Recall that the dynamics of the quantum system can be described by the Heisenberg equations

$$\dot{x} = \frac{i}{\hbar}[H, x] \qquad \dot{p} = \frac{i}{\hbar}[H, p]$$

(which are the same as (5.4) and (5.5)).

We note that for classical mechanics

$$\{x_i, x_j\} = \{k_i, k_j\} = 0 \quad \{k_i, x_j\} = \delta_{ij}$$

and for quantum mechanics

$$[x_i, x_j] = [p_i, p_j] = 0 \quad \frac{i}{\hbar}[p_i, x_j] = \delta_{ij}.$$

These are the *canonical commutation relations*. x and k are called *canonical variables* of classical mechanics, and x and p, *canonical operators* of quantum mechanics.

The following table provides a summary of the classical mechanical objects and their quantized counterparts:

Object	CM	QM
state space	$\mathbf{R_x}^3 \times \mathbf{R_k}^3$ and Poisson brackets	$L^2(\mathbb{R}^3_x)$ and commutator
evolution of state	path in phase-space	path in $L^2(\mathbb{R}^3)$
observable	real function on state space	self-adjoint operator on state space
result of measuring observable	deterministic	probabilistic
objects controlling dynamics	Hamiltonian	Schrödinger operator
canonical coordinates	x and k	operators x (mult.) and p

5.5 Pseudodifferential operators

The correspondence between classical observables and quantum observables is a subtle one. For canonical variables, we have that the variable x is mapped to the operator of multiplication by x, and the variable k is mapped to the operator $p = -i\hbar\nabla_x$. Continuing this, we should have a function $f(x)$ mapping to an operator of multiplication by $f(x)$, and a function $f(k)$ mapping to an operator $f(p)$. However,

the following simple case shows the ambiguity of this correspondence. The function $x \cdot k = k \cdot x$ could be mapped into any of the following three distinct operators:

$$x \cdot p, \quad p \cdot x, \quad \frac{1}{2}(x \cdot p + p \cdot x).$$

In this case, the ambiguity is resolved by requiring that the resulting operator is self-adjoint. But in the general situation

$$f(x, k) \to f(x, p),$$

showing that this condition resolves the ambiguity and that it can be implemented in terms of a mathematical formula requires some work.

In mathematics, operators obtained by a certain quantization rule from functions $f(x, k)$ satisfying certain estimates are called *pseudodifferential operators*. Differential operators with smooth coefficients, as well as certain integral and singular operators are examples of pseudodifferential operators.

Chapter 6

The uncertainty principle

One of the fundamental implications of quantum theory is the *uncertainty principle* - that is, the fact that certain physical quantities cannot be measured simultaneously with arbitrary accuracy. In this chapter, we establish precise mathematical statements of the uncertainty principle.

6.1 The Heisenberg uncertainty principle

We consider a particle in a state ψ and think of the observables x and p as random variables with probability distributions $|\psi|^2$ and $|\hat{\psi}|^2$ respectively. The *dispersion* of x_j in the state ψ is

$$(\Delta x_j)^2 \equiv < (x_j - < x_j >_\psi)^2 >_\psi$$

and the dispersion of p_j is

$$(\Delta p_j)^2 \equiv < (p_j - < p_j >_\psi)^2 >_\psi .$$

Theorem 6.1 (The Heisenberg uncertainty principle) *For any state ψ,*

$$\Delta x_j \Delta p_j \geq \hbar/2.$$

Proof: The basic ingredient is the commutation relation

$$\frac{i}{\hbar}[p, x] = \text{ id}$$

(this is a matrix equation, meaning $\frac{i}{\hbar}[p_j, x_k] = \delta_{j,k}$). For notational simplicity, we assume $< x >_\psi = < p >_\psi = 0$. Noting that for two self-adjoint operators A, B,

$$\langle i[A, B] \rangle_\psi = -2Im\langle A\psi, B\psi \rangle$$

we obtain

$$1 = \langle\psi,\psi\rangle = \langle\psi, \frac{i}{\hbar}[p_j, x_j]\psi\rangle$$
$$= -\frac{2}{\hbar} Im\langle p_j\psi, x_j\psi\rangle \leq \frac{2}{\hbar}|\langle p_j\psi, x_j\psi\rangle|$$
$$\leq \frac{2}{\hbar}\|p_j\psi\|\|x_j\psi\| = \frac{2}{\hbar}(\Delta p_j)(\Delta x_j).$$

This does it. □

6.2 Refined uncertainty principle

We also have the following related result.

Theorem 6.2 (Refined uncertainty principle) *On* $L^2(\mathbb{R}^3)$,

$$-\Delta \geq \frac{1}{4|x|^2}$$

(recall that for operators A, B, we write $A \geq 0$ if $\langle\psi, A\psi\rangle \geq 0$ for all ψ, and we write $A \geq B$ if $A - B \geq 0$).

Proof: Compute (formally!)

$$\sum_j i[|x|^{-1}p_j|x|^{-1}, x_j] = \hbar d|x|^{-2}$$

(d = space dimension = 3). Hence

$$\hbar d\||x|^{-1}\psi\|^2 = 2\sum Im\langle|x|^{-1}p_j|x|^{-1}\psi, x_j\psi\rangle$$

and therefore

$$\hbar(d-2)\||x|^{-1}\psi\|^2 = -2Im\sum_j\langle p_j\psi, \frac{x_j}{|x|^2}\psi\rangle.$$

Now the Cauchy-Schwarz inequality implies

$$|\sum_j\langle p_j\psi, \frac{x_j}{|x|^2}\psi\rangle| \leq \|p\psi\|\|\frac{1}{|x|}\psi\|$$

(prove this!), which together with the previous inequality gives the desired result. □

Problem 6.3 Show that the refined UP can be used to give a quick proof of the Heisenberg UP.

6.3 Application: stability of Hydrogen

In classical mechanics, the hydrogen atom is unstable: as the electron orbits the nucleus (proton), it radiates and falls onto the nucleus. One of the first triumphs of quantum mechanics was showing that this is not so in QM. The latter statement is expressed mathematically by the property that the Hamiltonian, H (and therefore the energy) is bounded from below.

The hydrogen atom is described by the Schrödinger operator

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|x|}$$

on $L^2(\mathbb{R}^3)$ (m and $-e$ are the mass and charge of the electron respectively). The refined uncertainty principle gives

$$H \geq \frac{\hbar^2}{8m|x|^2} - \frac{e^2}{|x|}.$$

The r.h.s here reaches its minimum at $|x|^{-1} = 4me^2/\hbar^2$ and so

$$H \geq -\frac{2me^4}{\hbar^2}.$$

Thus, the energy of the hydrogen atom is bounded from below, and so the electron does not collapse onto the proton.

Chapter 7

Spectral theory

Our next task is to classify the orbits (i.e. solutions) of the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi$$

with given initial condition

$$\psi|_{t=0} = \psi_0$$

according to their behaviour in space-time. Naturally, we want to distinguish between states which are localized for all time, and those whose essential support moves off to infinity. Such a classification is made with the help of a very important invariant - the *spectrum* of an operator. We begin by describing the general theory, and then we proceed to applications.

7.1 The spectrum of an operator

Definition 7.1 *The* spectrum *of an operator A on a Hilbert space $\mathcal{H}$ is the subset of $\mathbb{C}$ given by*

$$\sigma(A) \equiv \{\lambda \in \mathbb{C} \mid A - \lambda \textit{ is not invertible (has no bounded inverse)}\}$$

The usual reasons that $A - \lambda$ is not invertible are

1. $(A - \lambda)\psi = 0$ has a non-zero solution, $\psi \in \mathcal{H}$. Then λ is an *eigenvalue* of A.
2. $(A-\lambda)\psi = 0$ "almost" has a non-zero solution. More precisely, we say $\{\psi_n\} \subset \mathcal{H}$ is a *Weyl sequence* for A and λ if

(a) $\|\psi_n\| = 1$ for all n

(b) $\|(A-\lambda)\psi_n\| \to 0$ as $n \to \infty$

(c) $\psi_n \to 0$ *weakly* as $n \to \infty$ (this means $\langle \phi, \psi_n \rangle \to 0$ for all $\phi \in \mathcal{H}$).

This is what we mean by $(A-\lambda)\psi = 0$ "almost" having a non-zero solution.

Definition 7.2 *The* point spectrum *of A is*

$$\sigma_p(A) = \{\lambda \mid \lambda \textit{ is an isolated eigenvalue of } A \textit{ with finite multiplicity}\}$$

(isolated meaning some neighbourhood of λ is disjoint from $\sigma(A)$).

Here the *multiplicity* of an eigenvalue λ is the dimension of the subspace

$$\mathrm{N}ull(A-\lambda) \equiv \{v \in L^2 \ \mid \ (A-\lambda)v = 0\}.$$

Problem 7.3 Show $\mathrm{Null}(A-\lambda)$ is a vector space.

Problem 7.4 Show that for $A = A^*$, eigenfunctions of A corresponding to different eigenvalues are orthogonal.

Definition 7.5 *The* continuous spectrum *of A is*

$$\sigma_c(A) = \{\lambda \mid \ \textit{there is a Weyl sequence for } A \textit{ and } \lambda\}.$$

When A is self-adjoint, these two sets make up the whole spectrum:

Theorem 7.6 (Weyl) *If $A = A^*$, then the spectrum of A is the union of the point spectrum of A and the continuous spectrum of A:*

$$\sigma(A) = \sigma_p(A) \cup \sigma_c(A).$$

Problem 7.7 Show that for $U : \mathcal{H} \to \mathcal{H}$ unitary, $\sigma(U^*AU) = \sigma(A)$, $\sigma_p(U^*AU) = \sigma_p(A)$, and $\sigma_c(U^*AU) = \sigma_c(A)$.

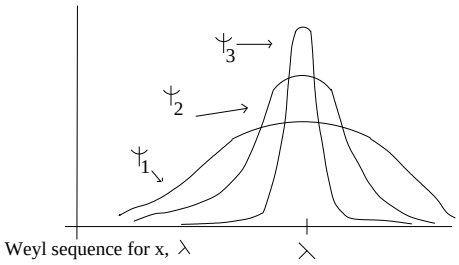
Example 7.8 We show that

1. $\sigma(p_j) = \sigma_c(p_j) = \mathbb{R}$
2. $\sigma(x_j) = \sigma_c(x_j) = \mathbb{R}$

Proof of the second fact: assume, for simplicity, $d = 1$. For any $\lambda \in \mathbb{R}$, we find a Weyl sequence for x and λ. This sequence is such that its square approximates the delta-function $\delta_\lambda(x) = \delta(\lambda - x)$ which solves the equation

$$(x - \lambda)\delta_\lambda = 0$$

exactly. Such a sequence is sketched in figure 7.1.



(7.1)

How do we find such a sequence ψ_n? Let ϕ be a fixed positive function supported on $[-1, 1]$, and such that

$$\int |\phi|^2 = 1.$$

We compress this function, increasing its height, and shift the result to λ:

$$\psi_n(x) = n^{1/2}\phi(n(x - \lambda)).$$

Then

$$\int |\psi_n|^2 = \int |\phi|^2 = 1$$

and

$$\|(x - \lambda)\psi_n\|^2 = \int |x - \lambda|^2 n|\phi(n(x - \lambda))|^2 dx$$

$$= \frac{1}{n^2} \int |y|^2 |\phi(y)|^2 dy \to 0$$

as $n \to \infty$. Thus $\lambda \in \sigma(x)$ at least. Now we show that $\psi_n \to 0$ weakly. Indeed,

$$|\int \bar{\psi_n} f| = |\int_{|x-\lambda| \le 1/n} \bar{\psi_n} f|$$

$$\le (\int |\psi_n|^2)^{1/2} (\int_{|x-\lambda| \le 1/n} |f|^2)^{1/2}$$

which $\to 0$ as $n \to \infty$ by a well-known result of analysis. Thus, $\lambda \in \sigma_c(x)$. It is easy to convince yourself that x has no eigenvalues.

Now we prove the first fact. Using properties of the FT, we have

$$\|(p-\lambda)\psi_n\| = \|\widehat{((p-\lambda)\psi_n)}\| = \|(k-\lambda)\hat{\psi}_n\|.$$

Take for $\hat{\psi}_n$ the Weyl sequence constructed above:

$$\hat{\psi}_n = n^{1/2}\hat{\phi}(n(k-\lambda))$$

with

$$\int |\hat{\phi}|^2 = 1.$$

So we have

$$\|\psi_n\| = \|\hat{\psi}_n\| = 1$$

and

$$\int \bar{f}\psi_n = \int \bar{\hat{f}}\hat{\psi}_n \to 0$$

for any $f \in L^2$. Further,

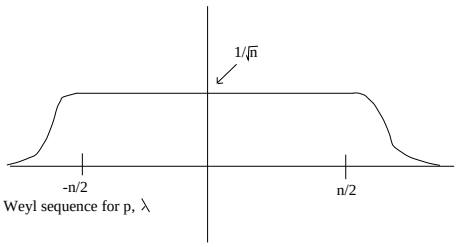
$$\|(k-\lambda)\hat{\psi}_n\| \to 0 \Rightarrow \|(p-\lambda)\psi_n\| \to 0$$

and so ψ_n is a Weyl sequence for p and λ. Thus $\sigma(p) = \sigma_c(p) = \mathbb{R}$. Now let us see how ψ_n looks. We have

$$\psi_n(x) = (2\pi\hbar)^{-1/2}\int e^{ik\cdot x/\hbar} n^{1/2}\hat{\phi}(n(k-\lambda))dk$$

$$= e^{-ix\cdot\lambda/\hbar} n^{-1/2}\phi(x/n).$$

We will assume $\phi \equiv 1$ for $|x| \le 1/2$. Then ψ_n looks like a plane wave (with amplitude $n^{-1/2}$ and wave vector λ), cut off at ∞ by $\phi(x/n)$ ($|\psi_n|$ is sketched in figure 7.2).



(7.2)

We remark that this fact also follows from the previous one, together with problem 7.7 and the Fourier transform.

The following exercise asks for the spectrum of two of our other favourite operators.

Problem 7.9 Prove

1. For $V : \mathbb{R}^d \to \mathbb{C}$ continuous, $\sigma(V) = \overline{\text{range}(V)}$
2. $\sigma(-\Delta) = \sigma_c(-\Delta) = [0, \infty)$

We now show that self-adjoint operators have real spectrum.

Theorem 7.10 *If $A = A^*$, then $\sigma(A) \subset \mathbb{R}$.*

Proof: Suppose $Im(\lambda) \neq 0$. Then we compute

$$\|(A-\lambda)\psi\|^2 = \langle (A-\lambda)\psi, (A-\lambda)\psi\rangle$$

$$= \|A\psi\|^2 - 2Re(\lambda)\langle\psi, A\psi\rangle + |\lambda|^2\|\psi\|^2$$

so

$$\|(A-\lambda)\psi\|^2 \geq \|A\psi\|^2 - 2|Re(\psi)|\|\psi\|\|A\psi\| + |\lambda|^2\|\psi\|^2$$
$$= (\|A\psi\| - |Re(\lambda)|\|\psi\|)^2 + |Im(\lambda)|^2\|\psi\|^2$$

and

$$\|(A-\lambda)\psi\| \geq |Im(\lambda)|\|\psi\|$$

and so $\lambda \notin \sigma(A)$ by the Weyl theorem. □

Proposition 7.11 *Let $A = A^*$. If λ is an accumulation point of $\sigma(A)$, then $\lambda \in \sigma_c(A)$.*

Proof: Suppose $\{\psi_n\}$ is a sequence of eigenfunctions with eigenvalues converging to λ. By problem 7.4, we can assume the ψ_n are orthonormal. Then $\sum |\langle f, \psi_n\rangle|^2 \leq \|f\|^2$ (Parseval's relation) implies $\langle f, \psi_n\rangle \to 0$ for all f, so $\psi_n \to 0$ weakly, and thus it is a Weyl sequence for H. □

If the operator A has the form of a Schrödinger operator on L^2, we can strengthen the Weyl theorem by showing that it is enough to consider Weyl sequences whose support moves off to infinity.

Definition 7.12 $\{\psi_n\} \subset L^2(\mathbb{R}^d)$ *is a* spreading sequence *for A and λ if*

1. $\|\psi_n\| = 1$ *for all* n
2. *for any bounded set* $B \subset \mathbb{R}^d$, $supp(\psi_n) \cap B = \emptyset$ *for* n *sufficiently large*
3. $\|(A - \lambda)\psi_n\| \to 0$ *as* $n \to \infty$.

Problem 7.13 Show that a spreading sequence for A, λ is also a Weyl sequence for A, λ.

Theorem 7.14 *If* $H = -\Delta + V$ *is a self-adjoint Schrödinger operator, then*

$$\sigma_c(H) = \{\lambda \mid \text{ there is a spreading sequence for } A \text{ and } \lambda\}.$$

We skip the proof of this theorem (see [HS]).

7.2 Applications to Schrödinger operators

In this section we address two central issues. Firstly, we want to know for which potentials, V, we can conclude that the Schrödinger operator $H = -\frac{\hbar^2}{2m}\Delta + V$ is self-adjoint. As we saw in Chapter 3, only when H is self-adjoint do we know that the quantum dynamics exist. Secondly, we wish to describe the spectrum of H. As we shall see in the next section, knowledge of $\sigma(H)$ gives us important information about the nature of the solutions of Schrödinger's equation (and hence, about the evolution of physical states).

Our fist result covers *confining* potentials - that is, potentials which increase to infinity with x.

Theorem 7.15 *Let* $V(x) \geq 0$ *and* $V(x) \to \infty$ *as* $|x| \to \infty$. *Then*

1. $H = -\Delta + V$ *is self-adjoint on* $L^2(\mathbb{R}^3)$
2. $\sigma(H)$ *consists of isolated eigenvalues* $\{\lambda_n\}_1^\infty$ *with* $\lambda_n \to \infty$ *as* $n \to \infty$.

Proof: The proof of self-adjointness is fairly technical, and can be found in [HS], for example. To prove the second part, suppose λ is in the continuous spectrum of H, and let $\{\psi_n\}$ be a corresponding spreading sequence. Then

$$0 \leftarrow \langle \psi_n, (H - \lambda)\psi_n \rangle = \langle \psi_n, -\Delta\psi_n \rangle + \langle \psi_n, V\psi_n \rangle - \lambda$$

$$= \int |\nabla\psi_n|^2 + \int V|\psi_n|^2 - \lambda \geq \inf_{y \in \text{supp}(\psi_n)} V(y) - \lambda \to \infty$$

(because $\{\psi_n\}$ is spreading), which is a contradiction. Thus the continuous spectrum is empty. Further, there must be eigenvalues tending to $+\infty$ or else H would be bounded from above (we clearly have $H \geq 0$, and operators with bounded spectrum are bounded). It is easy to show that H is not bounded. $\square$

Our next theorem covers the case when the potential tends to zero at infinity.

Theorem 7.16 *Let V be continuous, with $V(x) \to 0$ as $|x| \to \infty$. Then*

1. *$H = -\Delta + V$ is self-adjoint*
2. *$\sigma_c(H) = [0, \infty)$ (so H can have only negative isolated eigenvalues, possibly accumulating at 0).*

Proof: Again, for a proof self-adjointness, we refer the reader to [HS], for example. We prove the second part. We have, by the triangle inequality,

$$\|(H-\lambda)\psi_n\| - \|V\psi_n\| \leq \|(-\Delta-\lambda)\psi_n\| \leq \|(H-\lambda)\psi_n\| + \|V\psi_n\|.$$

Suppose $\{\psi_n\}$ is a spreading sequence. Then the term $\|V\psi_n\|$ goes to zero as $n \to \infty$ because V goes to zero at infinity and $\{\psi_n\}$ is spreading. So λ is in the continuous spectrum of H iff $\lambda \in$ contspec $(-\Delta)$. We have (see problem 7.9) contspec$(-\Delta) = [0, \infty)$. $\square$

We conclude this section with a characterization of the continuous spectrum of a Schrödinger operator in a manner similar to the characterization of the point spectrum as a set of eigenvalues.

Theorem 7.17 (Schnol-Simon) *For a Schrödinger operator, H, with bounded potential,*

$$\sigma(H) = \textit{ closure } \{\lambda \mid (H-\lambda)\psi = 0 \textit{ for } \psi \textit{ polynomially bounded }\}.$$

So we see that the continuous spectrum also arises from solutions of the eigenvalue equation, but these solutions may not live in the space $L^2(\mathbb{R}^3)$.

Proof: We prove only that r.h.s $\subset$ l.h.s., and refer the reader to [?] for a complete proof. Let ψ be a polynomially bounded solution of $(H-\lambda)\psi = 0$. Let C_r be the box of side-length $2r$ centred at the origin. Let j_r have support in C_{r+1} with $j_r \equiv 1$ on C_r, $0 \leq j_r \leq 1$, and $\sup_{r,x} |\partial_x^\alpha j_r(x)| < \infty$. Our candidate for a Weyl sequence is

$$w_r \equiv \frac{j_r\psi}{\|j_r\psi\|}.$$

Note that $\|w_r\| = 1$ and if $\psi \notin L^2$, then (since $\|j_r\psi\| \to \infty$)

$$\int_{|x|<R} |w_r|^2 \to 0$$

as $r \to \infty$ for all R. We show that

$$(H - \lambda)w_r \to 0.$$

Let $F(r) = \int_{C_r} |\psi|^2$, monotonically increasing. We claim there is a subsequence $\{r_n\}$ such that

$$\frac{F(r_n + 2)}{F(r_n - 1)} \to 1.$$

If not, then there is $a > 1$ and $r_0 > 0$ such that

$$F(r + 3) \geq aF(r)$$

for all $r \geq r_0$. Thus $F(r_0 + 3k) \geq a^k F(r_0)$ and so $F(r) \geq \text{const } b^r$ with $b = a^{1/3} > 1$. But $F(r) \leq Cr^N$ for some N (by assumption), a contradiction. Now,

$$(H - \lambda)j_r\psi = j_r(H - \lambda)\psi + [-\Delta, j_r]\psi$$

$$= (-\Delta j_r)\psi - 2\nabla j_r \cdot \nabla\psi.$$

Since $\|\nabla^n j_r\|_\infty$ is uniformly bounded,

$$\|(H - \lambda)j_r\psi\| \leq C \int_{C_{r+1} - C_r} (|\psi|^2 + |\nabla\psi|^2) \leq C \int_{C_{r+1} - C_r} |\psi|^2.$$

So

$$\|(H - \lambda)w_r\| \leq C\frac{F(r + 2) - F(r - 1)}{F(r)}$$

$$\leq C(\frac{F(r + 2)}{F(r - 1)} - 1)$$

and so $\|(H - \lambda)w_{r_n}\| \to 0$. $\square$

7.3 Spectrum and evolution

In this section we explain how the spectrum of a Schrödinger operator gives us useful information about the solutions of the Schrödinger equation. We begin with some simple notions.

Definition 7.18 *A subspace $W \subset L^2$ is* invariant *under an operator A if $Aw \in W$ whenever $w \in W$.*

Problem 7.19 Show that

1. The span of the eigenfunctions of A is invariant under A
2. For A symmetric, if W is invariant under A, then so is

$$W^\perp \equiv \{\psi \in L^2 \mid \langle \psi, w \rangle = 0 \ \ \forall w \in W\}$$

If we restrict a self-adjoint operator A to the invariant subspace orthogonal to the span of all its eigenfunctions, the Weyl theorem (plus some abstract spectral theory) imply that

$$A|_{\{\text{span of eigenfunctions of A}\}^\perp}$$

has a purely continuous spectrum.

Now we will see how the spectrum of a Schrödinger operator, H, gives us a space-time characterization of the quantum mechanical evolution, $\psi = e^{-iHt/\hbar}\psi_0$. We assume all functions below are normalized.

Suppose first that $\psi_0 \in \{$ span of eigenfunctions of $H\}$. Then for any $\epsilon > 0$, there is an R such that

$$\inf_t \int_{|x| \le R} |\psi|^2 \ge 1 - \epsilon.$$

To see this, note that if $H\psi_0 = \lambda\psi_0$, then $e^{-\frac{iHt}{\hbar}}\psi_0 = e^{-\frac{i\lambda t}{\hbar}}\psi_0$, and so

$$\int_{|x| \ge R} |\psi|^2 = \int_{|x| \ge R} |\psi_0|^2 \to 0$$

as $R \to \infty$. Such a ψ is called a *bound state*, as it remains essentially localized in space for all time. On the other hand, if

$$\psi_0 \in \{\text{span of eigenfunctions of } H\}^\perp$$

then for all R,

$$\int_{|x|\leq R} |\psi|^2 \to 0$$

as $t \to \infty$. Strictly speaking, this convergence is in the sense of *ergodic mean*: $f(t) \to 0$ in ergodic mean as $t \to \infty$ means

$$\frac{1}{T}\int_0^T f(t)dt \to 0$$

as $T \to \infty$. This result is called the *Ruelle theorem* (see, eg, [CFKS] for a proof). Such a state, ψ, is called a *scattering state*, as it eventually leaves any fixed ball in space.

We conclude that the classification of the spectrum into point and continuous parts corresponds to a classification of the dynamics into localized (bound) states and locally-decaying (scattering) states.

Chapter 8

Special cases

In this chapter we will solve the Schrödinger eigenvalue equation in a few special cases (ie, for a few particular potentials), which not only illustrate some of the general arguments presented above, but, in fact, form a basis for our intuition about quantum behaviour.

8.1 The infinite well

Let W be the box $[0, L]^3 \subset \mathbb{R}^3$. We take

$$V(x) = \begin{cases} 0 & x \in W \\ \infty & x \notin W \end{cases}$$

as our potential. This means that we impose Dirichlet boundary conditions

$$\psi|_{\partial W} = 0 \tag{8.1}$$

on the wave function. It is a simple matter to solve the eigenvalue equation

$$-\frac{\hbar^2}{2m}\Delta\psi = E\psi \tag{8.2}$$

in W with the boundary condition (8.1), using the method of separation of variables. Doing so, we obtain eigenvalues (energy levels)

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}\sum_{j=1}^{3} n_j^2$$

with corresponding eigenfunctions (bound states)

$$\psi_n = \prod_{j=1}^{3} \sin(\frac{\pi n_j x_j}{L})$$

for each integer triple $n = (n_1, n_2, n_3)$, $n_j \geq 1$. We see that the eigenvalue E_n appears with degeneracy equal to $|\{\{m_j\}| \sum m_j^2 = \sum n_j^2\}|$. We remark that the ground-state (lowest) energy $E_{(1,1,1)}$ is non-degenerate.

Problem 8.1 Determine the spectra of the operators x and p on the space $L^2(W)$ (with zero boundary conditions).

8.2 The torus

Now we consider a particle on a torus $T = \mathbb{R}^3/\mathbb{Z}^3$. This corresponds to taking $V \equiv 0$ in the cube W, but this time with periodic boundary conditions. That is, we solve the eigenvalue equation (8.2) with boundary conditions

$$\psi(x)|_{x_j=0} = \psi(x)|_{x_j=L}$$

$$\partial\psi/\partial x_k|_{x_j=0} = \partial\psi/\partial x_k|_{x_j=L}$$

for all j, k. This leads to (separation of variables again) eigenfunctions

$$\psi_n(x) = \prod_{j=1}^{3} \left\{ \begin{array}{c} \sin(\frac{2\pi n_j x_j}{L}) \\ \cos(\frac{2\pi n_j x_j}{L}) \end{array} \right\}$$

with eigenvalues

$$E_n = \frac{2\pi^2\hbar^2}{mL^2} \sum_{1}^{3} n_j^2$$

(greater spacing than for the infinite well, but with higher degeneracy).

Problem 8.2 Determine the spectra of the operators x and p for this space (ie, $L^2(W)$ with periodic boundary conditions).

8.3 A potential step

Here we take the one-dimensional potential

$$V(x) = \begin{cases} V_0 > 0 & x > 0 \\ 0 & x \leq 0. \end{cases}$$

Solving the eigenvalue problem separately in the two different regions gives us a general solution of the form

$$\psi = \begin{cases} Ae^{ik_0 x} + Be^{-ik_0 x} & x < 0 \quad (\frac{\hbar^2 k_0^2}{2m} = E) \\ Ce^{ik_1 x} + De^{-ik_1 x} & x > 0 \quad (\frac{\hbar^2 k_1^2}{2m} = E - V_0) \end{cases}.$$

There are no bound states, but we can say something about the scattering states. Suppose $E < V_0$, and take $k_1 = iK$ where $K = \sqrt{(2m/\hbar^2)(V_0 - E)} > 0$. Then for a bounded solution, we require $D = 0$. Imposing the condition that ψ be C^1 at 0, that is

$$\psi|_{0-} = \psi|_{0+} \qquad \partial\psi/\partial x|_{0-} = \partial\psi/\partial x|_{0+}$$

leads to the equations

$$A + B = C \qquad ik_0(A - B) = -KC$$

After manipulations, we find that

$$R \equiv \frac{B}{A} = \frac{k_0 - iK}{k_0 + iK}$$

(R is called the *reflection coefficient*), or, making the dependence on the energy E explicit,

$$R(E) = \frac{\sqrt{E} - i\sqrt{V_0 - E}}{\sqrt{E} + i\sqrt{V_0 - E}}.$$

Similarly, if $E > V_0$, we obtain

$$R(E) = \frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}.$$

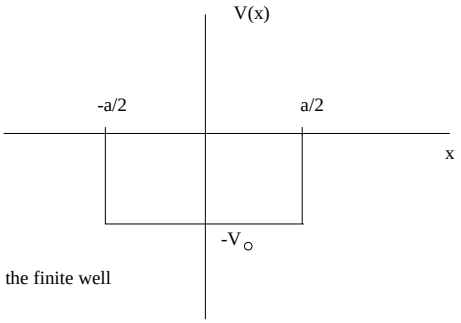
In particular, if $E - V_0 << 1$, then

$$R(E) \approx 1 - 2\sqrt{\frac{E - V_0}{E}}$$

and almost all of the wave is reflected. This is in spite of the fact that the energy of the particle is above the barrier. In classical mechanics, the particle would not feel the barrier at all.

8.4 The square well

Now we consider a potential well of finite depth V_0, and width a (see figure 8.3).



(8.3)

The determination of the point and continuous spectra is straightforward, and is left as an exercise.

Problem 8.3 Show

1. $\sigma_c(H) = [0, \infty)$
2. $\sigma_p(H) \subset (-V_0, 0)$
3. the equations for the eigenvalues are $(-V_0 \leq E \leq 0)$

$$k \tan(ak/2) = K \qquad k \cot(ak/2) = -K$$

where

$$K = \sqrt{-\frac{2mE}{\hbar^2}} \qquad k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

We now study the scattering states in more detail. If for $E \geq 0$ we write ψ in the form

$$\psi_{\text{inc}} = Ae^{-ik\cdot x/\hbar} \qquad x < -a/2$$

and

$$\psi_{\text{trans}} = AT(E)e^{-ik(x-a)/\hbar} \qquad x > a/2$$

($T(E)$ is the *transmission coefficient*) then

$$T(E) = \cos(\bar{k}a/\hbar) - i\frac{k}{\bar{k}}\sin(\bar{k}a/\hbar)$$

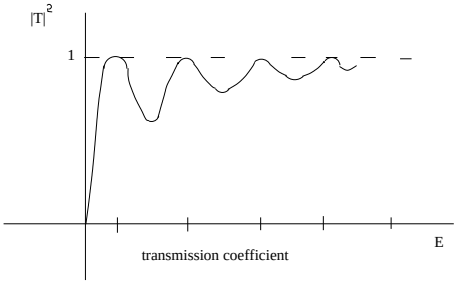
where

$$\bar{k} = \sqrt{2m(E - V_0)} \text{ and } \qquad k = \sqrt{2mE}.$$

This implies

$$|T(E)|^2 = \cos^2(\bar{k}a/\hbar) + \frac{E}{V_0 + E}\sin^2(\bar{k}a/\hbar)$$

which is sketched in figure 8.4.



(8.4)

We see that at the energies satisfying $\sin(\frac{\bar{k}a}{\hbar}) = 0$, i.e.

$$E = -V_0 + \frac{n^2\pi^2\hbar^2}{2ma} > 0, \qquad n = 1, 3, \ldots$$

$|T(E)|^2$ has maxima ($|T(E)|^2 = 1$) which are called *resonances*. The corresponding values of E are the *resonance energies*. We remark that for large n these are approximately equal to the energy levels of the infinite well of the same width.

8.5 The harmonic oscillator

The *harmonic oscillator* Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\omega^2|x|^2.$$

We will solve the eigenvalue problem explicitly for this operator. For simplicity, we consider the one-dimensional case. First, to remove all the constants we rescale: $x \mapsto \lambda x$ so that $p \mapsto \frac{1}{\lambda}p$ where $p = -i\hbar(d/dx)$. Setting $\lambda = \sqrt{\frac{\hbar}{m\omega}}$ gives $H \mapsto \hbar\omega H^{new}$ where

$$H^{new} = \frac{1}{2}((p^{new})^2 + x^2)$$

with $p^{new} = -i(d/dx)$. We introduce the *creation* and *annihilation* operators

$$a^* = \frac{1}{\sqrt{2}}(x - ip^{new})$$

$$a = \frac{1}{\sqrt{2}}(x + ip^{new}).$$

The commutation relation

$$[a, a^*] = 1 \tag{8.5}$$

is easily verified. We can rewrite H in terms of a and a^* as follows:

$$H^{new} = a^*a + \frac{1}{2}.$$

We say that this expression is in *normal form* as the a^* appears to the left of a. We introduce the *particle number* operator

$$N = a^*a$$

which satisfies the relations

$$Na = a(N - 1) \tag{8.6}$$

$$Na^* = a^*(N + 1) \tag{8.7}$$

(use (8.5) to see these). Clearly,

$$H^{new} = N + \frac{1}{2}.$$

Theorem 8.4 *We have*

1. $N \geq 0$
2. $\sigma(N) = \mathbb{Z}^+$ *(the non-negative integers), each eigenvalue having multiplicity* 1.

Proof:

1. This is easy, because a^* is the adjoint of a, so

$$< \psi, N\psi >= \|a\psi\|^2 \geq 0.$$

2. By the above, $N\psi = 0$ iff $a\psi = 0$. Note that the function

$$\psi_0 = ce^{-x^2/2}$$

(c a constant) is the unique family of solutions of

$$a\psi = (x + d/dx)\psi = 0$$

and hence of $N\psi = 0$. Thus ψ_0 (normalized by setting $c = (2\pi)^{-1/4}$) is the ground state. Now, the commutation relation (8.7) implies

$$Na^*\psi_0 = a^*\psi_0$$

and in general

$$N(a^*)^n\psi_0 = n(a^*)^n\psi_0.$$

Thus

$$\phi_n = (a^*)^n\psi_0$$

is an eigenfunction of N with eigenvalue n.

Problem 8.5 Show that $\|\phi_n\|^2 = n!$. Hint: write $\|\phi_n\|^2 =< \psi_0, a^n(a^*)^n\psi_0 >$, then push the a's through the a^*'s (including the necessary commutators) until they hit ψ_0 and annihilate it.

So

$$\psi_n = \frac{1}{\sqrt{n!}}(a^*)^n\psi_0$$

is a normalized eigenfunction of N with eigenvalue n. We now show that these are the only eigenfunctions. It follows from the commutation relations that if ψ is any eigenfunction of N with eigenvalue $\lambda > 0$, then

$$Na^m\psi = (\lambda - m)a^m\psi. \tag{8.8}$$

If we choose m so that $\lambda - m < 0$ we contradict $N \geq 0$ unless $a^m\psi = 0$. But this implies

$$a^j\psi = c\psi_0$$

for some integer j (c a constant), so by (8.8), $\lambda = j$. Applying now $(a^*)^j$ to this equation, and using the commutation relations, we can show $\psi = c\psi_j$ (c another constant). So we are done. □

Corollary 8.6

$$\sigma(H^{new}) = \{n + 1/2 \mid n = 0, 1, 2, \ldots\}$$

with eigenfunctions $\psi_n = (1/\sqrt{n!})(a^*)^n\psi_0$.

Finally, then, the spectrum of the original harmonic oscillator Hamiltonian is

$$\sigma(H) = \{\hbar\omega(n + 1/2) \mid n = 0, 1, 2, \ldots\}$$

with eigenfunctions obtained by rescaling the ψ_n's.

8.6 The Hydrogen atom

A hydrogen atom consists of a proton and an electron, interacting via a Coulomb force law. We will first make the simplifying assumption that the nucleus (the proton) is infinitely heavy, and so does not move. Thus we have the electron moving under the influence of the external potential $V(x) = -e^2/|x|$, where e is the charge of the proton, and $-e$ that of the electron. The appropriate Schrödinger operator is therefore

$$H = -\frac{\hbar^2}{2m}\Delta - e^2/|x|$$

acting on the Hilbert space $L^2(\mathbb{R}^3)$. In Chapter 9 we will see how to reduce the problem of the more realistic Hydrogen atom - when the nucleus has a finite mass (a two-body problem) - to the problem studied here.

As usual, we want to study the spectrum of H. The first step is to invoke theorem 7.16. However, the fact that our potential $V(x) = -e^2/|x|$ is singular at the origin is a possible obstacle. In fact, theorem 7.16 can be extended to cover this case (see, eg, [CFKS]), and we may conclude that H is self-adjoint, with continuous spectrum equal to the half-line $[0, \infty)$. Our goal, then, is to find the bound-states (eigenfunctions) and bound-state energies (eigenvalues). It is a remarkable fact that we can find these explicitly. Indeed, aside from the infinite well, the only multi-dimensional potentials for which the Schrödinger eigenvalue problem can be solved explicitly are the harmonic oscillator and the Coulomb potential.

Because the Coulomb potential is radially-symmetric (depends only on $r = |x|$), it is natural to work in spherical coordinates (r, θ, ϕ), where

$$x_1 = r\sin(\theta)\sin(\phi) \quad x_2 = r\sin(\theta)\cos(\phi) \quad x_3 = r\cos(\theta),$$

$0 \leq \theta < \pi$, $0 \leq \phi < 2\pi$. In spherical coordinates, the Laplacian becomes

$$\Delta = \Delta_r + \frac{1}{r^2}\Delta_\Omega$$

where

$$\Delta_r = \partial^2/\partial r^2 + \frac{2}{r}\partial/\partial_r$$

depends only on the radial variable, and

$$\Delta_\Omega = \frac{1}{\sin(\theta)}\partial/\partial\theta(\sin(\theta)\partial/\partial\theta) + \frac{1}{\sin^2(\theta)}\partial^2/\partial\phi^2$$

depends only on the "spherical" variables θ, ϕ.

The eigenfunctions of Δ_Ω are the well-known *spherical harmonics*, which take the form

$$Y_l^m(\theta, \phi) = c_{lm} P_l^{|m|}(\cos(\theta)) e^{im\phi} \tag{8.9}$$

where $l = 0, 1, \ldots$, $m = -l, -l+1, \ldots, l-1, l$, c_{lm} is a constant, and the *Legendre function* P_l^m can be written

$$P_l^m(u) = \frac{(1-u^2)^{m/2}}{2^l l!} d^{l+m}/du^{l+m}(u^2-1)^l. \tag{8.10}$$

In fact, we have

$$-\Delta_\Omega Y_l^m = l(l+1)Y_L^m. \tag{8.11}$$

Problem 8.7 Check (8.11) using (8.9) and (8.10) (a bit tedious).

It turns out that the spherical harmonics, Y_l^m, comprise an orthonormal basis of the Hilbert space $L^2(\mathbb{S}^2; d\Omega)$ of L^2 functions on the sphere $\mathbb{S}^2 = \{x \in \mathbb{R}^3 \mid |x| = 1\}$ with the measure $d\Omega = \sin^2(\theta) d\theta d\phi$ (see, eg, [LL]).

Before completing the solution of the eigenvalue problem for the hydrogen atom, we make a few remarks about the connection to angular momentum. The quantum-mechanical angular momentum $L = (L_1, L_2, L_3)$ is the self-adjoint (vector-valued) operator

$$L = x \times p$$

where $p = -i\hbar\nabla$ as usual. We define also the squared magnitude of the angular momentum, $L^2 = L_1^2 + L_2^2 + L_3^2$. The following facts are easily checked:

1. $L^2 = -\hbar^2\Delta_\Omega$ (hence $L^2 Y_l^m = \hbar^2 l(l+1)Y_l^m$)

2. $L_3 Y_l^m = \hbar m Y_l^m$.

Thus we see that the spherical harmonics are, in fact, simultaneous eigenfunctions of the angular momentum operators L_3 and L^2.

To complete the solution of the eigenvalue problem, we seek eigenfunctions of H in the separated-variables form

$$\psi(r, \theta, \phi) = R(r) Y_l^m(\theta, \phi).$$

Plugging this into the eigenvalue equation $H\psi = E\psi$, we obtain

$$(\frac{\hbar^2}{2m}[-\Delta_r + \frac{l(l+1)}{r^2}] - e^2/r)R = ER. \tag{8.12}$$

The solutions of the ODE (8.12) are well-studied (see, eg, [LL]). Without going into details, we remark that one can show (by power-series methods) that (8.12) has square-integrable solutions only for

$$n \equiv \frac{e^2}{\hbar}\sqrt{\frac{-m}{2E}} \in \{l+1, l+2, \ldots\}.$$

The corresponding eigenfunctions, R_{nl} are of the form

$$R_{nl}(r) = \rho^l e^{-\rho/2} F_{nl}(\rho)$$

where $\rho = \frac{2me^2}{n\hbar^2} r$, and F_{nl} is a polynomial.

In full, then, the solutions of the eigenvalue problem $H\psi = E\psi$ are

$$\psi(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$$

where

$$l = 0, 1, 2, \ldots \quad m = -l, -l+1, \ldots, l \quad n = l+1, l+2, \ldots$$

and

$$E(= E_n) = -(\frac{me^4}{2\hbar^2})\frac{1}{n^2}. \tag{8.13}$$

So we see that the Hydrogen atom has an infinite number of bound states below the continuous spectrum (which starts at zero), which accumulate at zero. The ground state energy, obtained for $l = m = 0, n = 1$, is $E_1 = -me^4/2\hbar^2$. An easy count finds the degeneracy of the energy level E_n to be

$$\sum_{l=0}^{n-1}(2l+1) = n^2.$$

Finally, we note that the expression (8.13) is in agreement with the empirical formula ("Balmer series")

$$\Delta E = R(\frac{1}{n_f^2} - \frac{1}{n_i^2})$$

($1 \leq n_f < n_i$ integers, R a constant) for differences ΔE in energy levels, which predates quantum mechanics, and was based on measurements of absorption and emission spectra.

8.7 A particle in an external EM field

Now we extend our quantization procedure to the case of a charged particle in an external electro-magnetic field. Of course, if the external field is purely electric, then it is a potential field, and fits within the framework we have considered already (as we saw in section 8.6).

Suppose, then, that a magnetic field B, and an electric field, E, are present (and are time-independent: $B, E : \mathbb{R}^3 \mapsto \mathbb{R}^3$). We know from the theory of electro-magnetism (Maxwell's equations) that these fields can be expressed in terms of the vector potential, $A : \mathbb{R}^3 \mapsto \mathbb{R}^3$, and the scalar potential, $\Phi : \mathbb{R}^3 \mapsto \mathbb{R}$ via

$$E = -\nabla\Phi \qquad B = curl A$$

(we are using units in which the speed of light, c, is equal to one).

According to our general quantization procedure, we write the classical Hamiltonian function for a particle of charge e subject to the fields E and B,

$$h(x,k) = \frac{1}{2m}(k - eA(x))^2 + e\Phi(x)$$

and then replace the canonical variables x and k with the quantum canonical operators x and p. The resulting Schrödinger operator is

$$H(A,\Phi) = \frac{1}{2m}(p - eA)^2 + e\Phi$$

acting on $L^2(\mathbb{R}^3)$. We remark that the self-adjointness of $H(A,\Phi)$ can be established by using *Kato's inequality* ([CFKS]).

An important feature of the operator $H(A,\Phi)$ is its *gauge invariance*. We recall that in the theory of electro-magnetism, the vector potential A is not uniquely

determined by the magnetic field B. In fact, if we add the gradient of any function χ to A (a *gauge transformation*), we obtain the same magnetic field B:

$$curl(A + \nabla\chi) = curl A = B.$$

Gauge invariance of the quantum Hamiltonian $H(A, \Phi)$ is reflected in the relation

$$H(A + \nabla\chi, \Phi) = e^{ie\chi} H(A, \Phi) e^{-ie\chi}. \tag{8.14}$$

Problem 8.8 Check that equation (8.14) holds.

Thus if A and $\tilde{A}$ differ by a gradient vector-field, then the operators $H(A, \Phi)$ and $H(\tilde{A}, \Phi)$ are unitarily equivalent via the unitary map

$$\psi \mapsto e^{ie\chi}\psi$$

on $L^2(\mathbb{R}^3)$. Thus the two Hamiltonians are physically equivalent. Of course, this is to be expected as A and $\tilde{A}$ correspond to the same magnetic field.

One can impose restrictions (called *gauge conditions*) on the vector potential A in order to remove some, or all, of the freedom involved in the choice of A. A common choice is $div A = 0$, known as the *Coulomb gauge*. By an appropriate gauge transformation, the Coulomb gauge can always be achieved.

We now consider an important special case - a constant magnetic field with no electric field present. A possible choice for A is

$$A(x) = \frac{1}{2} B \times x. \tag{8.15}$$

Another possibility, supposing B to be directed along the x_3 axis - $B = (0, 0, b)$ - is

$$A(x) = b(-x_2, 0, 0). \tag{8.16}$$

Problem 8.9 Check that both (8.15) and (8.16) yield the magnetic field B, and that the two are gauge-equivalent.

Using the second choice for A, the appropriate Schrödinger operator is

$$H(A) = \frac{1}{2m}[(p_1 + ebx_2)^2 + p_2^2 + p_3^2].$$

To analyze $H(A)$, we apply the Fourier transform to only the first and third variables ($x_{1,3} \mapsto k_{1,3}$). This results in the unitarily equivalent operator

$$\tilde{H} = \frac{1}{2m} p_2^2 + \frac{m\omega^2}{2}(x_2 + \frac{1}{eb} k_1)^2 + \frac{1}{2m} k_3^2$$

where $\omega = eb/m$ and k_1, k_3 act as multiplication operators. We remark that $\tilde{H}$ acts as a harmonic oscillator in the variable x_2, and as a multiplication operator in k_1 and k_3. In the following problem you are asked to determine the spectrum of this operator.

Problem 8.10

1. Show that the energy levels of $\tilde{H}$ (called *Landau levels*) are given by

$$(n + \frac{1}{2})\hbar\omega + \alpha^2/2m$$

where $n = 0, 1, 2, \ldots$ and $\alpha \in \mathbb{R}$. Show that the corresponding generalized eigenfunctions are

$$\psi_{n,\alpha}(k_1, x_2, k_3) = \phi_n(x_2 + k_1/eb)\delta(k_3 - \alpha)$$

where ϕ_n is the nth eigenfunction of the harmonic oscillator.

2. Analyze the same problem in two dimensions, with the magnetic field perpendicular to the plane.

Chapter 9

Many-particle systems

In this chapter we describe an extension of the concepts developed previously to many-particle systems. Specifically, we consider a physical system consisting of N particles of masses $m_1, \ldots, m_N$ which interact pairwise via the potentials $V_{ij}(x_i - x_j)$, where x_j is the position of the j-th particle. Examples of such systems include atoms or molecules - ie, a system consisting of electrons and nuclei interacting via Coulomb forces. We will write this example out explicitly later.

9.1 Quantization of a many-particle system

According to our general framework, we begin with the classical Hamiltonian formulation of this system. The appropriate phase-space is $\mathbb{R}^{3N}_x \times \mathbb{R}^{3N}_k$ where $x = (x_1, \ldots, x_N)$ are the particle coordinates, and $k = (k_1, \ldots, k_N)$ are the particle momenta. The Hamiltonian function is

$$H(x,k) = \sum_{j=1}^{N} \frac{1}{2m_j} k_j^2 + V(x)$$

where V is the total potential of the system, given in this case by

$$V(x) = \frac{1}{2} \sum_{i \neq j} V_{ij}(x_i - x_j).$$

The quantization proceeds in the standard way by replacing $\mathbb{R}^{3N}_x \times \mathbb{R}^{3N}_k$ with $L^2(\mathbb{R}^{3N}_x)$, x with the multiplication operator x, k with $p = -i\hbar\nabla_x$, and $H(x,k)$ with

the operator $H = H(x,p)$. Explicitly, the Schrödinger operator H is given by

$$H = \sum_1^N \frac{1}{2m_j} p_j^2 + V(x) \tag{9.1}$$

acting on $L^2(\mathbb{R}^{3N})$.

Example 9.1 Consider a molecule with N electrons of mass m and charge $-e$, and M nuclei of masses m_j and charges Z_j, $j = 1, \ldots, M$. In this case, the Schrödinger operator, H_{mol}, is

$$H_{mol} = \frac{1}{2m} \sum_1^N p_j^2 + \sum_1^M \frac{1}{2m_j} q_j^2 + V(x,y) \tag{9.2}$$

acting on $L^2(\mathbb{R}^{3(N+M)})$. Here $x = (x_1, \ldots, x_N)$ are the electron coordinates, $y = (y_1, \ldots y_M)$ are the nucleus coordinates, $p_j = -i\hbar\nabla_{x_j}$ is the momentum of the j-th electron, $q_j = -i\hbar\nabla_{y_j}$ is the momentum of the j-th nucleus, and

$$V(x,y) = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|} - \sum_{i,j} \frac{eZ_j}{|x_i - y_j|} + \frac{1}{2} \sum_{i \neq j} \frac{Z_i Z_j}{|y_i - y_j|}.$$

For a neutral molecule, we have

$$\sum_1^M Z_j = Ne.$$

If $M = 1$, the resulting system is called an atom, or Z-atom ($Z = Z_1$).

Since nuclei are much heavier than electrons, in the leading approximation one takes nuclei frozen at their positions, and considers, instead of (9.2), the Schrödinger operator

$$H_{BO} = \frac{1}{2m} \sum_1^N p_j^2 + V(x,y)$$

on $L^2(\mathbb{R}^{3N})$ with $y \in \mathbb{R}^{3M}$, the positions of the nuclei, playing the role of parameters. This is called the Born-Oppenheimer approximation. It plays a fundamental role in quantum chemistry, where most computations are done with the operator H_{BO}. The eigenvalues of the operator H_{BO} are functions of the coordinates, y, of the nuclei. Minimizing the lowest eigenvalue - the ground state energy - with respect to y gives the equilibrium positions of the nuclei, i.e. the shape of the molecule.

A spectral analysis of operator (9.1) is a more delicate problem than it is for one-particle operators. One adapts the tools we have seen so far to take into account the particle geometry. The resulting spectral analysis is described in [CFKS]. The main result, due to W. Hunziker, C. van Winter, and G.M. Zhislin (the *HWZ theorem*), gives a description of the spectra of many-particle Schrödinger operators, generalizing the results of Chapter 7. We will not go into the theory of many-body Schrödinger operators here. However, we will discuss two of its distinct features, which are not present in the one-body case.

9.2 Separation of the centre of mass motion

The Schrödinger operator (9.1) commutes with the operator of total translation of the system

$$\psi(x_1, \ldots, x_N) \mapsto \psi(x_1 + h, \ldots, x_N + h)$$

and one can show, therefore, that its spectrum is purely continuous. So in order to obtain interesting spectral information about our system, we have to remove this translational invariance ("break" it). One way of doing this is by fixing the centre of mass of the system at, say, the origin:

$$\sum_1^N m_j x_j = 0.$$

We will not describe a general mathematical procedure for fixing the centre of mass, but will show how to do it in the case of two particles, $N = 2$. In this case, we change the particle variables as follows:

$$x_1, x_2 \mapsto y = x_1 - x_2, z = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}. \tag{9.3}$$

Here y is the coordinate of the relative position of the two particles, and z is the coordinate of their centre of mass. Using this change of variables in the two-particle Schrödinger operator

$$H_2 = \frac{1}{2m_2} p_1^2 + \frac{1}{2m_2} p_2^2 + V(x_1 - x_2)$$

acting on $L^2(\mathbb{R}^6)$, we arrive easily at the operator

$$\tilde{H}_2 = \frac{1}{2\mu} p^2 + \frac{1}{2M} P^2 + V(y)$$

where $p = -i\hbar\nabla_y$, $P = -i\hbar\nabla_z$, $\mu = \frac{m_1 m_2}{m_1+m_2}$ (the *reduced mass*), and $M = m_1 + m_2$ (the total mass). In fact, it can be shown that H and $\tilde{H}$ are unitarily equivalent, with the equivalence given by a unitary realization of the change of coordinates (9.3).

The point now is that one can separate variables in the operator $\tilde{H}_2$. In formal language, this means that $\tilde{H}_2$ can be written in the form

$$\tilde{H}_2 = H \otimes \mathbf{1} + \mathbf{1} \otimes H_{CM}$$

on $L^2(\mathbb{R}^6) = L^2(\mathbb{R}_y{}^3) \otimes L^2(\mathbb{R}_z{}^3)$ where

$$H = \frac{1}{2\mu}p^2 + V(y)$$

acts on $L^2(\mathbb{R}_y{}^3)$, and

$$H_{CM} = \frac{1}{2M}P^2$$

acts on $L^2(\mathbb{R}_z{}^3)$. Clearly H and H_{CM} are the Schrödinger operators of the *relative motion* of the particles, and of their *center of mass motion* respectively. It is equally clear that of interest for us is H, and not H_{CM}. Note that H has the form of a one-particle Schrödinger operator with external potential $V(y)$. All the analysis we developed for such operators is applicable now to H.

9.3 Identical particles

Many-particle systems display a remarkable new feature of quantum physics. Unlike in classical physics, identical particles (i.e., particles with the same masses and charges, or, more generally, which interact in the same way) are indistinguishable in quantum physics. This means that all probability distributions which can be extracted from an N-particle wave function $\psi(x_1, \ldots, x_N)$, should be symmetric with respect to permutations of the coordinates of identical particles. This is equivalent to the property that $\psi(x_1, \ldots, x_N)$ is invariant under such a permutation modulo change of sign.

Assume for simplicity that all N particles are identical. Then the invariance property of $\psi(x_1, \ldots, x_N)$ formulated above means that $\psi(x_1, \ldots, x_N)$ belongs to a representation of the symmetric group S_N (the group of permutations of N indices) corresponding to a Young tableau with at most two columns. The shape of the Young tableau is determined by the *spin* of the particles involved. One-column Young tableaux - i.e. purely symmetric $\psi(x_1, \ldots, x_N)$ - correspond to particles with

integer spins, or *Bosons*, while two-column tableaux correspond to particles with half-integer spins, or *Fermions*. This relation between the symmetry properties of wave functions and the spin of particles, is known as the *relation between spin and statistics*. We will not go into this topic here, and refer the interested reader to any of the standard books on quantum mechanics given in the references.

Chapter 10

The Feynman path integral

In this chapter, we derive a convenient representation for the integral kernel of the Schrödinger evolution operator, $e^{-itH/\hbar}$. This is the "Feynman path integral." First, we need some mathematical tools.

10.1 Mathematical detour: the Trotter product formula

Let A, B, and $A+B$ be self-adjoint operators on a Hilbert space $\mathcal{H}$. If $[A,B] \neq 0$, then $e^{i(A+B)} \neq e^{iA}e^{iB}$ in general. But we do have the following.

Theorem 10.1 (Trotter product formula) *Let either A and B be bounded or A, B, and $A+B$ self-adjoint and bounded from below. Then for $Re(\lambda) \leq 0$,*

$$e^{\lambda(A+B)} = s - \lim_{n\to\infty} (e^{\lambda\frac{A}{n}} e^{\lambda\frac{B}{n}})^n$$

Remark 10.2 *The convergence here is in the sense of the* strong operator topology. *For operators A_n and A on a Hilbert space $\mathcal{H}$, $A_n \to A$ in the strong operator topology (written $s - \lim_{n\to\infty} A_n = A$) iff $\|A_n\psi - A\psi\| \to 0$ for all $\psi \in \mathcal{H}$. For bounded operators, we can take norm convergence. In the formula above we used a uniform decomposition of the interval $[0,1]$. The formula still holds for a non-uniform decomposition.*

Proof (for A,B bounded): We can take $\lambda = 1$. Let $S_n = e^{(A+B)/n}$ and $T_n = e^{A/n}e^{B/n}$. Now by telescoping,

$$S_n^n - T_n^n = S_n^n - T_n S_n^{n-1} + T_n S_n^{n-1} + \cdots - T_n^n$$

$$= \sum_{k=0}^{n-1} T_n^k (S_n - T_n) S_n^{n-k-1}$$

so

$$\|S_n^n - T_n^n\| \leq \sum_{k=0}^{n-1} \|T_n\|^k \|S_n - T_n\| \|S_n\|^{n-k-1}$$

$$\leq \sum_{k=0}^{n-1} (\max(\|T_n\|, \|S_n\|))^{n-1} \|S_n - T_n\|$$

$$\leq n e^{\|A\|+\|B\|} \|S_n - T_n\|.$$

Using a power series expansion, we see $\|S_n - T_n\| = O(1/n^2)$ and so $\|S_n^n - T_n^n\| \to 0$ as $n \to \infty$. □

10.2 Mathematical detour: integral operators

We consider integral operators, $\mathcal{K}$, on a function space:

$$(\mathcal{K}\psi)(x) = \int K(x,y)\psi(y)dy$$

($K(x,y)$ is the *kernel* of the operator). Examples include

1. $\mathcal{K} = g(-i\nabla)$ for which the kernel is

$$K(x,y) = (2\pi)^{-d/2} \check{g}(x-y) \tag{10.1}$$

2. $K = V$ (multiplication operator) for which the kernel is

$$K(x,y) = V(x)\delta(x-y).$$

Proposition 10.3 *If $\mathcal{K}_1$ and $\mathcal{K}_2$ are integral operators (with kernels K_1 and K_2), then the integral kernel of $\mathcal{K} \equiv \mathcal{K}_1\mathcal{K}_2$ is*

$$K(x,y) = \int K_1(x,z)K_2(z,y)dz.$$

Problem 10.4 Prove this.

Remark 10.5 *If $\mathcal{K}$ is an integral operator with kernel satisfying*

$$\int |K(x,x)|dx < \infty,$$

then the trace *of $\mathcal{K}$ is*

$$tr\ K = \int K(x,x)dx.$$

10.3 The Feynman path integral

Recall that the solution to the Schrödinger equation

$$i\hbar\partial\psi/\partial t = H\psi$$

with the initial condition

$$\psi|_{t=0} = \psi_0$$

is given in terms of the evolution operator $U(t) \equiv e^{-iHt/\hbar}$ as

$$\psi = U(t)\psi_0.$$

Here H is a self-adjoint Schrödinger operator, say

$$H = -\frac{\hbar^2}{2m}\Delta + V(x).$$

Our goal in this section is to understand the evolution operator $U(t) = e^{-\frac{iHt}{\hbar}}$ by finding a convenient representation of its integral kernel. We denote the integral kernel of $U(t)$ by $U_t(y,x)$ (also called the *propagator* from x to y).

Using the Trotter product formula, we have

$$e^{-\frac{iHt}{\hbar}} = e^{i(\frac{\hbar^2}{2m}\Delta t - Vt)/\hbar} = s - \lim_{n\to\infty} K_n^n$$

where $K_n \equiv e^{\frac{i\hbar t}{2mn}\Delta}e^{-\frac{iVt}{\hbar n}}$. So

$$U_t(y,x) = \lim_{n\to\infty}\int\cdots\int K_n(y,x_{n-1})\cdots K_n(x_2,x_1)K_n(x_1,x)dx_{n-1}\cdots dx_1. \quad (10.2)$$

Now,

$$K_n(y,x) = e^{\frac{i\hbar t\Delta}{2mn}}(y,x)e^{-\frac{iV(y)t}{\hbar n}}$$

as V, and hence $e^{-iVt/n\hbar}$ is a multiplication operator (check this).

Lemma 10.6 *For $Re(a) \geq 0$,*

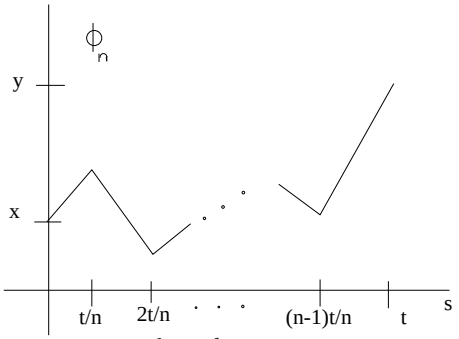
$$e^{\frac{1}{2a}\Delta}(x,y) = (\frac{2\pi}{a})^{-d/2} e^{-\frac{a}{2}|x-y|^2}.$$

Proof: For $Re(a) > 0$, problem 4.1 shows that the FT (with $\hbar = 1$) of $a^{d/2}e^{-\frac{a}{2}|x|^2}$ is $e^{-\frac{1}{2a}|k|^2}$, and the result follows from (10.1). In fact, this FT equality is valid for $Rea = 0$ as well (in a distributional sense). $\square$

Now setting $a = \frac{mn}{i\hbar t}$ and plugging into (10.2) gives us

$$U_t(y,x) = \lim_{n\to\infty} \int \cdots \int e^{iS_n/\hbar} (\frac{2\pi i\hbar t}{mn})^{-nd/2} dx_1 \cdots dx_{n-1}$$

where $S_n = \sum_{k=0}^{n-1} (mn|x_{k+1} - x_k|^2/2t - V(x_{k+1})t/n)$ with $x_0 = x$, $x_n = y$. Define the piecewise linear function ϕ_n such that $\phi_n(0) = x$, $\phi_n(t/n) = x_1$, $\cdots$, $\phi_n(t) = y$ (see figure 10.3).



piecewise linear function (10.3)

Then

$$S_n = \sum_{k=0}^{n-1} \{m\frac{|\phi_n((k+1)t/n) - \phi_n(kt/n)|^2}{2(t/n)^2} - V(\phi((k+1)t/n))\}t/n.$$

Now, S_n is a Riemann sum for the classical action

$$S(\phi,t) = \int_0^t \{\frac{m}{2}\dot{\phi}(s)^2 - V(\phi)\}ds$$

of the path ϕ_n. So we have shown

$$U_t(y,x) = \lim_{n\to\infty} \int_{P^n_{x,y,t}} e^{iS(\phi_n)/\hbar} D\phi_n \tag{10.4}$$

where $P^n_{x,y,t}$ is the $(n-1)$-dimensional space of paths ϕ_n with $\phi_n(0) = x$, $\phi_n(t) = y$, and which are linear on $(kt/n, (k+1)t/n)$ for $k = 0, 1, \ldots, n-1$, and $D\phi_n = (\frac{2\pi i\hbar t}{nm})^{-nd/2} d\phi_n(t/n) \cdots d\phi_n((n-1)t/n)$.

Heuristically, as $n \to \infty$, ϕ_n approaches a path from x to y (in time t). Thus we write

$$\boxed{U_t(y,x) = \int_{P_{x,y,t}} e^{iS(\phi,t)/\hbar} D\phi.} \tag{10.5}$$

Here $P_{x,y,t}$ is the space of paths from x to y defined as

$$P_{x,y,t} = \{\phi : [0,t] \to \mathbb{R}^d | \int_0^t |\dot{\phi}|^2 < \infty, \quad \phi(0) = x, \quad \phi(t) = y\}.$$

This is the *Feynman path integral.* It is not really an integral, but a formal expression whose meaning is given by (10.4). Useful results are obtained non-rigorously by treating it formally as an integral. Answers we get this way are intelligent guesses which must be justified by rigorous tools.

Note that $P^n_{x,y,t}$ is an $(n-1)$-dimensional subspace of the ∞-dimensional space $P_{x,y,t}$. It satisfies $P^n_{x,y,t} \subset P^{2n}_{x,y,t}$ and (in some sense) $\lim_{n\to\infty} P^n_{x,y,t} = P_{x,y,t}$. We call such subspaces *finite dimensional approximations* of $P_{x,y,t}$.

In (non-rigorous) computations, it is often useful to use finite-dimensional approximations to the path space other than the polygonal one above.

We can construct more general finite-dimensional approximations as follows. Pick a fixed function $\phi_{xy} \in P_{x,y,t}$. Then

$$P_{x,y,t} = \phi_{xy} + P_{0,0,t}.$$

Note $P_{0,0,t}$ is a Hilbert space. Choose an orthonormal basis $\{\xi_j\}$ in $P_{0,0,t}$ and define

$$P^n_{0,0,t} = \text{ span } \{\xi_j\}_1^n$$

and

$$P^n_{x,y,t} = \phi_{xy} + P^n_{0,0,t}.$$

Then $P^n_{x,y,t}$ is a finite dimensional approximation of $P_{x,y,t}$. Typical choices of ϕ_{xy} and $\{\xi_j\}$ are

1. ϕ_{xy} is piecewise linear and $\{\xi_j\}$ are splines. This gives the polygonal approximation introduced above.

2. ϕ_{xy} is a classical path (a critical point of the action functional $S(\phi)$) and $\{\xi_j\}$ are eigenfunctions of the Hessian of S at ϕ_{xy} (see the next section). In this case, if $\eta \in P^n_{0,0,t}$, then

$$D\eta = (\frac{2\pi it\hbar}{m})^{-d/2}(\frac{2\pi n}{t}\sqrt{\frac{m}{\hbar}})^n \prod_{j=1}^{n} da_j$$

where

$$\eta = \sum_{j=1}^{n} a_j \xi_j.$$

It is reasonable to expect that if

$$\lim_{n\to\infty} \int_{P^n_{x,y,t}} e^{iS(\phi,t)/\hbar} D\phi$$

exists, then it is independent of the finite-dimensional approximation, $P^n_{x,y,t}$, that we choose.

Problem 10.7

1. Compute (using (10.5) and a finite-dimensional approximation of the path space) U_t for

   (a) $V(x) = 0$ (free particle)

   (b) $V(x) = \frac{m\omega^2}{2}x^2$ (harmonic oscillator).

2. Derive a path integral representation for the integral kernel of $e^{-\frac{\beta H}{\hbar}}$.

3. Use this to find a path integral representation for $Z(\beta) \equiv \text{tr } e^{-\frac{\beta H}{\hbar}}$ (you should get the expression (13.9)).

10.4 Generalizations of the path integral

Here we mention briefly two extensions of the Feynman path integral we have just introduced.

1. Phase-space path integral:

$$U_t(y,x) = \int_{P_{x,y,t}\times \text{ anything}} e^{i\int_0^t (\dot\phi\pi - H(\phi,\pi))/\hbar} D\phi \not{D}\pi$$

where $\not{D}\pi$ is the *path measure*, normalized as

$$\int e^{-\frac{i}{2}\int_0^t \|\pi\|^2} \not{D}\pi = 1$$

(recall in QM $\not{d}^3 p = d^3p/(2\pi)^{3/2}$). To derive this representation, we use the Trotter product formula, the expression $e^{i\epsilon H} \approx 1 + i\epsilon H$ for ϵ small, and the symbolic (pseudo-differential) composition formula. Unlike the representation $\int e^{i\int_0^t S} D\phi$, this formula holds also for more complicated H, which are not quadratic in p!

2. A particle in a vector potential $A(x)$. In this case, the Hamiltonian is

$$H(x,p) = \frac{1}{2m}(p - eA(x))^2 + V(x)$$

and the Lagrangian is

$$L(x,\dot x) = \frac{m}{2}\dot x^2 - V(x) + e\dot x \cdot A(x).$$

The propagator still has the representation

$$U_t(y,x) = \int_{P_{x,y,t}} e^{iS(\phi)/\hbar} D\phi,$$

but with

$$S(\phi) = \int_0^t L(\phi,\dot\phi)ds = \int_0^t (\frac{m}{2}\dot\phi^2 - V(\phi))ds + e\int_0^t A(\phi)\cdot\dot\phi ds.$$

Since, in general, $A(x)$ does not commute with ∇, care should be exercised in computing a finite-dimensional approximation: one should take

$$\sum A(\frac{1}{2}(x_i + x_{i+1}))\cdot(x_{i+1} - x_i)$$

or

$$\sum \frac{1}{2}(A(x_i) + A(x_{i+1}))\cdot(x_{i+1} - x_i)$$

and not

$$\sum A(x_i)\cdot(x_{i+1} - x_i) \text{ or } \sum A(x_{i+1})\cdot(x_{i+1} - x_i).$$

Chapter 11

Mathematical detour: the calculus of variations

The calculus of variations, an extensive mathematical theory in its own right, plays a fundamental role throughout physics. This chapter contains an overview of some of the basic aspects of the variational calculus. We will use this material in Chapters 13 and 14, in conjunction with the path integral introduced in the previous chapter, to obtain useful quantitative results about quantum systems.

11.1 Functionals

The basic objects of study in the calculus of variations are *functionals*, which are just functions defined on function spaces. That is, we specify a space, X, of functions, and the *functionals* are just maps $S : X \to \mathbb{R}$.

Example 11.1 Here are some common examples of functionals, S, and the spaces X on which they are defined.

1. $X = L^2([a,b];\mathbb{R})$, $f \in X$ is fixed, and
$$S : \phi \mapsto \int_a^b f\phi.$$
2. Evaluation functional: $X = C([a,b])$, $x_0 \in [a,b]$ fixed, and
$$S : \phi \mapsto \phi(x_0)$$

(we can actually think of this as a special case of example 1 with $f(x) = \delta(x - x_0)$).

3. $X = \{\phi : \mathbb{R}^d \to \mathbb{R}^m | V(\phi) \in L^1(\mathbb{R}^d)\}$, $V : \mathbb{R}^m \to \mathbb{R}$, and
$$S : \phi \mapsto \int_{\mathbb{R}^d} V(\phi).$$

4. Dirichlet functional: $X = H^1(\mathbb{R}^d) \equiv \{\phi \in L^2(\mathbb{R}^d) \mid \nabla\phi \in L^2\}$, and
$$S : \phi \mapsto \frac{1}{2}\int_{\mathbb{R}^d} |\nabla\phi|^2.$$

5. Classical action: $X = \{\phi \in C^1([0,T];\mathbb{R}^m) \mid \phi(0) = a, \phi(T) = b\}$, and
$$S : \phi \mapsto \int_0^T \{\frac{1}{2}m|\dot{\phi}|^2 - V(\phi)\}.$$

6. Classical action: X as in the previous example, and
$$S : \phi \mapsto \int_0^T L(\phi, \dot{\phi})dt$$
(here $L : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ is the *Lagrangian*).

7. Action of a classical field theory: $X = \{\phi \in H^1(\mathbb{R}^d \times [0,T];\mathbb{R}^m) \mid \phi(x,0) = f(x), \phi(x,T) = g(x)\}$
$$S : \phi \mapsto \int_0^T \int_{\mathbb{R}^d} \{-\frac{1}{2}|\dot{\phi}|^2 + \frac{1}{2}|\nabla_x\phi|^2 + V(\phi)\}.$$

8. Quadratic form: $X = D(B)$, B a self-adjoint operator, and
$$S : \phi \mapsto \frac{1}{2}\langle\phi, B\phi\rangle. \tag{11.1}$$

9. Action of an EM field: $X = \{A \in H^1(\mathbb{R}^3 \times [0,T];\mathbb{R}^3) | \nabla \cdot A = 0\}$ and
$$S : A \mapsto \frac{1}{2}\int_0^T \int_{\mathbb{R}^3} \{-|\dot{A}|^2 + |\nabla \times A|^2\}.$$

10. Lagrangian functional: $\mathcal{L} : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$
$$S : \phi \mapsto \int \mathcal{L}(\phi(z), \nabla\phi(z))d^d z.$$

We will encounter many of these functionals in applications to quantum mechanics and quantum field theory.

11.2 The first variation and critical points

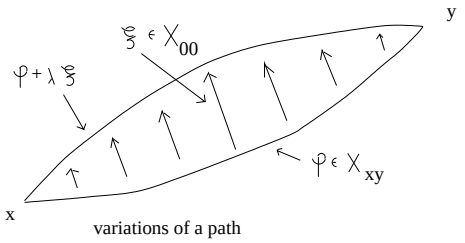
The notion of a *critical point* of a functional is a central one. It is a direct extension of the usual notion of a critical point of a function of finitely many variables (ie, a place where the derivative vanishes). The solutions of many physical equations are critical points of certain functionals (*action functionals*).

In what follows, X is some space of functions. It will almost always be a linear (ie vector) space, or an affine space, and will vary from example to example.

Definition 11.2 *A* variation *of $\phi \in X$ along ξ is a path, ϕ_λ in X (λ varying in a neighbourhood of 0), such that $\phi_0 = \phi$ and $\partial\phi_\lambda/\partial\lambda|_{\lambda=0} = \xi$.*

In this definition, if X is a linear space (as it usually is), we may take $\xi \in X$, and $\phi_\lambda = \phi + \lambda\xi$. More generally, X could be a manifold. In this case, the direction ξ of the variation lies in the tangent space $T_\phi X$.

Example 11.3 Define $X_{xy} = \{\phi \in C([a,b], X) | \phi(a) = x, \phi(b) = y\}$ (an affine space). Then $T_\phi X_{xy} = X_{00}$ (see figure 11.2), and an example of a variation of $\phi \in X_{xy}$ in the direction $\xi \in X_{00}$ is $\phi_\lambda = \phi + \lambda\xi \in X_{xy}$.



(11.2)

We now define a notion of differentiation of functionals which is a direct extension of usual differentiation of functions of finitely many variables.

Definition 11.4 *Let $S : X \to \mathbb{R}$ be a functional on a function space X. The* Fréchet derivative *(or* variational derivative *or* gradient map*) of S at ϕ is the function $\partial S(\phi)$ defined by*

$$\frac{\partial}{\partial\lambda} S(\phi_\lambda)|_{\lambda=0} = \int \partial S(\phi) \cdot \eta \tag{11.3}$$

for any η, and variation ϕ_λ of ϕ along η.

Remark 11.5 *This definition also applies to functionals defined on an abstract Hilbert space (eg (11.1)) with the integral replaced by the inner-product.*

It is a fairly easy matter to compute the Fréchet derivatives of the functionals in example (11.1) from the above definition, and the task is left as an exercise (hint: usually, one has to integrate by parts).

Problem 11.6 Referring to the list of functionals given in example 11.1, show that:

1. $\partial S(\phi) = f$
3. $\partial S(\phi) = \nabla V(\phi)$
4. $\partial S(\phi) = -\Delta\phi$
5. $\partial S(\phi) = -m\ddot{\phi} - \nabla V(\phi)$
6. $\partial S(\phi) = -\frac{d}{dt}(\partial_{\dot{\phi}} L) + \partial_\phi L$
7. $\partial S(\phi) = \Box\phi + \nabla V(\phi)$ where $\Box \equiv \partial_t^2 - \Delta$ is the *D'Alembertian* operator
8. $\partial S(\phi) = B\phi$ (in this case the variational derivative is defined with respect to the abstract inner-product rather than the integral)
9. $\partial S(A) = \Box A$
10. $\partial S(\phi) = -\nabla(\partial_{\nabla\phi} L) + \partial_\phi L$

As in the finite-dimensional case, a *critical point* is a place where the derivative vanishes.

Definition 11.7 *A function ϕ in X is a* critical point *(CP) of a functional S if* $\partial S(\phi) \equiv 0$.

In fact, many physical equations are critical point equations for certain functionals.

Example 11.8 Continuing with the same list of examples of functionals, we can write down some of the equations describing their critical points:

4. $\Delta\phi = 0$ (Dirichlet equation, ϕ harmonic)
5. $m\ddot{\phi} = -\nabla V(\phi)$ (Newton's equation)
6. $\frac{d}{dt}(\partial_{\dot{\phi}} L) = (\partial_\phi L)$ (Euler-Lagrange equation)
7. $\Box\phi + \nabla V(\phi) = 0$ (nonlinear wave/Klein-Gordon equation)

9. $\Box A = 0$ (wave equation)

10. $-\nabla(\partial_{\nabla\phi} L) + \partial_\phi L = 0$ (classical field equation)

Remark 11.9 *Strictly speaking, the Fréchet derivative, ∂S of a functional S, lives in the cotangent bundle T^*X over X. That is, for all $\phi \in X$, $\partial S(\phi)$ is the linear functional from $T_\phi X$ into $\mathbb{R}$ given by $\xi \mapsto \partial_\lambda S(\phi_\lambda)|_{\lambda=0}$ where ϕ_λ is a variation of ϕ in the direction ξ.*

The following connection between critical points and minima (or maxima) is familiar from multi-variable calculus.

Theorem 11.10 *If ϕ_0 minimizes a functional S, then ϕ_0 is a critical point of S.*

Problem 11.11 Prove this (similar to the usual finite-dimensional case).

As we have seen, the equations for a critical point of the functional

$$S(\phi) = \int_0^T (\frac{m}{2}\dot{\phi}^2 - V(\phi))$$

are exactly Newton's equation of classical mechanics. This is a special case of the *principle of minimal action*: solutions of physical equations minimize (more precisely, make stationary) certain functionals, called *action functionals*. It is one of the basic principles of modern physics.

11.3 The second variation

In the usual calculus, if one wishes to know if a critical point is actually a minimum (or maximum), one looks at the second derivative. For the same reason, we need to define the second derivative of a functional.

Definition 11.12 *A* variation of ϕ along η and ξ *is a two-parameter family, $\phi_{\lambda,\mu} \in X$, such that $\phi_{0,0} = \phi$, $\partial\phi/\partial\lambda|_{\lambda=\mu=0} = \xi$, and $\partial\phi/\partial\mu|_{\lambda=\mu=0} = \eta$.*

Definition 11.13 *Let S be a functional on a function space X. The* Hessian *(or* 2nd derivative*) of S at ϕ is the operator $\partial^2 S(\phi)$ (or $S''(\phi)$) such that*

$$(\partial^2/\partial\lambda\partial\mu) S(\phi_{\lambda,\mu})|_{\lambda=\mu=0} = \int \xi \cdot \partial^2 S(\phi)\eta \tag{11.4}$$

for all ξ, η, where $\phi_{\lambda,\mu}$ is a two-parameter variation of ϕ along ξ and η.

Computations of the second derivatives of the functionals in our list of examples are left as an exercise.

Problem 11.14 Continuing with our list of examples of functionals, show that

3. $S''(\phi) = HessV(\phi)$ (matrix multiplication operator).
4. $S''(\phi) = -\Delta$ (Laplacian).
5. $S''(\phi) = -m\partial_t^2 - HessV(\phi)$ (Schrödinger operator).
6. $$S''(\phi) = -d/dt(\partial_{\dot\phi}^2 L)d/dt - (d/dt\partial_{\phi\dot\phi}^2 L) + \partial_\phi^2 L. \tag{11.5}$$
7. $S''(\phi) = \Box + V''(\phi)$.
8. $S''(\phi) = B$.
9. $S''(\phi) = \Box$ (D'Alembertian).
10. $$S''(\phi) = -\nabla(\frac{\partial^2 L}{\partial\nabla\phi^2})\nabla - \nabla(\frac{\partial^2 L}{\partial\nabla\phi\partial\phi}) + \frac{\partial^2 L}{\partial\phi^2}.$$

The following criterion for a critical point to be a minimizer is similar to the finite-dimensional version, and the proof is left as an exercise.

Theorem 11.15 *If ϕ_0 is a critical point of S, and $\partial^2 S(\phi_0) > 0$ (a positive definite operator), then ϕ_0 is a local minimizer of S.*

Problem 11.16 Prove this.

Let us now pursue the question of whether or not a critical point of the classical action functional

$$S(\phi) = \int_0^T L(\phi(s), \dot\phi(s))ds$$

(which is a solution of the Euler-Lagrange equation - ie, a classical path) minimizes the action. As we have seen, the Hessian $S''(\phi)$ is given by (11.5). We call $\partial_{\dot\phi}^2 L$ the *generalized mass.*

Theorem 11.17 *Suppose $\partial_{\dot\phi^2}^2 L > 0$. Suppose further that $\partial_\phi^2 L$ is a bounded function. Then there is a $T_0 > 0$, such that $S''(\phi) > 0$ for $T \leq T_0$.*

Proof (for $L = \frac{m}{2}\dot{\phi}^2 - V(\phi)$): In this case $S''(\phi) = -m\partial^2/\partial s^2 - V''(\phi)$ on $L^2([0,T])$ with Dirichlet boundary conditions. The strong form of the uncertainty principle (see Chapter 6) says that $d^2/ds^2 \geq 1/(4s^2)$. So $S''(\phi) \geq m/4T^2 - \|V''\|_\infty$ which is > 0 for T sufficiently small. □

Corollary 11.18 *For T sufficiently small, a critical point of S (ie, a classical path) locally minimizes the action, S.*

We conclude this section with two further remarks about the variational calculus.

Remark 11.19 *In the finite-dimensional setting, the second derivative is obviously the derivative of the first derivative. The variational analogue can be written*

$$S''(\phi)\eta = \partial_\phi \langle \partial_\phi S(\phi), \eta \rangle.$$

Remark 11.20 (Lagrange multipliers) *Informally, ϕ is a critical point of a functional $E(\phi)$ under a constraint $C(\phi)$ (i.e. on the space $\{\phi \in X \mid C(\phi) = 0\}$) iff ϕ is a critical point of the functional $E(\phi) - \lambda C(\phi)$ for some λ (the Lagrange multiplier), and ϕ satisfies the constraint $C(\phi) = 0$.*

11.4 Application to the spectral problem: variational characterization of eigenvalues

For a moment, we consider an abstract self-adjoint operator H on some Hilbert space. By applying variational techniques to the "energy" functional $< \psi, H\psi >$, we will derive an important characterization of eigenvalues of H.

Theorem 11.21 *$\lambda \equiv \inf \sigma(H)$ is an eigenvalue of H iff there is a minimizer for $S(\psi) \equiv \frac{1}{2}\langle \psi, H\psi \rangle$ with the constraint $\|\psi\| = 1$.*

Proof: ψ_0 minimizes S with the given constraint iff ψ_0 is a CP of $S(\phi) - \lambda\|\psi\|^2$ (λ is a Lagrange multiplier) and $\|\psi_0\| = 1$. The variational derivative of this functional is $H\psi - \lambda\psi$, and its second variation is the operator $H - \lambda$. So ψ_0 minimizes S with the given constraint iff $H\psi_0 = \lambda\psi_0$, $H - \lambda \geq 0$, and $\|\psi_0\| = 1$, i.e. iff λ is an EV of H and $\lambda = \inf \sigma(H)$. □

This result leads us to the *variational principle of quantum mechanics*: for any ψ,

$$\langle \psi, H\psi \rangle \geq \lambda = \inf \sigma(H)$$

and equality holds iff $H\psi = \lambda\psi$.

This can be extended to higher eigenvalues:

Theorem 11.22 (MinMax principle) *The n^{th} EV of H, if it exists, is given by*

$$\lambda_n = \sup_{\dim X = n-1} \inf_{\psi \in X^\perp \mid \|\psi\|=1} \langle \psi, H\psi \rangle.$$

11.5 Conjugate points and Jacobi fields

In the remainder of this chapter, we study the classical action functional and its critical points (classical paths) in some detail. While such a study is of obvious importance in classical mechanics, it will also prove useful in the quasi-classical analysis of quantum systems that we undertake in chapters 13 and 14.

Thus we consider the action functional

$$S(\phi) = \int_0^t L(\phi(s), \dot{\phi}(s)) ds.$$

We have shown above that if t is sufficiently small, then $S''(\phi) > 0$, provided $(\partial^2 L/\partial \dot{\phi}^2) > 0$. So in this case if $\bar{\phi}$ is a critical path, then it minimizes $S(\phi)$. On the other hand, Theorem 11.15 implies that if $\bar{\phi}$ is a critical path such that $S''(\bar{\phi})$ has negative spectrum, then $\bar{\phi}$ is not a minimizer. We will show later that eigenvalues of $S''(\bar{\phi})$ decrease monotonically as t increases. So the point t_0 when the smallest eigenvalue of $S''(\bar{\phi})$ becomes zero, separates the t's for which $\bar{\phi}$ is a minimizer, from those for which $\bar{\phi}$ has lost this property. The points at which one of the eigenvalues of $S''(\bar{\phi})$ becomes zero play a special role in the analysis of classical paths. They are considered in this section.

In this discussion we have used implicitly the fact that because $S''(\bar{\phi})$ is a Schrödinger operator defined on $L^2([0,t])$ with Dirichlet (zero) boundary conditions, it has a purely point spectrum running off to ∞. We denote this spectrum by $\{\lambda_n(t)\}_1^\infty$ with $\lambda_n \to \infty$ as $n \to \infty$. Note that if $\bar{\phi}$ is a CP on $[0,t]$, then $\bar{\phi}_\tau \equiv \bar{\phi}|_{[0,\tau]}$ is a CP on $[0,\tau]$. Thus for $\tau \leq t$, $\{\lambda_n(\tau)\}$ is the spectrum of $S''(\bar{\phi}_\tau) = S''(\bar{\phi})$ on $[0,\tau]$ with zero boundary conditions..

We specialize now to the classical action functional

$$S(\phi) = \int_0^t \{\frac{m}{2}|\dot{\phi}|^2 - V(\phi)\}$$

on the space $X = \{\phi \in C^1([0,t];\mathbb{R}^d) \mid \phi(0) = x,\ \phi(t) = y\}$, and continue to denote by $\bar{\phi}$, a critical point of this functional (classical path).

Theorem 11.23 *$\lambda_n(\tau)$ is monotonically decreasing in τ.*

Proof: consider $\lambda_1(\tau)$, and let its normalized eigenfunction be ψ_1. Define $\tilde{\psi}_1$ to be ψ_1 extended to $[0, \tau+\epsilon]$ by 0. So by the variational principle,

$$\lambda_1(\tau+\epsilon) \leq \langle \tilde{\psi}_1, S''(\bar{\phi})\tilde{\psi}_1 \rangle = \lambda_1(\tau).$$

Further, equality here is impossible by the "unique continuation theorem" which states that if an eigenfunction of a Schrödinger operator is zero on an open set, it is everywhere zero. To extend the proof to the higher eigenvalues, one can use the MinMax principle. □

Definition 11.24 *A point $\bar{\phi}(\tau_0)$ such that $\lambda_n(\tau_0) = 0$ for some n is called a* conjugate point *to $\bar{\phi}(0) = x$ along $\bar{\phi}$.*

So if $c = \bar{\phi}(\tau_0)$ is a conjugate point to x, then $S''(\bar{\phi})$ on $[0, \tau_0]$ has a 0 eigenvalue. That is, there is some non-zero $\xi \in L^2([0,\tau_0])$ with $\xi(0) = \xi(\tau_0) = 0$ such that

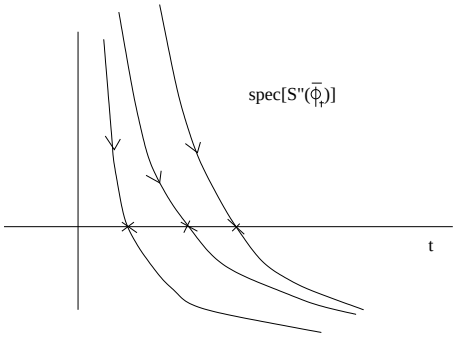
$$S''(\bar{\phi})\xi = 0. \tag{11.6}$$

This is the *Jacobi equation.* A solution of this equation with $\xi(0) = 0$ will be called a *Jacobi vector field.*

Definition 11.25 *The* index *of $S''(\bar{\phi})$ is the number of negative eigenvalues it has (counting multiplicity) on $L^2([0,t])$ with zero boundary conditions.*

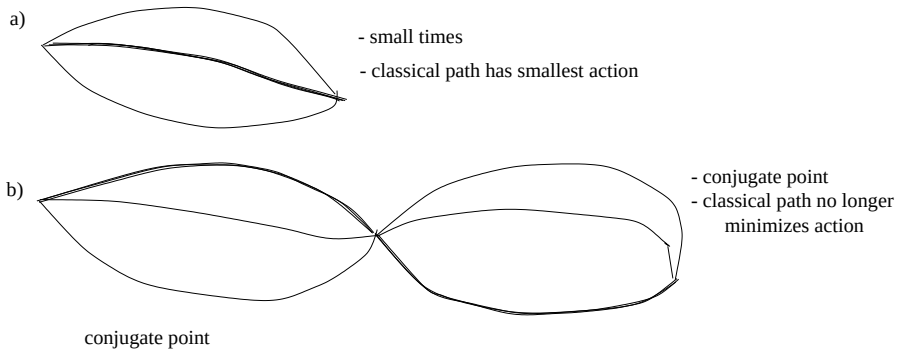
We recall that for τ small, $S''(\bar{\phi})$ has no zero eigenvalues on $[0,\tau]$ (Theorem 11.17). Combining this fact with Theorem 11.23 gives the following result.

Theorem 11.26 (Morse) *The index of $S''(\bar{\phi})$ is equal to the number of points conjugate to $\bar{\phi}(0)$ along $\bar{\phi}$, counting multiplicity (see figure 11.7).*



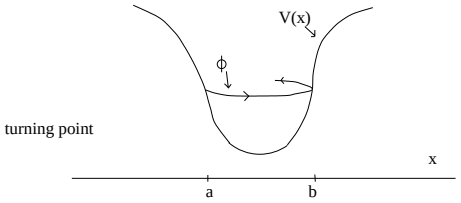
(11.7)

Thus the picture that has emerged is as follows. For sufficiently small times, there is a unique classical path with the smallest action. As time increases, the paths might lose this property. This happens if there is a point in the path conjugate to $\bar{\phi}(0)$ (see figure 11.8).



(11.8)

Example 11.27 An example of a conjugate point is a turning point in a one-dimensional potential (see figure 11.9).



(11.9)

The classical path ϕ starts at a, and turns back after hitting b at time τ. Now

$$S''(\phi) = -m\partial_s^2 - V''(\phi)$$

and it is easy to check that $S''(\phi)\dot{\phi} = 0$ (just differentiate Newton's equation). Since $\dot{\phi}(0) = \dot{\phi}(\tau) = 0$ (the velocity at a turning point is zero), b is conjugate to a. It is clear here that ϕ ceases to be a minimal action path after hitting b.

Now we return to the Jacobi equation (11.6), and consider its *fundamental solution* $J(s)$. $J(s)$ is the $d \times d$ matrix satisfying

$$S''(\bar{\phi})J = 0$$

with the initial conditions

$$J(0) = 0 \text{ and } \dot{J}(0) = id.$$

J is called the *Jacobi matrix*.

Proposition 11.28 *The Jacobi matrix has the following properties*

1. *For any $h \in \mathbb{R}^d$, Jh is a Jacobi field. Conversely, any Jacobi field is of the form Jh for some $h \in \mathbb{R}^d$.*

2. *$\bar{\phi}(\tau_0)$ is a conjugate point to $\bar{\phi}(0)$ iff $J(\tau_0)$ has a zero-eigenvalue, i.e.* $\det J(\tau_0) = 0$.

Proof:

1. The first part is obvious. To prove the second part let ξ be a Jacobi field, and let $h = \dot{\xi}(0)$. Then $\tilde{\xi} \equiv Jh$ satisfies the same differential equation as ξ with the same initial conditions. Hence $\xi = \tilde{\xi}$.

2. $\bar{\phi}(\tau_0)$ is a conjugate point iff there is a Jacobi field ξ such that $\xi(\tau_0) = 0$. By the previous statement, there is $h \neq 0$ such that $\xi = Jh$, which implies $J(\tau_0)h = 0$. So $J(\tau_0)$ has a zero eigenvalue (with the eigenvector h), and $\det J(\tau_0) = 0$.

□

Now we give the defining geometric/dynamic interpretation of J. Consider a family of critical paths $\phi_v(s)$ starting at $\bar{\phi}(0)$ with various initial velocities $v \in \mathbb{R}^d$. Denote $\bar{v} = \dot{\bar{\phi}}(0)$. Then

$$J(s) = \frac{\partial \phi_v(s)}{\partial v}|_{v=\bar{v}}$$

is the Jacobi matrix (along $\bar{\phi}$). Indeed, ϕ_v satisfies the equation $\partial S(\phi_v) = 0$. Differentiating this equation with respect to v, and using that $S''(\phi) = \partial_\phi \partial_\phi S(\phi)$, we find by the definition of ∂_ϕ that

$$0 = \frac{\partial}{\partial v} \partial_\phi S(\phi_v) = S''(\phi_v) \frac{\partial \phi_v}{\partial v}.$$

Thus, $\partial \phi_v / \partial v|_{v=\bar{v}}$ satisfies the Jacobi equation. Next,

$$\frac{\partial}{\partial v} \phi_v(0) = \frac{\partial}{\partial v} \bar{\phi}(0) = 0$$

and

$$\frac{\partial}{\partial v} \dot{\phi}_v(0) = \frac{\partial}{\partial v} v = id$$

which completes the proof.

11.6 Action of the critical path

Suppose $\bar{\phi}$ is a critical path for S with $\phi(0) = x$ and $\phi(t) = y$. Then the *action from x to y* is $S_0(x, y) \equiv S(\bar{\phi})$. In what follows,

$$S(\phi) = \int_0^t L(\phi, \dot{\phi}) ds.$$

Lemma 11.29 *Define $k = (\partial L/\partial \dot{\phi})(\bar{\phi})|_{t=0}$. Then*

$$\partial S_0(x, y)/\partial x = -k.$$

Proof: Again, we specialize to $L = m|\dot{\phi}|^2/2 - V(\phi)$. Using the chain rule and integration by parts, we find

$$\partial S(\bar{\phi})/\partial x = \int_0^t \{m\dot{\bar{\phi}}\partial\dot{\bar{\phi}}/\partial x - V'(\bar{\phi})\partial\bar{\phi}/\partial x\}$$

$$= \int_0^t \{(-m\ddot{\bar{\phi}} - V'(\bar{\phi}))\partial\bar{\phi}/\partial x\} + m\dot{\bar{\phi}}\partial\bar{\phi}/\partial x|_0^t$$

which, as $\bar{\phi}$ is a critical point and $(\partial\bar{\phi}/\partial x)(t) = 0$, is just $-m\dot{\phi}(0) = -k$ as claimed. □

This lemma implies $\partial k/\partial y = -\partial^2 S_0(x, y)/\partial x \partial y$. On the other hand, $\partial k/\partial y = (\partial y/\partial k)^{-1} = mJ^{-1}(k, t)$. This gives us

$$\frac{\partial^2 S_0(x, y)}{\partial x \partial y} = -mJ^{-1}(k, t)$$

which establishes the following result.

Proposition 11.30 *If y is a conjugate point to x then* $\det(\frac{\partial^2 S_0(x,y)}{\partial x \partial y}) = \infty$.

The following exercise illustrates this result for the example of the classical harmonic oscillator.

Problem 11.31 Consider the harmonic oscillator, whose Lagrangian is $L = \frac{m}{2}\dot{\phi}^2 - \frac{m\omega^2}{2}\phi^2$. Compute

$$S_0(x, y) = \frac{\omega}{2\sin(\omega t)}[(x^2 + y^2)\cos(\omega t) - 2xy]$$

and so compute

$$\partial^2 S_0(x,y)/\partial x \partial y = -\frac{\omega}{\sin \omega t}.$$

Note that this is infinite for $t = n\pi/\omega$ for all integers n. Thus $\phi(n\pi/\omega)$ are conjugate to $\phi(0)$.

Lemma 11.32 (Hamilton-Jacobi equation) *S_0 satisfies the Hamilton-Jacobi equation*

$$\partial S_0/\partial t = -h(x, \partial S_0/\partial x) \tag{11.10}$$

where h is the classical Hamiltonian function associated with L.

Proof: Since $S_0 = S(\bar{\phi}) = \int_0^t L(\bar{\phi}, \dot{\bar{\phi}})$, we have

$$\partial S(\bar{\phi})/\partial t = L(\bar{\phi}, \dot{\bar{\phi}})|_{s=t} + \int_0^t (\partial L/\partial \bar{\phi} \cdot \partial \bar{\phi}/\partial t + \partial L/\partial \dot{\bar{\phi}} \cdot \partial \dot{\bar{\phi}}/\partial t) ds$$

$$= L(\bar{\phi}, \dot{\bar{\phi}})|_{s=t} + \partial L/\partial \dot{\bar{\phi}} \cdot \partial \bar{\phi}/\partial t|_{s=0}^{s=t} + \int_0^t (\partial L/\partial \bar{\phi} - d/ds(\partial L/\partial \dot{\bar{\phi}}))\partial \bar{\phi}/\partial t$$

and since $\bar{\phi}$ is a CP of S, and $\partial \bar{\phi}/\partial t|_{s=0}^{s=t} = -\dot{\bar{\phi}}|_{s=t}$, this is

$$L(\bar{\phi}, \dot{\bar{\phi}}) - (\partial L/\partial \dot{\bar{\phi}})\dot{\bar{\phi}}|_{s=t}.$$

$$= -(k\dot{\bar{\phi}} - L(\bar{\phi}, \dot{\bar{\phi}}))\big|_{k=\partial L/\partial \dot{\bar{\phi}}} = -h(x,k).$$

Since $k = \partial L/\partial \dot{\bar{\phi}}|_{s=t} = \partial S_0/\partial x$ we are done. □

Lemma 11.33 (Conservation of energy)

$$\textit{energy } (\bar{\phi}) \equiv \frac{\partial L}{\partial \dot{\phi}}\dot{\phi} - L|_{\bar{\phi}} = \textit{ const.}$$

Proof: We compute

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{\phi}}\dot{\phi} - L) = \frac{\partial^2 L}{\partial \dot{\phi}^2}\ddot{\phi}\dot{\phi} + \frac{\partial^2 L}{\partial \dot{\phi}\partial \phi}\dot{\phi}^2$$

$$+\frac{\partial L}{\partial \dot{\phi}}\ddot{\phi} - \frac{\partial L}{\partial \dot{\phi}}\ddot{\phi} - \frac{\partial L}{\partial \phi}\dot{\phi}$$

$$= (\frac{d}{dt}\frac{\partial L}{\partial \dot{\phi}} - \frac{\partial L}{\partial \phi})\dot{\phi}$$

so $\frac{\partial L}{\partial \dot{\phi}}\dot{\phi} - L|_{\bar{\phi}}$ is a constant (which we will denote by E). Now

$$\frac{\partial L}{\partial \dot{\phi}}\dot{\phi} - L = h(\phi, \frac{\partial L}{\partial \dot{\phi}}),$$

hence E is the energy of $\bar{\phi}$. $\square$

We want now to pass from a time-dependent to a time-independent picture of classical motion. We perform a Legendre transform on $S_0(x, y, t)$ to obtain $W_0(x, y, E)$ via

$$W_0 = S_0 + Et|_{t:\partial S/\partial t = -E}.$$

Note that from the energy conservation law

$$\frac{\partial L}{\partial \dot{\phi}}\dot{\phi} - L|_{\bar{\phi}} = E$$

we have

$$W_0 = \int_0^t \frac{\partial L}{\partial \dot{\phi}}\dot{\phi}|_{\bar{\phi}} = \int_{\bar{\phi}} k \cdot dx.$$

Let $\bar{t}$ be such that $\partial S/\partial t|_{t=\bar{t}} = -E$.

Lemma 11.34 *$\bar{\phi}|_{t=\bar{t}}$ is a classical path at energy E.*

Proof: Let $S = S_0$. Then

$$\frac{\partial S}{\partial t} = L + \int_0^t (\frac{\partial L}{\partial \dot{\phi}}\frac{\partial \dot{\phi}}{\partial t} + \frac{\partial L}{\partial \phi}\frac{\partial \phi}{\partial t})ds$$

$$= L + \frac{\partial L}{\partial \dot{\phi}}\frac{\partial \phi}{\partial t}|_0^t = L + \frac{\partial L}{\partial \dot{\phi}}\frac{\partial \phi}{\partial t}|_{s=t}.$$

Since $\phi(s) = y + \dot{\phi}(t)(s-t) + O((s-t)^2)$, we have

$$\frac{\partial \phi}{\partial t}|_{s=t} = -\dot{\phi}(t)$$

$$\Rightarrow \frac{\partial S}{\partial t} = L - \frac{\partial L}{\partial \dot{\phi}}\dot{\phi}.$$

Hence

$$\frac{\partial S}{\partial t}|_{t=\bar{t}} = -E \Rightarrow \text{ energy } (\bar{\phi}) = E$$

$\square$

Lemma 11.35 *W_0 satisfies the Hamilton-Jacobi equation*

$$h(x, \partial W_0/\partial x) = E. \tag{11.11}$$

Proof: Setting $t = \bar{t}$ in (11.10), and using that $\partial S/\partial t|_{t=\bar{t}} = -E$, we find

$$h(x, \partial S/\partial x)|_{t=\bar{t}} = E.$$

Finally, we note that

$$\frac{\partial W_0}{\partial x} = \frac{\partial S}{\partial x}|_{t=\bar{t}} + (\frac{\partial S}{\partial t} + E)|_{t=\bar{t}}\frac{\partial \bar{t}}{\partial x} = \frac{\partial S}{\partial x}|_{t=\bar{t}}$$

which completes the proof. □

Remark 11.36 *If w is a critical path from x to y in time t, then $w|_{t=\bar{t}}$ is a classical path from x to y at energy E, and we denote $w|_{t=\bar{t}} \equiv w_E$.*

Finally, consider a classical particle in $\mathbb{R}^d$ with a potential $V(x)$.

Theorem 11.37 (Jacobi theorem) *The classical trajectory of a particle at an energy E is a geodesic in the Riemannian metric*

$$< u, v >_x = 2(E - V(x))_+ u \cdot v$$

(where $u \cdot v$ is the inner product in $\mathbb{R}^n$) on the set $\{x \in \mathbb{R}^n | V(x) \leq E\}$ (the classically allowed region).

Proof: w is a geodesic iff w obeys the Euler-Lagrange equation

$$\ddot{w}_l = \Gamma^l_{ij}\dot{w}^i\dot{w}^j$$

where the Christoffel symbols can be computed to be

$$\Gamma^l_{ij}(x) = -\frac{1}{2}(E - V)^{-1}_+ \frac{\partial V}{\partial x^l}\delta_{ij}.$$

Thus the geodesic equation becomes

$$\ddot{w} = -\frac{1}{2}(E - V)^{-1}_+ \nabla V(w)\|\dot{w}\|^2.$$

Now if γ is a classical path at energy E, then it obeys the Newton equation

$$m\ddot{\gamma} = -\nabla V(\gamma).$$

Energy conservation says

$$\frac{m}{2}\|\dot{\gamma}\|^2 + V(\gamma) = E$$

and these two equations imply

$$\ddot{\gamma} = -\frac{1}{2}(E - V)_+^{-1}\nabla V(\gamma)\|\dot{\gamma}\|^2$$

□.

Chapter 12

Mathematical detours: the stationary phase method and operator determinants

In this chapter we describe the mathematics which we will use to derive useful formulas from the path integral. These formulas are *semi-classical*, or *quasi-classical*, meaning they are leading-order asymptotic expressions as the "parameter" $\hbar \to 0$.

12.1 The stationary phase method

We would like to determine the asymptotics of oscillatory integrals of the form

$$\int_{\mathbb{R}^d} e^{iS(\phi)/\hbar} d\phi$$

as $\hbar \to 0$ (here ϕ is a finite dimensional variable). The basic idea is that as $\hbar \to 0$, the integrand is highly oscillating and yields a small contribution except where $\nabla S(\phi) = 0$ (ie, critical points).

We study

$$I(\hbar) \equiv \int f(\phi) e^{iS(\phi)/\hbar} d^n\phi$$

where $f \in C_0^\infty$ and consider two cases:

1. $\mathrm{supp}(f)$ contains no critical points of S. Define

$$L = \frac{\hbar}{i} \langle \frac{\partial S(\phi)}{\|\partial S(\phi)\|^2}, \partial_\phi \rangle.$$

Note $Le^{iS(\phi)/\hbar} = e^{iS(\phi)/\hbar}$, so

$$\int f e^{iS/\hbar} = \int f L^m e^{iS/\hbar}$$

$$= \int (L^*)^m f e^{iS/\hbar} = O(\hbar^m)$$

for any m.

2. $\mathrm{supp}(f)$ contains only one CP, $\bar{\phi}$ of S. Expand $S(\phi)$ around $\bar{\phi}$. Writing $\phi - \bar{\phi} = \sqrt{\hbar}\alpha$ we obtain

$$S(\phi)/\hbar = S(\bar{\phi})/\hbar + \frac{1}{2} < \alpha, S''(\bar{\phi})\alpha > + O(\sqrt{\hbar}\alpha^3)$$

$$\Rightarrow I(\hbar) = \hbar^{d/2} e^{iS(\bar{\phi})/\hbar} \int f(\bar{\phi} + \sqrt{\hbar}\alpha) e^{i<\alpha, S''(\bar{\phi})\alpha>/2} e^{iO(\sqrt{\hbar}\alpha^3)} d^n\alpha.$$

Now we use the formula

$$\int_{\mathbb{R}^d} e^{i<\alpha, S''(\bar{\phi})\alpha>/2} d\alpha = (2\pi i)^{d/2} [\det S''(\bar{\phi})]^{-1/2}$$

(we can derive this expression from, say, analytic continuation of $\int e^{-a<\alpha, S''\alpha>}$ from $Re(a) > 0$, though the integrand is not integrable in the usual sense). Noting that $f(\bar{\phi} + \sqrt{\hbar}\alpha) = f(\bar{\phi}) + O(\sqrt{\hbar})$, we have the *stationary phase expansion* (for one critical point):

$$I(\hbar) = (2\pi i\hbar)^{d/2} [\det S''(\bar{\phi})]^{-1/2} f(\bar{\phi}) e^{iS(\bar{\phi})/\hbar} [1 + O(\sqrt{\hbar})]. \tag{12.1}$$

12.2 Operator determinants

For square matrices, the determinant function has the properties

1. A is invertible iff $\det A \neq 0$
2. $A = A^* \Rightarrow \det A \in \mathbb{R}$
3. $\det(AB) = \det(A)\det(B)$
4. $A > 0 \Rightarrow \det A = e^{\mathrm{tr}(\ln A)}$

5. $\det A = \prod_{\lambda \text{ ev of } A} \lambda$

We would like to define the determinant of a Schrödinger operator.

Example 12.1 Let $H = -\Delta + V$ on $[0, L]$ with zero boundary conditions (assume V is bounded and continuous). Then

$$\|(H - (2\pi n/L)^2)\sin(2\pi nx/L)\| = \|V(x)\sin(2\pi nx/L)\| \leq (\sup|V|)\|sin(2\pi nx/L)\|$$

and spectral theory tells us that H has an eigenvalue in the interval $[(2\pi n/L)^2 - \sup|V|, (2\pi n/L)^2 + \sup|V|]$. Thus,

$$\sigma(H) = \{(2\pi n/L)^2 + O(1)|n \in \mathbb{Z}\}.$$

So trying to compute the determinant directly, we get $\prod_{\lambda \text{ ev } H} \lambda = \infty$.

For a positive matrix, A, we can define $\zeta_A(s) \equiv \text{tr } A^{-s} = \sum_{\lambda \text{ ev of } A} \lambda^{-s}$.

Problem 12.2 Show in this case that $\det(A) = e^{-\zeta_A'(0)}$

Now for $H = -\Delta + V$ on $[0, L]^d$ with zero boundary conditions,

$$\zeta_H(s) = \text{trace} H^{-s} \equiv \sum_{\lambda \text{ ev of } H} \lambda^{-s}$$

exists for $Re(s) > 1/2$ (see example 12.1 for $d = 1$). If ζ_H has an analytic continuation into $\{Re(s) \geq 0\}$, then we define

$$\det H \equiv e^{-\zeta_H'(0)}.$$

So defined, $\det H$ has properties 1-4 above, but not property 5. It turns out that when $H = -\Delta + V$, for example, ζ_H does have an analytic continuation to a neighbourhood of 0, and this definition applies.

It is difficult, however, to compute a determinant from this definition. In what follows, we describe some useful techniques for computation of determinants.

Using the formula

$$\lambda^{-s} = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t\lambda} dt$$

for each $\lambda_n \in \sigma(H)$ leads to

$$\zeta_H(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \sum_n e^{-t\lambda_n} dt.$$

By the spectral mapping theorem, $e^{-t\lambda_n}$ is the n^{th} eigenvalue of e^{-tH}. So

$$\zeta_H(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \text{ tr } e^{-tH} dt.$$

This formula can be useful, as it may be easier to deal with $tr(e^{-tH}) = \int e^{-tH}(x,x)dx$ than $tr(H^{-s})$.

Example 12.3 We consider $H = -\Delta$ in a "box" $B = [-L/2, L/2]^d$ with periodic boundary conditions. In this case

$$e^{-tH}(x,y) \approx (2\pi t)^{-d/2} e^{-|x-y|^2/2t}$$

in $B \times B$, and so

$$\text{tr } e^{-tH} = \int_{B\times B} e^{-tH}(x,x)dx \approx \int_B (2\pi t)^{-d/2} = (2\pi t)^{-d/2} \text{vol}(B).$$

But calculation of $\det H$ by this method is still a problem.

The most useful calculational technique for us is as follows. Let A and B be Schrödinger operators on $L^2([0,T];\mathbb{R}^d)$ with Dirichlet boundary conditions. Denote by J_A the solution to $AJ_A = 0$ with $J_A(0) = 0$, $\dot{J}_A(0) = id$ (J a $d \times d$ matrix valued function on $[0,T]$). Then one can show

Theorem 12.4

$$\frac{\det A}{\det B} = \frac{\det J_A(T)}{\det J_B(T)}. \tag{12.2}$$

Remark 12.5 *If $A = S''(\bar{\phi})$ for a critical path $\bar{\phi}$, then J_A is the Jacobi matrix along $\bar{\phi}$.*

Problem 12.6 Let $A(T)$ be the operator $-\partial_t^2 + q(t)$ defined on $L^2([0,T];\mathbb{R}^d)$ with Dirichlet boundary conditions, and let $J_A(T)$ be the corresponding Jacobi matrix. Show that the functions $\det A(t)$ and $\det J(t)$ have the same zeros of the same multiplicities (t_0 is a zero of $f(t)$ of multiplicity n if $\partial^k/\partial t^k f(t_0) = 0$ for $k = 0, \ldots, n-1$ and $\partial^n/\partial t^n f(t_0) \neq 0$).

Chapter 13

Quasi-classical analysis

An extremely useful approach to the study of quantum systems (which are typically difficult to solve analytically) is to exploit the fact that $\hbar$ is a small constant, and to seek asymptotic expressions for physical quantities as we let $\hbar \to 0$. This is called *quasi-classical* (or *semi-classical*) analysis, and is the subject of the present chapter.

13.1 Quasi-classical asymptotics of the propagator

The path integral (10.5) has the form of the oscillatory integrals we studied in section 12.1. It is natural, then, to apply (formally) the method of stationary phase (with small parameter $\hbar$) to the path integral, in order to derive a quasi-classical expression for the Schrödinger propagator $e^{-itH/\hbar}(y,x)$. That is, we simply plug the path integral expression (10.5) into the stationary phase expansion formula (12.1). Denoting $S(\phi) = S(\phi, t)$, the result is

$$e^{-iHt/\hbar}(y,x) = \int_{P_{x,y,t}} e^{iS(\phi)/\hbar} D\phi = \sum_{\bar{\phi} \text{ cp of } s} M_{\bar{\phi}} (\det S''(\bar{\phi}))^{-1/2} e^{iS(\bar{\phi})/\hbar} (1 + O(\sqrt{\hbar})) \tag{13.1}$$

where $M_{\bar{\phi}}$ is some normalization constant. We determine $M_{\bar{\phi}} \equiv M$, assuming it is independent of $\bar{\phi}$ and V. For $V = 0$, we know the kernel of the propagator explicitly:

$$e^{-iH_0 t/\hbar}(y,x) = (2\pi i\hbar t/m)^{-d/2} e^{im|x-y|^2/2\hbar t}.$$

So in particular, $e^{-iH_0 t/\hbar}(x,x) = (2\pi i\hbar t/m)^{-d/2}$. Now the right-hand side of the expression (13.1) for $e^{-itH_0/\hbar}(x,y)$ is (to leading order) $M(\det S_0''(\phi_0))^{-1/2} e^{iS_0(\phi_0)/\hbar}$

where the critical point is $\phi_0(s) = x + (y-x)s/t$. Thus $S_0(\phi_0) = m(y-x)^2/2t$ and $S_0''(\phi_0) = -m\partial_s^2$ with Dirichlet boundary conditions.

Comparison thus gives us

$$M = (\det(-m\partial_s^2))^{1/2}(2\pi i\hbar t/m)^{-d/2}$$

and therefore

$$e^{-iHt/\hbar}(y,x) = \sum_{\text{cps } \bar{\phi}} (2\pi i t\hbar/m)^{-d/2} \left(\frac{\det(-m\partial_s^2)}{\det S''(\bar{\phi})}\right)^{1/2} e^{iS(\bar{\phi})/\hbar}(1 + O(\sqrt{\hbar})) \quad (13.2)$$

as $\hbar \to 0$. This is precisely the quasi-classical expression we were looking for.

We now give a "semi-rigorous" derivation of this expression. We assume for simplicity that S has only one critical point, $\bar{\phi}$. Let $\{\xi_j\}$ be the normalized eigenfunctions of $S''(\bar{\phi})$ which form a basis of $L^2([0,t])$ (with zero boundary conditions). For the n^{th} order finite dimensional approximation to the space of paths in the path integral, we take the n-dimensional space of functions of the form

$$\phi^{(n)} = \bar{\phi} + \sum_{j=1}^{n} a_j \xi_j.$$

Expanding $S(\phi^{(n)})$ around $\bar{\phi}$ gives

$$S(\phi^{(n)}) = S(\bar{\phi}) + \frac{1}{2}\langle \xi, S''(\bar{\phi})\xi\rangle + O(\xi^3)$$

where

$$\xi \equiv \phi^{(n)} - \bar{\phi} = \sum_{1}^{n} a_j \xi_j.$$

We also have

$$D\phi^{(n)} = C_n \prod_{1}^{n} da_j$$

(C_n some constant). Now using the fact that

$$\langle \xi, S''(\bar{\phi})\xi\rangle = \sum_{i,j} a_i a_j \langle \xi_i, S''(\bar{\phi})\xi_j\rangle = \sum_j \mu_j a_j^2$$

(where $S''(\bar{\phi})\xi_j = \mu_j \xi_j$) we have

$$\int_{\phi^{(n)}: x \to y} e^{iS(\phi^{(n)})/\hbar} D\phi^{(n)} = e^{iS(\bar{\phi})/\hbar} \int e^{i\sum \mu_j a_j^2/2\hbar}(1 + O(a^3/\hbar)) C_n d^n a.$$

Setting $b \equiv a_j/\sqrt{\hbar}$ this becomes

$$\hbar^{n/2} C_n e^{iS(\bar{\phi})/\hbar} \int e^{i\sum \mu_j b_j^2/2}(1 + O(b^3\sqrt{\hbar}))d^n b$$

which is

$$C_n(2\pi i\hbar)^{n/2}(\det(S''(\bar{\phi})|_{F_n}))^{-1/2} e^{iS(\bar{\phi})/\hbar}(1 + O(\sqrt{\hbar}))$$

where $F_n \equiv \{\sum_1^n a_j\xi_j\}$ so that $\det S''(\bar{\phi})|_{F_n} = \prod_1^n \mu_j$. To avoid determining the constants C_n arising in the "measure" $D\phi$, we compare again with the free ($V = 0$) propagator. Taking a ratio gives us

$$\frac{e^{-iHt/\hbar}(y,x)}{(\frac{2\pi i\hbar t}{m})^{-d/2}} = \lim_{n\to\infty} \frac{C_n(2\pi i\hbar)^{n/2}(\det(S''(\bar{\phi})|_{F_n}))^{-1/2} e^{iS(\bar{\phi})/\hbar}}{C_n(2\pi i\hbar)^{n/2}(\det(-m\partial_s^2|_{F_n}))^{-1/2}}$$

which reproduces (13.2), as expected.

13.2 Quasi-classical asymptotics of the Greens function

Definition 13.1 *The* Greens function, $G_A(x,y,z)$, *of the operator* A *is* $(A-z)^{-1}(y,x)$, *the integral kernel of the resolvent* $(A-z)^{-1}$.

Now, for A self-adjoint

$$(A-z)^{-1} = i\int_0^\infty e^{-iAt+izt}dt$$

which converges if $Im(z) > 0$. Taking $z = E + i\epsilon$ (E real, $\epsilon > 0$ small), and letting $\epsilon \to 0$ defines

$$(A - E - i0)^{-1}(y,x) = \frac{i}{\hbar}\int_0^\infty e^{-iAt/\hbar}(y,x)e^{iEt/\hbar}dt.$$

Using our quasi-classical expression (13.2) for the propagator $e^{-iHt/\hbar}$, we have in the leading order as $\hbar \to 0$ (dropping the $-i0$ from the notation)

$$(H-E)^{-1}(y,x) = \frac{i}{\hbar}\sum_{\omega \text{ a CP}} \int_0^\infty K_\omega e^{i(S(\omega,t)+Et)/\hbar}dt$$

where ω is the critical path from x to y in time t, $S_\omega(x,y) = S(\omega)$, and

$$K_\omega \equiv (\frac{m}{2\pi i t\hbar})^{d/2}(\frac{\det(-m\partial_s^2)}{\det S''(\omega)})^{1/2}.$$

Now we want to use the stationary phase approximation again, but this time in the t variable. Denote by t_ω the critical points of the phase $S(\omega)+Et$. They satisfy the equation

$$\partial S(\omega)/\partial t = -E.$$

As in Chapter 11, $\omega_E \equiv \omega_{t=t_\omega}$ is a classical path at energy E. Let $S_\omega(x,y;t) \equiv S(\omega,t)$ for a path going from x to y in time t. Then the stationary phase formula gives

$$(H-E)^{-1}(y,x) = \frac{i}{\hbar}\sum_\omega \sum_{t_\omega} D_{\omega_E}^{1/2} e^{iW_{\omega_E}/\hbar}, \tag{13.3}$$

where we use the notation $D_{\omega_E}^{1/2} \equiv K_{\omega_E}(2\pi i\hbar)^{1/2}(\partial^2 S_\omega/\partial t^2)^{-1/2}|_{t=t_\omega}$ and $W_{\omega_E}(y,x,E) = S_\omega(x,y) + Et|_{t=t_\omega}$ (so W_{ω_E} is the Legendre transform of S_ω).

Lemma 13.2

$$D_{\omega_E} = -(2\pi i\hbar)^{d-1}\det\begin{pmatrix} \partial^2 W/\partial x\partial y & \partial^2 W/\partial x\partial E \\ \partial^2 W/\partial y\partial E & \partial^2 W/\partial E^2 \end{pmatrix} \tag{13.4}$$

where W is $W_{\omega_E}(x,y,E)$.

Sketch of proof: We first establish

$$\frac{\det(-m\partial_s^2)}{\det(S''(\omega))} = (-\frac{m}{t})^{-d}\det(\partial^2 S_\omega/\partial x\partial y). \tag{13.5}$$

To do this we recall that if for an operator A we denote the $d\times d$ matrix solving $AJ=0$ (the Jacobi equation) with $J(0)=0$ and $\dot J(0)=1$ by J_A then

$$\frac{\det(-m\partial_s^2)}{\det(S''(\omega))} = \frac{\det J_{-m\partial_s^2}(t)}{\det J_{S''(\omega)}(t)}.$$

Next we use that

$$-\frac{1}{m}J_{S''(\omega)}(t) = (\frac{\partial^2 S_\omega}{\partial x\partial y})^{-1}$$

and

$$-\frac{1}{m}J_{-m\partial_s^2}(t) = (\frac{\partial^2 S_{0,\omega}}{\partial x \partial y})^{-1} = -(\frac{m}{t})^{-1}$$

to arrive at (13.5).

We can then show that

$$\det(\partial^2 S_\omega/\partial x \partial y)(\frac{\partial^2 S_\omega}{\partial t^2})^{-1}|_{t=t_\omega}$$

equals the r.h.s. in equation (13.4) (see appendix for details). □

Now, differentiating the equation (11.11) (the Hamilton-Jacobi equation) with respect to y gives

$$(\partial h/\partial k)(\partial^2 W/\partial x \partial y) = 0$$

so the matrix $(\partial^2 W/\partial x \partial y)$ has a zero-eigenvalue, and so has determinant zero, and thus

$$D_{\omega_E} = (2\pi i\hbar)^{d-1}(\partial^2 W/\partial x \partial E)(\partial^2 W/\partial y \partial E). \tag{13.6}$$

Formula (13.3), together with (13.6), is our desired quasi-classical expression for the Greens function $(H-E)^{-1}(y,x)$.

13.2.1 Appendix

Proposition 13.3 *At $t = t_\omega$,*

$$\det(-\frac{\partial^2 S_\omega}{\partial x \partial y}) = (\frac{\partial^2 S_\omega}{\partial t^2}) \det \begin{pmatrix} \frac{\partial^2 W}{\partial x \partial y} & \frac{\partial^2 W}{\partial x \partial E} \\ \frac{\partial^2 W}{\partial y \partial E} & \frac{\partial^2 W}{\partial E^2} \end{pmatrix}$$

Proof: We drop the subindices for simplicity of notation. Differentiating $W = S + Et|_{t=t_\omega}$ with respect to x, we obtain

$$\frac{\partial W}{\partial x} = \frac{\partial S}{\partial x} + \frac{\partial S}{\partial t}\frac{\partial t}{\partial x} + E\frac{\partial t}{\partial x},$$

which due to $\partial S/\partial t = -E$ gives

$$\frac{\partial W}{\partial x} = \frac{\partial S}{\partial x}.$$

Similarly,

$$\frac{\partial W}{\partial y} = \frac{\partial S}{\partial y} \quad \text{and} \quad \frac{\partial W}{\partial E} = t.$$

This last equation, together with $\partial S/\partial t = -E$ yields

$$\frac{\partial^2 W}{\partial E^2} = \frac{\partial t}{\partial E} = -(\frac{\partial^2 S}{\partial t^2})^{-1}.$$

Furthermore,

$$\frac{\partial^2 S}{\partial x \partial y} = \frac{\partial^2 W}{\partial x \partial y} - \frac{\partial^2 W}{\partial x \partial E}\frac{\partial E}{\partial t}\frac{\partial t}{\partial y}$$

$$= \frac{\partial^2 S}{\partial t^2}[-\frac{\partial^2 W}{\partial x \partial y}\frac{\partial^2 W}{\partial E^2} + \frac{\partial^2 W}{\partial x \partial E}\frac{\partial^2 W}{\partial E \partial y}]$$

$$= -\frac{\partial^2 S}{\partial t^2}\det\begin{pmatrix} \frac{\partial^2 W}{\partial x \partial y} & \frac{\partial^2 W}{\partial x \partial E} \\ \frac{\partial^2 W}{\partial y \partial E} & \frac{\partial^2 W}{\partial E^2} \end{pmatrix}.$$

□

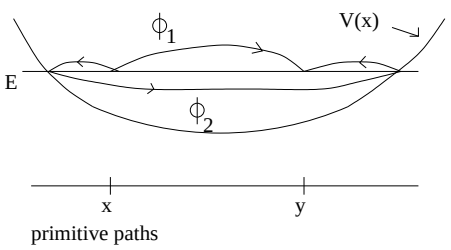
13.3 Bohr-Sommerfeld semi-classical quantization

In this section we derive a semi-classical expression for the eigenvalues (energy levels) of the Schrödinger operator $H = -\frac{\hbar^2}{2m}\Delta + V$. We use the Greens function expansion (13.3) from the last chapter. For simplicity, we will assume $d = 1$.

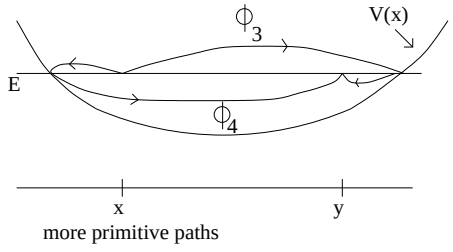
Application of the expression (13.3) requires a study of the classical paths at fixed energy. Consider the trajectories from x to y at energy E. We can write them (using informal notation) as

$$\phi_n = \phi_{xy} \pm n\alpha$$

where α is a periodic trajectory (from y to y) of minimal period, at the energy E, while ϕ_{xy} is one of the four "primitive" paths from x to y at energy E (see figure 13.7).



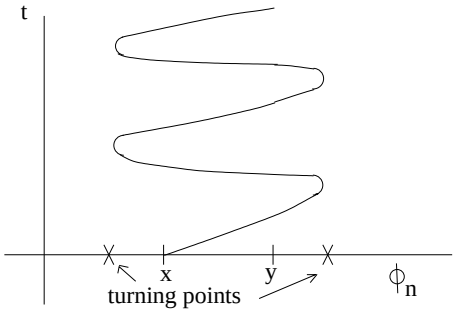
primitive paths



more primitive paths

(13.7)

All these paths are treated in the same way, so we consider only one, say the first one. The space time picture of ϕ_n in this case is sketched in figure 13.8.



(13.8)

For this path we compute

$$W_{\phi_n} = W_\phi + nI$$

where

$$I = \int_0^t L(\alpha, \dot{\alpha}) ds + Et.$$

But α is a critical path so

$$\frac{m}{2}\dot{\alpha}^2 + V(\alpha) = E$$

and

$$I = \int_0^t \{m\dot{\alpha}^2 - E\} + Et = \int_\alpha p \cdot dx$$

(where $p = m\dot{\alpha}$ and $dx = \dot{\alpha} ds$).

We now determine D_ϕ. We have $p(x) = \partial W/\partial x$. The H-J equation (11.11) implies

$$\partial W/\partial x = \pm\sqrt{2m(E - V(x))}$$

so

$$\partial^2 W/\partial x \partial E = \pm m/p(x).$$

Using (13.6), we have

$$D_\phi = \frac{m^2}{p(x)p(y)}.$$

At a turning point x_0, $p(x_0) = 0$ and p changes sign (we think about $p(x)$ as a multi-valued function, or a function on the Riemann surface of $\sqrt{z}$, so at a turning point $\sqrt{p(x)}$ crosses to a different sheet of the Riemann surface).

Because p changes sign at each of the two turning points of the periodic trajectory, we conclude that

$$D_{\phi_n}^{1/2} = D_{\phi}^{1/2}(-1)^n.$$

So our semi-classical expression (13.3) for the Greens function $G_E(y,x)$ is

$$G_E(y,x) = \sum_{n=0}^{\infty} N \exp[i(W_\phi/\hbar + n[\frac{1}{\hbar}\int_\alpha p\cdot dx - \pi])]$$

(N is a constant)

$$= Ne^{iW_\phi/\hbar}\frac{1}{1-e^{i(\int_\alpha p\cdot dx/\hbar - \pi)}}$$

We conclude that as $\hbar \to 0$, $G_E(y,x)$ has poles (and hence H has eigenvalues) when

$$\boxed{\int_\alpha p\cdot dx = 2\pi\hbar(k+1/2)}$$

(for an integer k). This is the *Bohr-Sommerfeld semi-classical quantization condition* (for $d=1$). It is an expression for the quantum energy levels (the energy E appears in the left hand side through the path α at energy E), which uses purely classical data!

Problem 13.4 Show that for the harmonic oscillator potential, the Bohr-Sommerfeld condition gives all of the energy levels exactly.

13.4 Quasi-classical asymptotics for the ground state energy

Here we derive a quasi-classical expression for the ground state energy (lowest eigenvalue) of the Schrödinger operator $H = -\frac{\hbar^2}{2m}\Delta + V$ when $V(x) \to \infty$ as $|x| \to \infty$ (a confining potential).

We first define a couple of quantities which are familiar from statistical mechanics.

Definition 13.5 *The* partition function, $Z(\beta)$, *at inverse temperature* $\beta > 0$ *is*

$$Z(\beta) \equiv \ tr\ e^{-\beta H}$$

(the trace is well-defined as $\sigma(H) = \{E_n\}_0^\infty$ *with* $E_n \to \infty$*).*

Definition 13.6 *The* free energy, F, *is*

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta).$$

The free energy is a useful quantity for us here because of the following connection with the ground state energy of the Schrödinger operator H.

Theorem 13.7 (Feynman-Kac)

$$\lim_{\beta \to \infty} F(\beta) = E_0.$$

Proof:

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta E_n} = e^{-\beta E_0}(1 + \sum_{n=1}^{\infty} e^{-\beta(E_n - E_0)})$$

so

$$\ln Z = -\beta E_0 + \ln(1 + R)$$

where

$$R \equiv \sum_{1}^{\infty} e^{-\beta(E_n - E_0)} \to 0 \text{ as } \beta \to \infty.$$

This does it. □

Our goal then, is to find the asymptotics for E_0 by determining an asymptotic expression for $Z(\beta)$ using a path integral.

As we have seen (problem 10.7), the path integral expression for $Z(\beta)$ is

$$Z(\beta/\hbar) = \int_{\phi \text{ a path of period } \beta} e^{-S_e(\phi)/\hbar} D\phi \tag{13.9}$$

where $S_e(\phi) = \int_0^\beta \{\frac{m}{2}\dot{\phi}^2 + V(\phi)\}$ (note that this is not the usual action - the potential enters with the opposite sign).

Remark 13.8 *This path integral can actually be put on a rigorous mathematical foundation.*

Mimicking the procedure we used for the Schrödinger propagator (ie, the stationary phase method), we see that the quasi-classical expansion for $Z(\beta/\hbar)$ is

$$\sum_{\text{minimal paths } \omega} N B_\omega^{1/2} e^{-S_e(\omega)/\hbar}$$

(N a constant) where

$$B_\omega = \frac{\det S_0''(\omega_0)}{\det S_e''(\omega)}$$

and $S_0(\phi) = \int_0^\beta (m/2)\dot{\phi}^2$. A *minimal path* for S_e is a classical path for the inverted potential $-V$. We specialize to $d = 1$ for simplicity, and we assume V has only one minimum at x_0. Then the minimal path is $\omega(s) \equiv x_0$ (a constant path), and

$$S_e''(\omega) = -m\partial_s^2 + V''(x_0).$$

Because x_0 minimizes V, $V''(x_0) > 0$ and we write it as $m\omega^2$. Then using the method (12.2) of computing ratios of determinants, we easily obtain

$$B_\omega = \frac{2\omega\beta}{e^{\omega\beta} - e^{-\omega\beta}}.$$

Also, $S_e(\omega) = \beta V(x_0)$. We can now compute $Z(\beta/\hbar)$, and hence (all straightforward computations) arrive at

$$F(\beta/\hbar) = V(x_0) + \hbar\omega/2 + O(1/\beta)$$

(in the leading order as $\hbar \to 0$). Letting $\beta \to \infty$ and using the Feynman-Kac formula, we obtain

$$\boxed{E_0 \approx V(x_0) + \frac{1}{2}\hbar\omega}$$

which is the desired asymptotic (as $\hbar \to 0$) expression for the ground state energy. It is equal to the classical ground state energy, $V(x_0)$, plus the ground state of the harmonic oscillator with the frequency $\sqrt{V''(x_0)/m}$. This indicates that the low energy excitation spectrum of a particle in the potential $V(x)$ is the low energy spectrum of this harmonic oscillator.

Chapter 14

Resonances

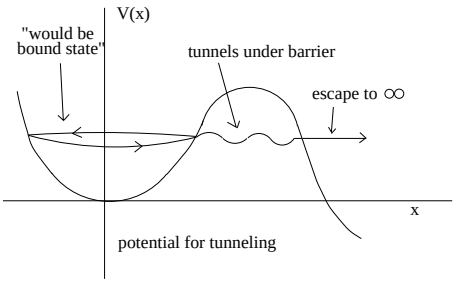
The notion of a resonance is a key notion in quantum physics. It refers to meta-stable states - i.e., to states which for long time intervals behave as stable states, but eventually break up. In other words, these are states of the continuous spectrum (i.e. scattering states), which for a long time behave as if they were bound states. In fact, the notion of the bound state is an idealization: most of the states which are (taken to be) bound states in certain models, turn out to be resonance states in a more realistic approach.

We sketch briefly the mathematical theory of resonance states. To characterize them in terms of spectral characteristics, we have to use more detailed notions than the spectrum, such as spectral densities, or generalize the notion of the spectrum altogether. The resulting theory, which is elegant and powerful, is not considered here. Here we consider a particular, but central case of resonances due to tunneling, on which we illustrate some of the mathematics and physics involved.

14.1 Tunneling and resonances

Consider a particle in a potential $V(x)$, of the form shown in figure 14.1. If $V(x) \to -\infty$ as $x \to \infty$ (in some directions), then such a potential is called *unstable*. In this

case, the corresponding Schrödinger operator, H, is not bounded from below.



(14.1)

If the barrier is very thick, then the particle spends lots of time in the well, and behaves as if it were a bound state. However, eventually it tunnels through the barrier (*quantum tunneling*) and escapes to ∞. Thus the state of the particle is a scattering one. It is intuitively reasonable that

1. energy of resonance $\approx$ energy of bound state in well
2. resonance lifetime is determined by barrier thickness and height, and $\hbar$.

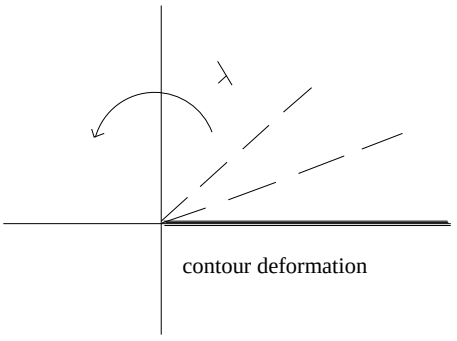
Since the resonances are very close to bound states if the barrier is large, or $\hbar$ is small, we try to mimic our treatment of the ground state (section 13.4). But right away we run into a problem: if $V(x) \not\to \infty$ as $x \to \infty$ in some directions, then

$$Z(\beta) = \text{ tr } e^{-\beta H} = \infty.$$

The paradigm of this problem is the divergence of the integral

$$Z(\lambda) = \int_0^\infty e^{-\lambda a^2/2} da$$

for $\lambda \leq 0$. However, we can define this integral by an analytic continuation. $Z(\lambda)$ is well-defined for $Re(\lambda) > 0$. Continue it analytically into $\lambda \in \mathbb{R}^-$ as follows. We move λ from $Re(\lambda) > 0$ into $Re(\lambda) \leq 0$, and deform the contour of integration at the same time, in such a way that $Re(\lambda a^2) > 0$ (see figure 14.2).



(14.2)

Of course, in this particular case we know the result:

$$Z(\lambda) = (\frac{2\lambda}{\pi})^{-1/2} = -i(\frac{2|\lambda|}{\pi})^{-1/2}$$

for $\lambda < 0$ (which is purely imaginary!).

There is a powerful method of rotating the contour which is applicable much beyond the simple integral we consider. It goes as follows. For $\theta \in \mathbb{R}$, we change variables via $a = e^{-\theta}b$. This gives

$$Z(\lambda) = e^{-\theta} \int_0^\infty e^{-\lambda e^{-2\theta} b^2/2} db. \tag{14.3}$$

The integral here is convergent and analytic in θ as long as

$$Re(\lambda e^{-2\theta}) > 0. \tag{14.4}$$

We continue it analytically in θ and λ, preserving this condition. In particular, for $\lambda \in \mathbb{R}^-$, we should have $\pi/4 < Im(\theta) < 3\pi/4$.

Now observe that the r.h.s. of (14.3) is independent of θ. Indeed, it is analytic in θ as long as (14.4) holds, and is independent of $Re(\theta)$ since the latter can be changed without changing the integral, by changing the variable of integration ($b \mapsto e^{-\theta'}b$, $\theta' \in \mathbb{R}$). Thus we constructed an analytic continuation of $Z(\lambda)$ with $Re(\lambda) > 0$ into a region with $Re(\lambda) < 0$. In fact, we continued this function onto the second sheet of its Riemann surface!

Finally, we define $Z(\lambda)$, $\lambda < 0$, by (14.3) with θ obeying (14.4).

14.2 Free resonance energy

With some wisdom gained, we return to the problem of defining the partition function $Z(\beta)$ and free energy $F(\beta)$ in the case when $V(x) \not\to \infty$ as $x \to \infty$ in some directions (or more precisely, $\sup_{x\in\Gamma} V(x) < \infty$ for some cone Γ). We begin with a definition.

Definition 14.1 *A family $H(\theta)$ in a complex disc $\{|\theta| \le \epsilon\}$, will be called a complex deformation of H if $H(0) = H$, $H(\theta)$ is analytic in $\{|\theta| \le \epsilon\}$, and there is a one-parameter unitary group $U(\lambda)$, $\lambda \in \mathbb{R}$, such that*

$$H(\theta + \lambda) = U(\lambda)^{-1} H(\theta) U(\lambda)$$

for $\lambda \in \mathbb{R}$.

If $V(x)$ has certain analytic properties, then $H(\theta)$ can be constructed by changing the variables in H as $x \mapsto xe^{-\theta}$ for $\theta \in \mathbb{R}$, and then continuing the result analytically in θ. Let, for example, $V(x) = -Cx^3$ as $x \to +\infty$. Then $V(e^\theta x) = -Ce^{3\theta}x^3$. Take $\theta = -i\pi/3$. Then $V(e^\theta x) = Cx^3$ is stable in the direction $x \to +\infty$. The group $U(\lambda)$ here is the *group of dilations*:

$$U(\lambda) : \psi(x) \mapsto e^{n\theta/2}\psi(e^\theta x)$$

for $\psi \in L^2(\mathbb{R}^n)$.

Assume that we can construct a complex deformation, $H(\theta)$, of H, such that

$$Z(\beta) = \text{ tr } e^{-\beta H(\theta)} < \infty \tag{14.5}$$

for $Im(\theta) > 0$ (or more generally for $|\theta| \leq \epsilon$, $Im(\theta) > 0$).

Proposition 14.2 *If tr* $e^{-\beta H(\theta)} < \infty$ *for* $\theta \in \Omega \subset \{|\theta| < \epsilon\}$, *then tr* $e^{-\beta H(\theta)}$ *is independent of* θ.

Proof: $e^{-\beta H(\theta)}$ is analytic in $\{|\theta| \leq \epsilon\}$ and satisfies

$$e^{-\beta H(\theta+s)} = U(s)^{-1} e^{-\beta H(\theta)} U(s)$$

for $s \in \mathbb{R}$, and consequently,

$$\text{tr } e^{-\beta H(\theta+s)} = \text{tr } e^{-\beta H(\theta)}.$$

Hence, tr $e^{-\beta H(\theta)}$ is independent of $Re(\theta)$, and so is independent of θ. $\square$.

If there is a complex deformation, $H(\theta)$, of H, such that (14.5) holds, we call $Z(\beta) = \text{tr } e^{-\beta H(\theta)}$ an *adiabatic partition function* for H, and $F(\beta) = -(1/\beta)\ln Z(\beta)$ the *free resonance energy* for H We interpret

$$E(\beta) \equiv ReF(\beta)$$

as the *resonance energy* at the temperature $1/\beta$,

$$\Gamma(\beta) \equiv -ImF(\beta)$$

as the *resonance decay probability per unit time* (or *resonance width*) at the temperature $1/\beta$, and

$$T(\beta) \equiv \frac{1}{\Gamma(\beta)}$$

as the *resonance lifetime* at the temperature $1/\beta$. The *resonance eigenvalue* for zero temperature is given by

$$z_r = E_r - i\Gamma_r \equiv \lim_{\beta\to\infty} F(\beta).$$

Usually, $|ImZ| << |ReZ|$. Hence,

$$E = ReF \approx -\frac{1}{\beta}\ln(ReZ)$$

and

$$\Gamma = -ImF = \frac{1}{\beta} Im \ln(1 + i\frac{ImZ}{ReZ}) \approx \frac{1}{\beta}\frac{ImZ}{ReZ}.$$

In fact, one can show that for $1 << t << \Gamma^{-1}$,

$$e^{-iHt/\hbar}\psi_0 = e^{-iz_r t/\hbar}\psi_0 + \text{ small}$$

if ψ_0 lies near E_r in the spectral decomposition of H. Note that

$$e^{-iz_r t/\hbar} = e^{-\Gamma_r t/\hbar} e^{-iE_r t/\hbar}$$

exhibits exponential decay at the (slow) rate Γ_r. This is consistent with our picture of a resonance as a meta-stable state.

14.3 Instantons

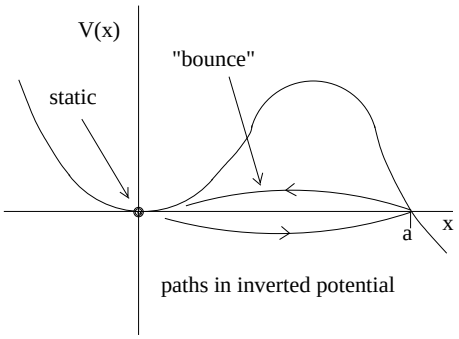
To compute $Z(\beta)$ we proceed as in the ground state problem; we represent $Z(\beta)$ formally as a path integral, and then apply the formal quasiclassical expansion (cf (13.9)):

$$Z(\beta/\hbar) = \sum_\omega N B_\omega^{1/2} e^{-S_e(\omega)/\hbar}$$

(as always we ignore the factor $(1 + O(\sqrt{\hbar}))$). Here, as before, ω are critical points of $S_e(\phi)$ of period β, N is a normalization factor independent of ω and H, and

$$B_\omega = \frac{\det S_0''(\omega_0)}{\det S_e''(\omega)}.$$

Now ω is a periodic classical path in imaginary time (or in inverted potential $-V(x)$), with period β large (see figure 14.6).



(14.6)

Two periodic solutions of arbitrarily large period are

$$\omega_s(s) \equiv 0$$

("s" for "static") and

$$\omega_b(s) : 0 \mapsto a \mapsto 0$$

("b" for "bounce"). ω_b is called an *instanton* or *bounce*. Since ω_s is a minimum of V, $V''(w_s) > 0$, and so

$$S_e''(\omega_s) = -\partial_s^2 + \Omega^2$$

where $\Omega^2 = V''(0)$. We computed before

$$B_{\omega_s} = \frac{\Omega\beta}{\sinh(\Omega\beta)} \approx \frac{\Omega\beta}{e^{\Omega\beta}}$$

for β large. Moreover, $S_e(\omega_s) = 0$. We will show later (section 14.5) that

$$B_{\omega_b}^{1/2} = -i\beta S_b^{-1/2} \left(\frac{\det{}^{\perp} S_e''(\omega_b)|}{\det S_0''(\omega_0)} \right)^{-1/2} \tag{14.7}$$

where

$$S_b \equiv S_e(\omega_b) = \int_{\omega_b} p \cdot dx$$

is the action of the "bounce", and

$$\det{}^{\perp} A \equiv \det(A|_{(\text{null } A)^{\perp}}). \tag{14.8}$$

Collecting these results, we have (for large β)

$$E = -\frac{1}{\beta}\ln(ReZ) \approx \frac{\hbar\Omega}{2}$$

and

$$\Gamma \approx -\frac{1}{\beta}\frac{ImZ}{ReZ} \approx \hbar S_b^{-1/2}\left(\frac{|\det{}^{\perp} S_e''(\omega_b)|}{\det S_e''(w_s)}\right)^{-1/2} e^{-S_b/\hbar}.$$

So the probability of decay of the state inside the well is

$$\Gamma = \text{ const } e^{-S_b/\hbar}$$

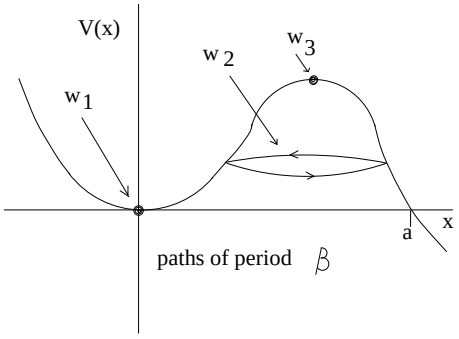
where $S_b = S(\omega_b)$ is the action of the instanton (which equals the length of the minimal geodesic in the Agmon metric $ds^2 = (V(x) - E)_+ dx^2$). This explains the sensitivity of the lifetimes of unstable nuclei to small variations of parameters (for example, weight determines isotopes).

Finally, we note that

$$\det S_e''(\omega_s) \approx \frac{e^{\Omega\beta}}{2\Omega}.$$

14.4 Finite temperatures (Josephson junction)

Consider quantum tunneling at finite temperatures ($\beta < \infty$). Now we have to consider all three critical paths of period β (see figure 14.9), $\omega_1 = \omega_s \equiv x_{min}$, $\omega_2 = \omega_b$, $\omega_3 \equiv x_{max}$.



(14.9)

Since $V''(x_{min}) > 0$, ω_1 is a minimal trajectory. As we will see, ω_b is a saddle point of Morse index 1. Finally, $V''(x_{max}) < 0$, and so ω_3 is also a saddle point.

For $k = 1, 3$,

$$S_e(\omega_k) = V(x_k)\beta$$

and for $k = 2, 3$,

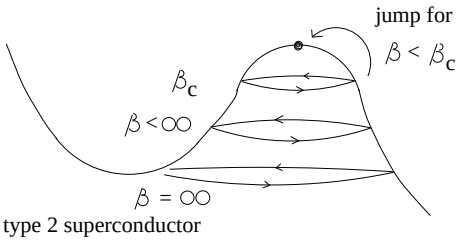
$$S_e(\omega_1) < S_e(\omega_k).$$

In this case, the quasi-classical expression for the decay probability is

$$\Gamma = -\frac{1}{\beta B_{\omega_1}}(ImB_{\omega_2}e^{-S(\omega_2)/\hbar} + ImB_{\omega_3}e^{-S(\omega_3)/\hbar}).$$

Through which trajectory, ω_2 or ω_3, does the tunneling take place? ω_3 corresponds to a thermally driven escape (due to thermal fluctuations), and ω_2 corresponds to a quantum tunneling escape. If β is very small (large temperature), the transition occurs through ω_3, as only ω_3 can have arbitrarily small period. On the other hand, if β is very large (small temperature), ω_2 sits close to the bottom of the well, and one can show that $S_e(\omega_2) < S_e(\omega_3)$. In this case, the transition occurs through ω_2.

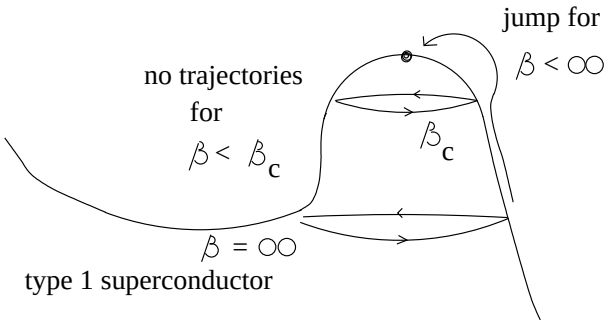
For intermediate temperatures, the tunneling depends radically on the geometry of the barrier. There is a critical value of β, $\beta_c \approx 2\pi/\Omega_{max}$ where $\Omega_{max}^2 = -V''(x_{max})$, at which a phase transition occurs; the transition is between the situations where decay is due to tunneling, and due to thermal fluctuations (crossover). In a superconductor of the second type the transition is continuous: as temperature decreases below $1/\beta_c$ (i.e. β increases above β_c) the tunneling trajectory bifurcates from ω_3 and slips down the barrier (see figure 14.10). For $\beta < \beta_c$ tunneling takes place through ω_3.



type 2 superconductor (14.10)

In a superconductor of the first type (see figure 14.11), there are no closed trajectories with period $> \beta_c$, so the transition is discontinuous: decay jumps from ω_3 to a

trajectory at the bottom of the barrier.



(14.11)

The result above supports the following physical picture of the tunneling process. With the Boltzmann probability $e^{-E/T}$, the particle is at an energy level E. The probability of tunneling from an energy level E is e^{-S_E} where S_E is the action of the minimal path at energy E. The probability of this process is $e^{-E/T-S_E}$. Thus the total probability of tunneling is

$$\int e^{-E/T-S_E} \approx Ce^{-E_0/T-S_{E_0}}$$

where E_0 solves the stationary point equation

$$\partial/\partial E(E/T + S_E) = 1/T + \partial S_E/\partial E = 0.$$

But $-\partial S_E/\partial E$ is the period of the trajectory under the barrier at the energy level $-E$, and $S_{E_0} + E_0/T$ is the action of a particle (in imaginary time) at the energy E_0 corresponding to the period $1/T$.

14.5 Pre-exponential factor for the bounce

The bounce solution, ω_b, presents some subtleties. ω_b breaks the translational symmetry of $S_e(\phi)$, and hence $\dot{\omega}_b$ is a zero-mode of $S_e''(\omega_b)$:

$$S_e''(\omega_b)\dot{\omega}_b = 0.$$

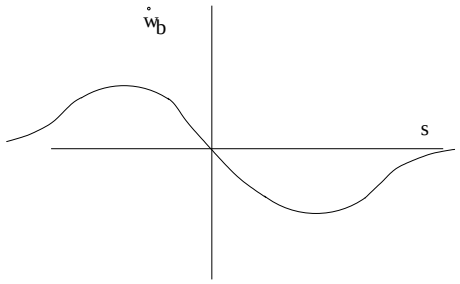
To establish this, simply differentiate the equation $\partial S_e(\omega_b) = 0$ with respect to s.

Thus we have two problems:

1. $S_e''(\omega_b)$ has a zero eigenvalue, so formally

$$[\det S_e''(\omega_b)]^{-1/2} = \text{ const } \int e^{-<\xi, S_e''(\omega_b)\xi>/2\hbar} D\xi = \infty \tag{14.12}$$

2. $\dot{\omega}_b$ has one zero (see figure 14.13), and so the Sturm-Liouville theory (from ordinary differential equations) tells us that, in fact, $S_e''(\omega_b)$ has exactly one negative eigenvalue.



(14.13)

This gives a second reason for the integral (14.12) to diverge.

To illustrate these divergences, we change variables. Write, for ϕ near ω_b, $\phi = \omega_b + \xi$ with

$$\xi = \sum_0^\infty a_k \xi_k,$$

where $\{\xi_k\}$ are the eigenfunctions of $S''(\omega_b)$ with eigenvalues λ_k (in increasing order). Then

$$S_e(\phi) \approx S_e(\omega_b) + \sum_0^\infty \lambda_k a_k^2.$$

But $\lambda_0 < 0$ and $\lambda_1 = 0$, hence we have two divergent integrals:

$$\int_{-\infty}^{\infty} e^{-\lambda_j a_j^2/2\hbar} da_j = \infty$$

for $j = 0, 1$. We already know that we can define the first integral by an analytic continuation to be

$$\int_{-\infty}^{\infty} e^{-\lambda_0 a_0^2/2\hbar} da_0 = \left(\frac{2\lambda_0}{\pi\hbar}\right)^{-1/2} = -i\left|\frac{2\lambda_0}{\pi\hbar}\right|^{-1/2}.$$

The second integral, correctly treated, is shown to contribute (see the following section)

$$S_b^{-1/2}\beta\sqrt{2\pi\hbar} \tag{14.14}$$

where S_b is the action of the "bounce", $S_e(\omega_b)$. Hence

$$\int_{\text{near } \omega_b} e^{-S_e(\phi)/\hbar} = B_{\omega_b} e^{-S(\omega_b)/\hbar}$$

where

$$B_{\omega_b}^{1/2} = -i\beta S_b^{-1/2} \left(\frac{|\det{}^{\perp} S_e''(\omega_b)|}{\det S_0''(\omega_0)} \right)^{-1/2}$$

(this is (14.7)) and $\det^{\perp}$ is defined in (14.8).

14.6 Contribution of the zero-mode

The virial theorem of classical mechanics gives

$$\int \dot{\omega_b}^2 = S(\omega_b) = S_b.$$

Define the normalized zero eigenfunction

$$\xi_1 = S_b^{-1/2} \dot{\omega_b}.$$

Then

$$(\omega_b + c_1\xi_1)(s) = \omega_b(s) + c_1 S_b^{-1/2} \dot{\omega_b}(s) \approx \omega_b(s + c_1 s_b^{-1/2}).$$

Hence

$$\phi \approx \omega_b(s + c_1 S_b^{-1/2}) + \sum_{n \neq 1} c_n \xi_n$$

and therefore

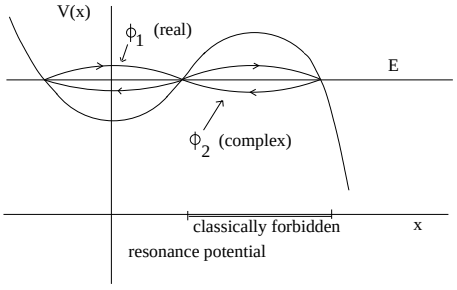
$$\prod_n dc_n = S_b^{-1/2} ds \prod_{n \neq 1} dc_n.$$

Integrating gives (14.14).

14.7 Bohr-Sommerfeld quantization for resonances

The goal of this section is derive a semi-classical formula for the resonance eigenvalues of a Schrödinger operator with a tunneling potential. We proceed by analogy with the treatment of a confining potential in section 13.3 which lead to the Bohr-Sommerfeld quantization rule.

As in the rest of this chapter, we consider a tunneling potential of the form sketched in figure 14.15.

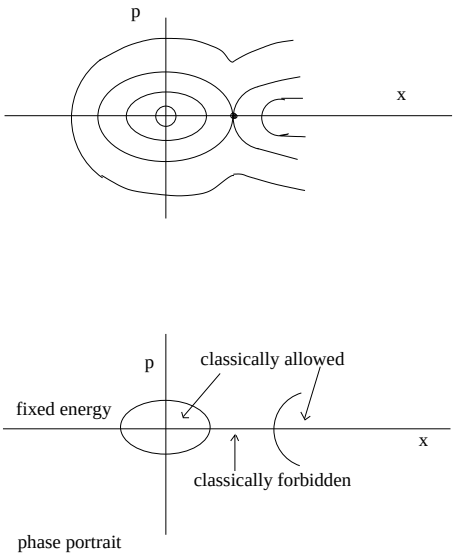


(14.15)

The path-integral expression for the Greens function of H is, as in section 13.2,

$$G_H(E, y, x) = \int_0^\infty \int_{P_{x,y,t}} e^{i(S(\phi,t)+Et)/\hbar}. \tag{14.16}$$

We seek critical points (because, as always, we wish to apply the method of stationary phase) which are closed trajectories ($x = y$) at the fixed energy E. The trajectories in phase space are shown in figure 14.17.

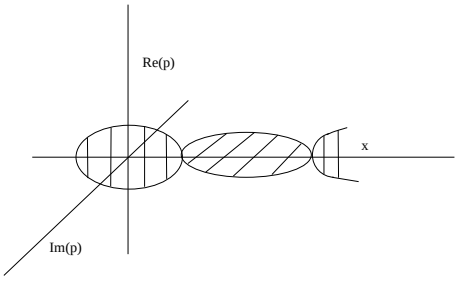


(14.17)

At energy E, phase-space is partitioned into classically allowed, and classically forbidden regions (as in figure 14.17). If we complexify the phase space

$$\mathbb{R} \times \mathbb{R} \mapsto \mathbb{C} \times \mathbb{C}$$

the picture becomes that shown in figure 14.18.



(14.18)

Thus we consider complex paths of the form $\alpha(\sigma) = \psi(-i\sigma)$, and $t = -i\tau$. Let

$$A(\psi, \tau) = \int_0^\tau \frac{m}{2}\dot{\psi}^2 + V(\psi).$$

Then

$$S(\alpha, -i\tau) = \int_0^\tau (-\frac{m}{2}\dot{\psi}^2 - V(\psi))(-i)d\sigma = iA(\psi, \tau)$$

and so

$$\partial_\alpha S = i\partial_\psi A, \qquad \text{and} \qquad \frac{\partial S(\alpha, -i\tau)}{\partial \tau} = i\frac{\partial A(\psi, \tau)}{\partial \tau}.$$

Thus the phase factor in (14.16) is

$$S(\alpha, -i\tau) + E(-i\tau) = i(A(\psi, \tau) - E\tau).$$

Now, the real critical point (ϕ_1, t) satisfies

$$\partial_\phi S = 0, \qquad \frac{\partial S(\phi_1, t)}{\partial t} = -E,$$

so ϕ_1 has period t, and $m\ddot{\phi_1} = -\nabla V(\phi_1)$ (as in figure 14.17). This has a phase

$$W_1 = S(\phi_1, t) - Et|_{\partial S/\partial t = -E}.$$

The complex critical point $(\phi_2(\sigma) = \psi_2(-i\sigma), i\tau)$ satisfies

$$\partial_\phi S(\alpha, -i\tau) = i\partial_\psi A(\psi, \tau) = 0$$

and

$$\frac{\partial S(\phi_2, -i\tau)}{\partial \tau} = i\frac{\partial A(\psi_2, \tau)}{\partial \tau} = iE,$$

so ψ_2 has period τ, and $m\ddot{\psi_2} = \nabla V(\psi_2)$ (as in figure 14.17). Hence the phase is

$$iW_2 = i(A(\psi_2, \tau) - E\tau)|_{\frac{\partial A(\psi_2,\tau)}{\partial \tau}=E}$$

We can characterize a general closed critical orbit by the list

$$(1, m_1, 1, m_2, 1, m_3, \ldots),$$

meaning the real closed CP is traversed once, the complex closed CP is traversed m_1 times, the real CP is followed again, then the complex CP m_2 times, etc. (we follow the real CP several times in succession if some of the m_i are zero). Applying the stationary phase method, we obtain the following contribution to the path integral:

$$\sum_{n=0}^{\infty} \sum_{m_1 \ldots m_n} e^{i(1+n)W_1/\hbar - (m_1+\cdots+m_n)W_2/\hbar}$$

$$= e^{iW_1/\hbar} \sum_{n\geq 0} (e^{iW_1/\hbar} \sum_{m=0}^{\infty} e^{-mW_2/\hbar})^n$$

$$= e^{iW_1/\hbar} \sum_{n=0}^{\infty} (e^{iW_1/\hbar} \frac{1}{1-e^{-W_2/\hbar}})^n = e^{iW_1/\hbar} \frac{1}{1 - e^{iW_1/\hbar} \frac{1}{1-e^{-W_2/\hbar}}}$$

$$= \frac{e^{iW_1/\hbar}(1 - e^{-W_2/\hbar})}{1 - e^{iW_1/\hbar} - e^{-W_2/\hbar}}.$$

Writing the lowest resonance eigenvalue as $E_0 - i\Delta E$ and expanding $e^{iW_1(E)/\hbar}$ to first order around E_0, and $e^{-W_2(E)/\hbar}$ to zeroth order, gives the equation

$$e^{iW_1(E_0)/\hbar} = 1$$

for E_0 (i.e. E_0 is the ground state energy, as before), and the expression

$$\Delta E = \hbar \left(\frac{\partial W_1(E_0)}{\partial E} \right)^{-1} e^{-W_2(E_0)/\hbar}$$

for ΔE. The last two equations represent the Bohr-Sommerfeld quantization for resonances.

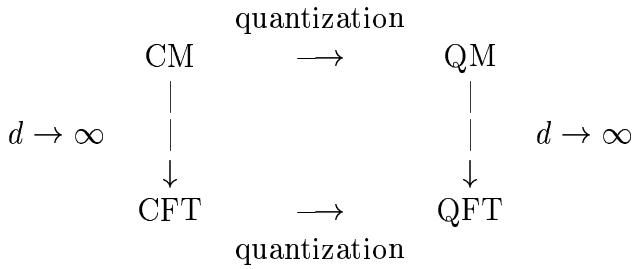
Chapter 15

Introduction to quantum field theory

The goal of quantum field theory (which we will often abbreviate as QFT) is to describe elementary particles and their interactions. Its mathematical framework can be thought of as partial differential equations (PDEs) in infinitely many variables. QFT has deep connections with a variety of disciplines, including statistical mechanics and condensed matter physics, probability theory (ie stochastic PDEs), and nonlinear PDEs.

15.1 The place of QFT

All physical theories can be classified by two sets of parameters: whether they describe particles (point or localized objects) or fields (extended objects), and whether they are classical (e.g. the results of experiments are deterministic) or quantum (measurement results are probabilistic). With this classification in mind, we have the following diagram displaying the place of QFT relative to classical mechanics (CM), classical field theory (CFT), and quantum mechanics (QM) (here d is the number of degrees of freedom):



The two physical CFTs are electro-magnetism (EM) (governed by Maxwell's equations) and gravity (governed by Einstein's equations). When one "quantizes" Maxwell's equations, one obtains the theory of quantum electrodynamics (QED). The appropriate quantization of the Einstein equations is unknown.

In addition, there are many "mock" CFTs (ie non-physical ones) which exist only to be quantized. These include the theories given by the Klein-Gordon equation, and the Yang-Mills equations (gauge field theory). These are both variations on the EM theory. The former is obtained by replacing the vector structure of EM by a complex one, and the latter is a non-commutative generalization.

15.1.1 Physical Theories

A physical theory specifies what it means for a system to be in a particular "state" (the state space), how this state evolves in time (evolution law), and how this state corresponds to the outcomes of physical measurements on the system (observables). The table (5.4) displays the objects describing CM and QM.

We will introduce QFT by quantizing CFT. We do this by analogy with the quantization of CM (ie, the passage to QM). We will see later that this analogy suggests we have to put CFT, which is originally given in terms of a PDE, into Hamiltonian form. This is done in two steps: introducing the principle of minimal action, and the Legendre transform.

15.1.2 Principle of minimal action

The principle of minimal action (properly, of "stationary" action) states that evolution equations for physical states are Euler-Lagrange equations for a certain functional called the *action* (see Chapter 11 for examples of functionals and Euler-Lagrange equations).

More precisely, we define on our space of possible fields, ϕ, a functional, S, such that ϕ is a solution to the CFT equation if and only if $\delta S(\phi) = 0$. In particular, we

consider a class of examples from Chapter 11:

$$S(\phi) = \int_0^T \int_{\mathbb{R}^d} \mathcal{L}(\phi(x,t), \nabla_x \phi(x,t), \dot{\phi}(x,t)) d^d x dt \tag{15.1}$$

for $\phi : \mathbb{R}^d_x \times \mathbb{R}_t \to \mathbb{R}$. Here, $\mathcal{L}$ is the *Lagrangian density*. Specializing further, we have the following important example of a classical field theory:

Example 15.1 [Klein-Gordon field theory] The KG Lagrangian density is

$$\mathcal{L}(\phi, \dot{\phi}) = \frac{1}{2}(\dot{\phi})^2 - \frac{1}{2}|\nabla_x \phi|^2 - F(\phi).$$

The corresponding *Lagrangian functional*,

$$L(\phi, \dot{\phi}) = \int_{\mathbb{R}^d} \left\{ \frac{1}{2}(\dot{\phi}^2 - |\nabla_x \phi|^2) - F(\phi) \right\}$$

is defined on $H^1(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$ (at least if $F(0) = \nabla F(0) = 0$). We recall from Chapter 11 that the corresponding critical point equation is

$$\Box \phi + \nabla F(\phi) = 0 \tag{15.2}$$

the *Klein-Gordon equation*.

The set of functions ϕ on which S is defined will, in general, be a space of paths

$$\phi : [0, T] \to X$$

in some (infinite dimensional) space X. X is called the *configuration space* of the physical system, and its elements are called fields. In our case, X is always a space of functions on some finite-dimensional manifold. In general, X could be curved, but for simplicity we assume X is a Hilbert space. We remark that in general, the Lagrangian functional is defined on (a subspace of) TX, the tangent bundle of X.

15.2 Klein-Gordon theory as a Hamiltonian system

In this section we describe (infinite-dimensional) Hamiltonian systems, and write the Klein-Gordon theory as a Hamiltonian system.

15.2.1 Legendre transform

Definition 15.2 *If f is a convex, differentiable function/functional, ($\partial^2 f > 0$) on an inner-product space, the* Legendre transform*, g, of f, is defined by*

$$g(\pi) \equiv sup_u(\langle u, \pi\rangle - f(u)) \tag{15.3}$$
$$= (\langle u, \pi\rangle - f(u))|_{u:\partial f(u)=\pi}.$$

Problem 15.3 Show that g is also convex, and that (Legendre transform)$^2 = id$.

Example 15.4 The Legendre transform maps the given functions/functionals as follows (these are easily verified):

1. $f(v) = \frac{m|v|^2}{2} \mapsto g(k) = \frac{|k|^2}{2m}$
2. $f(\psi) = \frac{1}{2}\int |\psi|^2 \mapsto g(\pi) = \frac{1}{2}\int |\pi|^2$
3. $L(x,v) = \frac{mv^2}{2} - V(x) \mapsto$ (Leg. trans. in v) $H(x,k) = \frac{k^2}{2m} + V(x)$
4. $L(\phi,\psi) = \int\{\frac{1}{2}(|\psi|^2 - |\nabla\phi|^2) - F(\phi)\}d^nx \mapsto$ (Leg. trans. in ψ) $H(\phi,\pi) = \int\{\frac{1}{2}(|\pi|^2 + |\nabla\phi|^2) + F(\phi)\}d^nx$

15.2.2 Hamiltonians

Suppose the dynamics of a system are determined by the principle of minimal action with a Lagrangian function/functional on a configuration space X,

$$L : TX \to \mathbb{R}.$$

Then a *Hamiltonian function/functional* for the system is the Legendre transform (in the tangent space variable) of L

$$H : T^*X \to \mathbb{R}.$$

15.2.3 Poisson brackets

Let Z be a vector space, which we call the *state space*. For example, the classical mechanics state space for a single particle is $Z = \mathbb{R}^3 \times \mathbb{R}^3$, and the Klein-Gordon state space is $Z = H^1(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$. Suppose F and G are differentiable functions/functionals on Z. Then a *Poisson bracket* of F and G is a function(al), $\{F, G\}$, on Z, satisfying

1. $\{\cdot,\cdot\}$ is bilinear
2. $\{F,G\} = -\{G,F\}$ (skew-symmetry)
3. $\{A,\{B,C\}\} + \{B,\{C,A\}\} + \{C,\{A,B\}\} = 0$ (Jacobi identity).

Remark 15.5 *The set of functionals, with the Poisson bracket, form a* Lie Algebra.

Example 15.6 If Z is an inner-product space, the following construction produces a Poisson bracket:

1. Assume there is a linear operator J on Z such that $J^* = -J$ (J is a *symplectic* operator). Then
$$\{F,G\} =< \partial F, J\partial G >$$
is a Poisson bracket (check this).
2. (CM) If $Z = \mathbb{R}^3 \times \mathbb{R}^3$, then
$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{15.4}$$
is a symplectic operator, giving the Poisson bracket
$$\{F,G\} = \nabla_x F \cdot \nabla_k G - \nabla_k F \cdot \nabla_x G.$$
3. (KG) If $Z = H^1(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$ and J is as in (15.4), the Poisson bracket is
$$\{F,G\} = \int \{\partial_\pi F \partial_\phi G - \partial_\phi F \partial_\pi G\}. \tag{15.5}$$

Definition 15.7 *A* Hamiltonian system *is a Poisson space (a vector space Z with a Poisson bracket) together with a Hamiltonian defined on that space.*

Example 15.8 Our two main examples of Hamiltonian systems are

1. (CM) $Z = \mathbb{R}^3 \times \mathbb{R}^3$ with bracket as above, and Hamiltonian
$$h(x,k) = \frac{1}{2m}|k|^2 + V(x)$$
2. (KG) $Z = H^1(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$ with bracket as above and Hamiltonian
$$H(\phi,\pi) = \frac{1}{2}\int \{|\pi|^2 + |\nabla\phi|^2 + F(\phi)\}$$

15.2.4 Hamilton's equations

Suppose Z is a Hamiltonian system, and assume Z is a function space over $\mathbb{R}^n$. The functional on Z which maps $\Phi \mapsto \Phi(x)$ is called the *evaluation functional* (at x), which we denote (with some abuse of notation) as $\Phi(x)$.

Definition 15.9 Hamilton's equations *are*

$$\dot{\Phi}(x) = \{\Phi(x), H\} \tag{15.6}$$

for all x.

Example 15.10 If the Poisson structure is given by a symplectic operator J, then

$$\{\Phi(x), H\} = \int \partial_\Phi \Phi J \partial_\Phi H = \int \delta_x J \partial_\Phi H = J \partial_\Phi H(x)$$

which leads to Hamilton's equation

$$\dot{\Phi} = J \partial_\Phi H(\Phi). \tag{15.7}$$

We have the following basic result, whose proof if left as an exercise:

Theorem 15.11 *1. A path Φ_t in Z solves (15.6) iff*

$$d/dt F(\Phi_t) = \{F(\Phi_t), H\}$$

for all functionals F.

2. If $L(\phi, \psi)$ and $H(\phi, \pi)$ are related by a Legendre transform (in $\psi \leftrightarrow \pi$), then the Euler-Lagrange equations for

$$S(\phi, \dot{\phi}) = \int_0^T L(\phi, \dot{\phi}) dt$$

are equivalent to the Hamilton equation (15.6).

Problem 15.12 Prove this theorem.

We verify this result in the KG case. With

$$\Phi = \begin{pmatrix} \phi \\ \pi \end{pmatrix}$$

a path in $H^1(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$, equation (15.7) is

$$\begin{pmatrix} \dot{\phi} \\ \dot{\pi} \end{pmatrix} = J \begin{pmatrix} -\Delta\phi + F'(\phi) \\ \pi \end{pmatrix}$$

and we immediately recover the Klein-Gordon equation.

Problem 15.13 Show formally, that with the Poisson bracket given in (15.5),

$$\{\pi(x), \phi(y)\} = \delta(x - y). \tag{15.8}$$

Remark 15.14 *Equation (15.8) says that the evaluation functionals, π, and ϕ, are* canonical coordinates. *We can make (15.8) rigorous by introducing, for $f \in C_0^\infty$, the functionals $\phi(f) : (\phi, \pi) \mapsto < f, \phi >$ and $\pi(f) : (\phi, \pi) \mapsto < f, \pi >$. The rigorous version of (15.8) is then $\{\pi(f), \phi(g)\} = < f, g >$.*

15.3 Maxwell's equations as a Hamiltonian system

Here we write Maxwell's equations in Hamiltonian form, as a prelude to quantizing EM.

The Maxwell equations in a vacuum are

$$\nabla \cdot E = 0 \qquad \nabla \times B = \partial E/\partial t \tag{15.9}$$

$$\nabla \times E = -\partial B/\partial t \qquad \nabla \cdot B = 0 \tag{15.10}$$

for vector fields $E : \mathbb{R}^{3+1} \to \mathbb{R}^3$ (the electric field) and $B : \mathbb{R}^{3+1} \to \mathbb{R}^3$ (the magnetic field).

The equations (15.10) imply the existence of potentials $U : \mathbb{R}^{3+1} \to \mathbb{R}$ and $A : \mathbb{R}^{3+1} \to \mathbb{R}^3$ such that

$$E = -\partial A/\partial t - \nabla U \qquad B = \nabla \times A.$$

There is a redundancy in the choice of A, U. Specifically, any *gauge transformation*

$$A \mapsto A + \nabla\chi \qquad U \mapsto U - \partial\chi/\partial t$$

for $\chi : \mathbb{R}^{3+1} \mapsto \mathbb{R}$ leaves Maxwell's equations invariant. By appropriate choice of χ, we may take

$$U \equiv 0 \qquad \nabla \cdot A = 0$$

(ie A is *transverse*) which is called the *Coulomb gauge*. From now on, we work in this gauge. Thus, we have

$$E = -\partial A/\partial t \qquad B = \nabla \times A$$

and using the second equation of (15.9) results in

$$\Box A = 0 \qquad \nabla \cdot A = 0. \tag{15.11}$$

We recall from Chapter 11, that equation (15.11) is the Euler-Lagrange equation for the action

$$S(A) = \frac{1}{2}\int\int \{|\dot{A}|^2 - |\nabla \times A|^2\} \tag{15.12}$$

where the variation is among transverse vector fields.

Problem 15.15 Show that the Hamiltonian corresponding to (15.12) is

$$H(A, E) = \frac{1}{2}\int \{|E|^2 + |\nabla \times A|^2\} = \frac{1}{2}\int \{|E|^2 + |B|^2\}$$

where E is the dual field to A, and $\nabla \cdot E = 0$.

The phase space for this Hamiltonian is

$$Z = H^{1,trans}(\mathbb{R}^3; \mathbb{R}^3) \oplus L^{2,trans}(\mathbb{R}^3; \mathbb{R}^3),$$

a Sobolev space of transverse vector fields.

Let T be the projection operator of vector fields onto transverse vector fields:

$$TF \equiv F - (\Delta)^{-1}\nabla(\nabla \cdot F).$$

Problem 15.16 Check that $\nabla \cdot (TF) = 0$.

We define the Poisson bracket on Z by

$$\{F, G\} = \langle \partial_{A,E} F, J_T \partial_{A,E} G \rangle$$

where

$$J_T \equiv \begin{pmatrix} 0 & -T \\ T & 0 \end{pmatrix}.$$

Problem 15.17 Check that Maxwell's equations are equivalent to the Hamilton equations

$$\dot{\phi} = J_T \partial_\phi H(\phi) \qquad \phi = (A, E).$$

We make two final comments.

1. Note that
$$\{E_i(x), A_j(y)\} = T_{ij}(x - y)$$
where $T_{ij}(x-y)$ is the matrix integral kernel of T. We still refer to A and E as canonical variables, but with *constraints*.

2. The first Hamilton equation
$$\dot{A} = T \partial_E H(A, E) = -TE = -E$$
shows that the conjugate field E is, in fact, the electric field, as the notation suggested in the first place.

15.4 Quantization of Klein-Gordon and Maxwell equations

We are now ready to attempt to quantize the Klein-Gordon theory. We begin with Klein-Gordon theory in Hamiltonian form, and proceed, naively at first, by analogy with the passage from classical mechanics to quantum mechanics (which is summarized in the table (5.4)). We take, for now,

$$F(\phi) = \frac{1}{2} m^2 |\phi|^2$$

with $m > 0$.

15.4.1 The quantization procedure

Under quantization, the classical phase space

$$Z = H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$$

with the Poisson bracket arising from the symplectic matrix J, becomes the quantum state space

$$L^2(H^1(\mathbb{R}^3), D\phi)$$

(i.e. L^2(config. space) with respect to a "Lebesgue measure" on configuration space) together with the commutator $\frac{i}{\hbar}[\cdot,\cdot]$ of operators on the state space. The classical observables, real-valued functionals on the phase space, become quantum observables - self-adjoint operators on the state space $L^2(H^1)$. In particular, the classical canonical variables

$$\phi^{cl}(x) \quad \text{and} \quad \pi^{cl}(x)$$

become the operators

$$\phi^{op}(x) = \text{ mult. by } \phi(x) \qquad \pi^{op}(x) = -i\hbar\partial_{\phi(x)}$$

on the state space $L^2(H^1)$.

The classical KG dynamics are generated by the Hamiltonian functional

$$H(\phi,\pi) = \frac{1}{2}\int \{|\pi|^2 + |\nabla\phi|^2 + m^2|\phi|^2\}$$

which, under quantization, becomes the Schrödinger operator

$$H = H(\phi^{op}, \pi^{op})$$

on state space.

Before proceeding to discuss the problems with this naive approach, we remark that the state space $L^2(H^1)$ is a space of functionals on an infinite-dimensional space of functions, and the quantum observables can be thought of as infinite-dimensional pseudo-differential operators.

Right away, our approach has serious problems.

Problem 1: There is, in fact, no Lebesgue (translation invariant, sigma-finite) measure on infinite-dimensional spaces. We are forced to resort to measures known to exist on such spaces: Gaussian measures.

Correction 1: We replace $D\phi$ with $d\mu_C(\phi)$, the Gaussian measure of mean 0 and covariance operator C. The operator C acts on $L^2(\mathbb{R}^3)$.

One way to describe $d\mu_C$ is through finite-dimensional approximations of the function space. Suppose

$$\cdots \subset F_n \subset F_{n+1} \subset \cdots$$

is a sequence of finite-dimensional subspaces of H^1, whose limit is H^1. Then

$$d\mu_c|_{F_n}(\phi) = M_n(\det C_n)^{-1/2} e^{-<\phi, C_n^{-1}\phi>/2} D\phi$$

where $D\phi$ is the usual Lebesgue measure on a finite-dimensional space, C_n is C restricted to F_n, and M_n is a normalization constant chosen such that

$$\int_{F_n} d\mu_C(\phi)|_{F_n} = 1.$$

We introduce the *expected value* of a functional F with respect to $d\mu_C$

$$E(F) \equiv \int F(\phi) d\mu_C(\phi).$$

The terminology "mean 0" and "covariance C" corresponds to the properties

$$E(\phi(x)) = 0$$

and

$$E(\phi(x)\phi(y)) = C(x,y)$$

where $C(x,y)$ is the integral kernel of C. For the Klein-Gordon theory, we take

$$C = \frac{1}{2}(-\Delta + m^2)^{-1/2}$$

(recall $-\Delta + m^2 > 0$, so this makes sense). To get an idea of the origin of this choice, note that the classical Klein-Gordon Hamiltonian is

$$H(\phi,\pi) = \frac{1}{2}\int \{\pi^2 + |\nabla\phi|^2 + m^2|\phi|^2\}$$

$$= \frac{1}{2}\int \{\pi^2 + \phi(-\Delta + m^2)\phi\} = \frac{1}{2}\int \{\pi^2 + |(-\Delta + m^2)^{1/2}\phi|^2\} \qquad (15.13)$$

$$= \frac{1}{2}\int \{\pi^2 + |\frac{1}{2}C^{-1}\phi|^2\}.$$

But we are not out of the woods yet.

Problem 2: It turns out that

$$\mu_C(H^1(\mathbb{R}^3)) = 0.$$

To see that there is a problem, we compute formally

$$E(\int |\nabla\phi|^2) = \int\int \delta(x-y)\nabla_x\nabla_y E(\phi(x)\phi(y))d^3x d^3y$$

$$= \int\int \delta(x-y)\nabla_x\nabla_y C(x,y)d^3x d^3y.$$

If $C = c(-i\nabla_x)$ then $C(x,y) = \check{c}(x-y)$ and so

$$E(\int |\nabla\phi|^2) = (\Delta\check{c})(0).$$

For $C = (-\Delta + m^2)^{-1/2}$, we have

$$\check{c}(x) = (2\pi)^{-3/2}\int e^{ik\cdot x}(|k|^2 + m^2)^{-1/2}d^3k$$

$$= const.|x|^{-2} + o(|x|^{-2}) \quad \text{as} \quad |x| \to 0.$$

Thus $E(\int |\nabla\phi|^2) = \infty$, indicating that $\mu_C(H^1(\mathbb{R}^3)) = 0$.

This argument suggests that $\check{c}(x)$ must be *integrated* at least $d-1 = 2$ times in order to remove the singularity at $x = 0$. We expect, then, that $E(\int |\nabla^{-s}\phi|^2) < \infty$ for $s > (d-1)/2 = 1$, and

$$\mu_C(H^{-s}(\mathbb{R}^d)) = \begin{cases} 0 & s < (d-1)/2 \\ 1 & s > (d-1)/2 \end{cases}$$

Here $H^s(\mathbb{R}^d)$ is the Sobolev space of order s:

$$H^s(\mathbb{R}^d) = \{f \mid (1-\Delta)^{s/2}f \in L^2\}$$

(note $H^{s'} \subset H^s \subset L^2 \subset H^{-s} \subset H^{-s'}$, $s' > s > 0$).

Vectors in the space $L^2(H^{-s}, d\mu_C)$ are functionals $F(\phi)$ on H^{-s} such that

$$\int |F(\phi)|^2 d\mu_C(\phi) < \infty.$$

The most basic example of such a functional is as follows. Fix $f \in H^s$. Then the map

$$\phi \in H^{-s} \mapsto \int f\phi \equiv f(\phi) \equiv \phi(f)$$

is a linear functional on H^{-s} which is in $L^2(H^{-s}, d\mu_C)$. We compute formally

$$E(|\int f\phi|^2) = \int\int f(x)f(y)E(\phi(x)\phi(y)) =< f, Cf > < \infty.$$

More generally, let $p(t_1, \ldots, t_n)$ be a polynomial in $t_1, \ldots, t_n$ and fix $f_1, \ldots, f_n \in H^s$. Then the functional

$$F : \phi \in H^{-s} \mapsto p(\phi(f_1), \ldots, \phi(f_n))$$

is an element of $L^2(H^{-s}, d\mu_C)$.

To summarize then, we have made the following correction:

Correction 2: replace $L^2(H^1(\mathbb{R}^3), D\phi)$ by $L^2(H^{-s}(\mathbb{R}^3), d\mu_C)$ where $C = (-\Delta + m^2)^{-1/2}$ and $s > (d-1)/2$.

Unfortunately, the first correction has generated a further problem: $-i\partial_\phi$ is not symmetric on $L^2(H^{-s}, d\mu_C)$. In fact, we have the following integration by parts formula

$$\int \bar{F}(-i\partial_\phi G)d\mu_C(\phi) = \int \overline{(-i\partial_\phi F)}Gd\mu_C(\phi) + i\int \bar{F}G\partial_\phi d\mu_C(\phi)$$

$$= \int \overline{(-i\partial_\phi + iC^{-1}\phi)F}Gd\mu_C(\phi)$$

where we have used

$$\partial_\phi d\mu_C(\phi) = -C^{-1}\phi d\mu_C(\phi).$$

To see this, think formally about the Gaussian measure as being

$$d\mu_C(\phi) = \text{ const } e^{-<\phi, C^{-1}\phi>/2}D\phi.$$

Thus we have

$$(-i\partial_\phi)^* = -i\partial_\phi + iC^{-1}\phi$$

which leads us to the following correction.

Correction 1a:

$$-i\hbar\partial_\phi \mapsto \pi \equiv -i\hbar\partial_\phi + \frac{\hbar}{2}iC^{-1}\phi.$$

Note now that $\pi^* = \pi$, as desired.

Problem 15.18 Derive formally the commutation relations

$$\frac{i}{\hbar}[\pi(x), \phi(y)] = \delta(x-y) \tag{15.14}$$

$$\frac{i}{\hbar}[\pi(x), \pi(y)] = \frac{i}{\hbar}[\phi(x), \phi(y)] = 0.$$

We have improved our situations somewhat, but a serious problem still remains:
Problem 3: $H(\phi, \pi) = \infty$.
Specifically, we will prove the following a bit later:

Proposition 15.19

$$\frac{1}{2}\int \{\pi^2 + |\nabla\phi|^2 + m^2\phi^2\} = \infty.$$

Note, however, that ϕ and π are operator-valued distributions ($\in H^{-s}$), and there is no reason to expect this expression to be finite.

Correction 3: We "Wick order" H

$$H(\phi^{cl}, \pi^{cl}) \mapsto : H(\phi, \pi) :$$

We will postpone the description of this procedure for a little while.

Let us now pause and summarize our corrected quantization procedure in the table below.

	KGCFT	KGQFT
state space	$H^1(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$	$L^2(H^{-s}(\mathbb{R}^3), d\mu_C)$, $s > 1$
canonical variables	$\phi^{cl}(x)$ $\pi^{cl}(x)$	$\phi(x) =$ mult by $\phi(x)$ $\pi(x) = -i\hbar\partial_{\phi(x)} + \frac{i\hbar}{2}C^{-1}\phi(x)$
observables	$F(\phi^{cl}, \pi^{cl}) : H^1 \times L^2 \to \mathbb{R}$	self-adjoint operators $: F(\phi, \pi) :$ on $L^2(H^{-s}, d\mu_C)$
dynamics	Hamiltonian $H(\phi^{cl}, \pi^{cl})$ Poisson brackets $\{\pi^{cl}(x), \phi^{cl}(y)\} = \delta(x-y)$	Schrödinger operator $H =: H(\phi, \pi) :$ $\frac{i}{\hbar}$ (commutator) $\frac{i}{\hbar}[\pi(x), \phi(y)] = \delta(x-y)$

Before moving on, we make a remark about mathematical rigor. Strictly speaking, ϕ and π are operator-valued distributions. Though $\phi(x)$, for example, is not well-defined, $\phi(f)$ (for a test function $f \in H^s$) is well-defined. We think formally of $\phi(f)$ as $\int \phi(x)f(x)dx$. In particular, the correct expression for the commutation relation (15.14) is

$$\frac{i}{\hbar}[\pi(f), \phi(g)] = < f, g > .$$

Theorem 15.20 *For all $f \in H^s$, $\phi(f)$ and $\pi(f)$ are self-adjoint operators on $L^2(H^{-s}, d\mu_C)$.*

We omit the proof.

15.4.2 Creation and annihilation operators

Definition 15.21 *The* annihilation operator $a(f)$, *and the* creation operator $a^*(f)$ *are defined by*

$$a(f) = \frac{1}{2}\phi(C^{-1/2}f) + i\pi(C^{1/2}f) \tag{15.15}$$

$$a^*(f) = \frac{1}{2}\phi(C^{-1/2}f) - i\pi(C^{1/2}f). \tag{15.16}$$

Problem 15.22 Establish the commutation relations

$$[a(f), a^*(g)] = \hbar < f, g >$$

$$[a(f), a(g)] = [a^*(f), a^*(g)] = 0$$

for $f, g \in H^s$.

We now find the expression for the Hamiltonian operator

$$H(\phi, \pi) = \frac{1}{2}\int \{\pi^2 + |\nabla\phi|^2 + m^2\phi^2\}$$

in terms of the creation and annihilation operators. As in (15.13), we can write

$$H(\phi, \pi) = \frac{1}{2}\int \{\pi^2 + (\frac{1}{2}C^{-1}\phi)^2\} = \frac{1}{2}\int \{[\frac{i}{2}C^{-1/2}(a^* - a)]^2 + [\frac{1}{2}C^{-1/2}(a^* + a)]^2\}$$

$$= \frac{1}{4}\int \{C^{-1/2}a^*C^{-1/2}a + C^{-1/2}aC^{-1/2}a^*\} = \frac{1}{2}\int a^*C^{-1}a + \frac{\hbar}{4}\int (C^{-1}\delta)(0)dx$$

where we have used the commutation relation for a and a^*, and the self-adjointness of C. The first term is non-negative, and the second is infinite, which establishes, formally, proposition 15.19.

We can make this argument rigorous as follows. First, we move to momentum space via the Fourier transform: $a(x) \mapsto \hat{a}(k)$, $a^*(x) \mapsto \hat{a}^*(k)$. We wish to show that $\int \omega(k)\hat{a}(k)\hat{a}^*(k)dk = \infty$, where $\omega(k) = (|k|^2 + m^2)^{1/2}$ (the *dispersion law*). Let $\mathbb{R}^3 = \cup_{\alpha\in\mathbb{Z}^3} B_\alpha$ (a disjoint union), $a_\alpha = \int_{B_\alpha} \hat{a}$, and $\omega_\alpha = \min_{k\in B_\alpha} \omega(k)$. Then

$$[a_\alpha, a_\beta^*] = (\text{ vol } B)\delta_{\alpha,\beta}$$

so that

$$\int \omega \hat{a}\hat{a}^* \geq \text{ vol } B \sum_{\alpha\in\mathbb{Z}^3} \omega_\alpha a_\alpha a_\alpha^*.$$

On the other hand,

$$\sum \omega_\alpha a_\alpha a_\alpha^* = \sum \omega_\alpha a_\alpha^* a_\alpha + \text{ vol } B \sum \omega_\alpha = \infty.$$

15.4.3 Wick ordering

We now describe the process of *Wick ordering* or *Wick quantization* mentioned in an earlier section.

Let $A(\phi^{cl}, \pi^{cl})$ be a classical observable.

1. We express $A(\phi^{cl}, \pi^{cl})$ in terms of α and α^*, where

$$\alpha = \frac{1}{2}C^{-1/2}\phi^{cl} + iC^{1/2}\pi^{cl}$$

and

$$\alpha^* = \frac{1}{2}C^{-1/2}\phi^{cl} - iC^{1/2}\pi^{cl}$$

to obtain

$$A(\phi^{cl}, \pi^{cl}) = B(\alpha, \alpha^*).$$

2. In the expression for B, move all α^*'s to the left of the α's, to obtain an expression of the form

$$B(\alpha, \alpha^*) = \sum_{n,m} \int B_{n,m}(\alpha^*)^n \alpha^m.$$

3. Now we quantize the observable A as follows:

$$A(\phi^{cl}, \pi^{cl}) \mapsto : A(\phi, \pi) :\equiv \sum_{n,m} \int B_{n,m} (a^*)^n a^m.$$

This is the Wick ordered observable.

Here are some examples of Wick ordering:

Example 15.23

1.
$$\begin{aligned} &: \phi^2 :=: [C^{1/2}(a + a^*)]^2 : \\ =&: (C^{1/2}a)^2 + (C^{1/2}a^*)^2 + C^{1/2}a^*C^{1/2}a + C^{1/2}aC^{1/2}a^* \\ &= (C^{1/2}a)^2 + (C^{1/2}a^*)^2 + 2C^{1/2}a^*C^{1/2}a. \end{aligned}$$

2. As before,

$$H = \frac{1}{2} : \int \{\pi^2 + |\nabla\phi|^2 + m^2\phi^2\} := \frac{1}{2} \int a^* C^{-1} a.$$

Problem 15.24 [see [GJ]] Let $c =< f, Cf >= E(\phi(f)^2)$. Show

1. $: \phi(f)^n := c^{n/2} P_n(c^{-1/2}\phi(f))$ where P_n is the n^{th} Hermite polynomial
2. $: e^{\phi(f)} := e^{\phi(f) - c/2}$.

15.4.4 Quantizing Maxwell's equations

The procedure described above for the quantization of the Klein-Gordon theory carries over to the case of Maxwell's equations, whose Hamiltonian formulation was given in section 15.3.

There are two essential differences, which we list here.

1. There is no mass, $m = 0$, in the EM case. That is, the dispersion law in this case is $\omega(k) = |k|$ (equivalently, the covariance operator is $\frac{1}{2}(-\Delta)^{-1/2}$).
2. The quantized $A(x)$ and $E(x)$ are operator-valued transverse vector fields. That is, our quantum state space is $L^2(H^{-s,trans})$

The Hamiltonian for the quantized EM theory is, of course, just

$$H = \frac{1}{2}\int : |E|^2 + |\nabla \times A|^2 :$$

and the non-trivial commutation relation is

$$\frac{i}{\hbar}[E(x), A(y)] = T(x-y)(id)$$

where $T(x-y)$ is the integral kernel of the operator of projection onto the transverse vector fields.

15.5 Fock space

We return now to the Klein-Gordon theory. We will revise slightly our definitions of the annihilation and creation operators, $a(x)$ and $a^*(x)$, which were originally defined by (15.15-15.16), and which act on $L^2(H^{-s}, d\mu_C)$. We will now take

$$a(f) = \frac{1}{2}\phi(C^{-1/2}f) + \frac{i}{\hbar}\pi(C^{1/2}f)$$

$$a^*(f) = \frac{1}{2}\phi(C^{-1/2}f) - \frac{i}{\hbar}\pi(C^{1/2}f).$$

Note that

$$a = \frac{1}{2}C^{-1/2}\phi + \frac{i}{\hbar}C^{1/2}\pi = C^{1/2}\partial_\phi.$$

Thus the only solution to the equation $a\Omega = 0$ is $\Omega = \text{const}$. We thus set $\Omega \equiv 1$, and call it the *vacuum*.

Theorem 15.25 *Any vector $\phi \in L^2(H^{-s}, d\mu_C)$ can be written as*

$$\phi = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \int \phi_n(x_1, \ldots, x_n) a^*(x_1) \cdots a^*(x_n) \Omega dx_1 \cdots dx_n$$

where $\phi_n \in L^2_{sym}(\mathbb{R}^{nd}) = \otimes^n_{sym,1} L^2(\mathbb{R}^d)$

For simplicity, we denote the r.h.s. by

$$\sum_n \frac{1}{\sqrt{n!}} \int \phi_n (a^*)^n \Omega.$$

Proof:

1. We first remark that

$$\int \phi_n(a^*)^n\Omega = \int \phi_n^{sym}(a^*)^n\Omega$$

where

$$\phi^{sym}(x_1,\dots,x_n) = \frac{1}{n!}\sum_{\pi\in S_n}\phi(x_{\pi(1)},\dots,x_{\pi(n)}) \in L^2_{sym}(\mathbb{R}^{nd})$$

is the *symmetrization* of ϕ (here S_n the group of permutations of the n variables).

2. We use the fact that vectors of the form $\prod_1^n \phi(f_j)\Omega$, $n \geq 1$, are dense in L^2. Note

$$\prod_1^n \phi(f_j)\Omega = \prod_1^n (a(C^{1/2}f_j) + a^*(C^{1/2}f_j))\Omega.$$

Using the commutation relations, we write $\prod(a+a^*)$ in the normal form

$$\prod_1^n (a+a^*)\Omega = \sum_{k+l\leq n}\int A_{kl}(a^*)^k a^l\Omega.$$

But $(a^*)^k a^l\Omega = 0$ unless $l=0$, so

$$\prod_1^n \phi(f_j)\Omega = \sum_{k\leq n}\int A_{k0}(a^*)^k\Omega.$$

Thus vectors of the form

$$\sum \frac{1}{n!}\int \phi_n(a^*)^n\Omega$$

are dense in L^2.

3. We have by straightforward computation

$$\langle \int \phi_n(a^*)^n\Omega, \int \chi_m(a^*)^m\Omega\rangle = \begin{cases} 0 & n\neq m \\ n! < \phi_n, \chi_n > & n=m \end{cases} \tag{15.17}$$

Problem 15.26 Show (15.17).

Thus

$$\{\phi = \sum_n \frac{1}{\sqrt{n!}} \int \phi_n (a^*)^n \Omega \ \mid \ \phi_n \in \otimes^n_{sym,1} L^2(\mathbb{R}^d)\} \approx \bigoplus_{n=0}^{\infty} [\otimes^n_{sym,1} L^2(\mathbb{R}^d)]$$

is closed, contains a dense set, and hence is the whole L^2 space. $\square$

Definition 15.27 *The (bosonic) Fock space is*

$$\mathcal{F} \equiv \bigoplus_{1}^{\infty} [\otimes^n_{sym,1} L^2(\mathbb{R}^d)].$$

We call

$$\mathcal{F}_n \equiv \otimes^n_{sym,1} L^2(\mathbb{R}^d)$$

the n-particle sector. *By convention,* $\mathcal{F}_0 = \mathbb{C}$.

The previous theorem provides a unitary isomorphism

$$L^2(H^{-s}, d\mu_C) \approx \mathcal{F}$$

given by

$$\sum \frac{1}{\sqrt{n!}} \int \phi_n (a^*)^n \Omega \leftrightarrow \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \vdots \end{pmatrix}.$$

Moreover it is easily checked that on F,

$$a(f) : \phi_n \in \mathcal{F}_n \mapsto \sqrt{n} < f, \phi_n > \in \mathcal{F}_{n-1}$$

and

$$a^*(f) : \phi_n \in \mathcal{F}_n \mapsto \sqrt{n+1} f \otimes_{sym} \phi_n \in \mathcal{F}_{n+1}.$$

Problem 15.28 Check that in this setting,

$$[a(f), a^*(g)] = \int \bar{f} g.$$

Proposition 15.29 *Consider the Hamiltonian,* $H = \int a^* C^{-1} a$, *and* particle number, $N = \int a^* a$, *operators. In the Fock space representation,*

$$H\phi \leftrightarrow (\sum_1^n C_{x_j}^{-1} \phi_n)$$

$$N\phi \leftrightarrow (n\phi_n).$$

Proof: This is simply a matter of using the commutation relations. We leave the details as an exercise.

Thus we have obtained a very simple realization of our state space $L^2(H^{-s}, d\mu_C)$ which is independent of C, and in which the Klein-Gordon Hamiltonian acts as a direct sum of simple one-variable operators in a finite but increasing number of variables:

$$H \approx \oplus_{n=0}^{\infty} \sum_1^n \sqrt{-\Delta_{x_i} + m^2}.$$

In particular, the spectrum of H is

$$\sigma(H) = \{0\} \cup \{\cup_{n \geq 1} [nm, \infty)\}$$

where the zero-eigenfunction is the vacuum, Ω.

Physically, this theory describes non-interacting particles (bosons) of mass m.

15.6 Generalized Free Theory

Let Λ be a self-adjoint operator on $L^2(\mathbb{R}^d)$. We consider the Hamiltonian

$$H_\Lambda = \frac{1}{2} \int \{|\pi|^2 + \phi \Lambda^2 \phi\}$$

(KG corresponds to $\Lambda = \sqrt{-\Delta + m^2}$).

Defining creation and annihilation operators as in the KG case (eg. $a(x) = 1/2\Lambda\phi + \frac{i}{\hbar}\Lambda^{-1}\pi$) leads to

$$H_\Lambda = \int a^*(x) \Lambda a(x) dx.$$

We may now quantize as with the KG case, and construct Fock space analogously. As with KG, the one-particle operator Λ determines all the properties of H_Λ. In particular,

$$H_\Lambda \approx \oplus_{n=0}^{\infty} \sum_1^n \Lambda_{x_i}.$$

Again, this describes a free (non-interacting) theory.

15.7 Interactions

The quadratic Hamiltonians studied above correspond to non-interacting or "free" quantum field theories. The central goal of QFT is to understand how the interactions modify the picture constructed for the free theories.

There are two ways of introducing interaction into a QFT. The first way is to add to the quadratic Hamiltonian in question a functional of ϕ of degree higher than two. Such a term represents a self-interaction of the field ϕ. The second way is to consider an interaction of several fields or an interaction of a field with a quantum-mechanical system. An interaction of this type will be considered in the next chapter. In this section we make a few remarks on the (very difficult) problem of constructing self-interacting quantum field theories. A more detailed treatment of this subject is beyond the scope of this book. It can be found in [GJ,Si].

We consider a Hamiltonian

$$H = H_{KG} + \lambda W$$

where H_{KG} is the Klein-Gordon Hamiltonian treated in the previous section, $\lambda > 0$, and

$$W = \int : P(\phi) :$$

where P is a polynomial which is bounded from below.

The problem here is that if P has order ≥ 3, then $W(\phi)$ is not well-defined. This problem can be remedied via *ultra-violet (UV)* and *infra-red (IR)* cut-offs.

We replace $W(\phi)$ with

$$W_\epsilon = \sum a_n \int : w_{n,\epsilon} \phi^{\otimes n} : \tag{15.18}$$

where $w_{n,\epsilon} \in L^2(\mathbb{R}^{dn})$, $w_{n,\epsilon} \to 1$ as $\epsilon \to 0$, and

$$\phi^{\otimes n}(x_1, \ldots, x_n) = \prod_1^n \phi(x_j).$$

If we approximate $w_{n,\epsilon}$ by $\sum f_1 \otimes \cdots \otimes f_n$, then

$$\int w_{n,\epsilon} \phi^{\otimes n} \approx \phi(f_1) \cdots \phi(f_n)$$

is well-defined as a product of commuting, self-adjoint operators. Put differently, if we write

$$\phi^n(x) = \int \prod_1^n \delta(x_i - x)\phi(x_1)\cdots\phi(x_n),$$

then expression (15.18) corresponds to smoothing out the delta functions. This is equivalent to cutting-off their Fourier transforms at large momenta: hence, a UV cut-off.

Another way to do a UV cut-off is via a *lattice approximation*. In this case we replace $\mathbb{R}^n$ with the lattice $(\epsilon\mathbb{Z})^n$, and let $\epsilon \to 0$.

We describe here a convenient mathematical method for smoothing out a rough function ϕ. Let θ be a C^∞ function such that $\theta \geq 0$, $\int \theta = 1$, and $\theta(0) = 1$. Define

$$\theta_\epsilon(x) = \epsilon^{-d}\theta(x/\epsilon).$$

Now we set $\phi_\epsilon = \theta_\epsilon * \phi$. Then ϕ_ϵ is smooth, and $\phi_\epsilon \to \phi$ as $\epsilon \to 0$. Note that

$$\hat{\phi}_\epsilon(k) = \hat{\theta}_\epsilon(k)\hat{\phi(k)} = \hat{\theta}(\epsilon k)\hat{\phi}(k).$$

So $\hat{\phi}_\epsilon$ is essentially $\hat{\phi}$ cut off at the momentum scale $|k| \leq 1/\epsilon$.

We note now that the condition $w_{n,\epsilon} \in L^2$ is incompatible with the translation invariance of H. That is, if P is the momentum operator ($P = \int a^*(k)ka(k)dk$), then $[W_\epsilon, P] = 0$ iff $w_{n,\epsilon}$ is independent of $\sum x_i$. Thus we require first that $w_{n,\epsilon} \in L^2(X_n)$ where $X_n = \{\underline{x} \in \mathbb{R}^{3n} \mid \sum x_i = 0\}$ and then set

$$w_{n,\epsilon,\delta} = w_{n,\epsilon}\chi_{|\sum x_i| \leq 1/\delta}.$$

This $\chi_{|\sum x_i| \leq 1/\delta}$ constitutes an infra-red (IR) cut-off.

It turns out that removing the IR cut-off ($\delta \to 0$) is not too difficult. Removing the UV cut-off ($\epsilon \to 0$), however, is very difficult, and not always possible.

15.8 Quadratic approximation

Presently, we understand quadratic Hamiltonians rather well. The first step in investigating more general non-quadratic Hamiltonians is finding the correct quadratic approximation. This is completely analogous to the situation in non-linear differential equations where the first step is practically always a linearization around a solution of interest. Indeed, quadratic Hamiltonians are in one-to-one correspondence with linear (Heisenberg) equations of motion.

In the simplest situations, for example

$$H = H_{KG} + W \tag{15.19}$$

where

$$W = \lambda^{-2} \int : P(\lambda\phi) :$$

with $P(\phi) = o(\phi^2)$, the quadratic approximation is obvious (here we presented W in a conveniently rescaled form). It corresponds to the linearization around a trivial solution $\phi_0 \equiv 0$ in non-linear differential equations. However, there are many important cases where finding a correct quadratic approximation constitutes a considerable conceptual step. In these cases one deals with quantum fluctuations around *nontrivial classical solutions* rather than trivial ones. These are exactly the cases we discuss briefly in this section.

Before proceeding to this discussion, we give two simple, but rather important examples of non-trivial classical solutions ϕ_0. Both examples are in dimension one, $d = 1$. Let

$$V(\phi) = \int \left\{ \frac{1}{2} |\nabla\phi|^2 + \lambda^{-2} F(\lambda\phi) \right\}$$

where (in order to identify this with (15.19))

$$F(\phi) = \frac{1}{2} m^2 \phi^2 + P(\phi).$$

For our first example, we take

$$F(\phi) = \frac{1}{2}(\phi^2 - a^2)^2$$

for some $a > 0$. In this case, the functional $V(\phi)$ has a minimizer in a class of functions $\phi : \mathbb{R} \to \mathbb{R}$ with the boundary conditions

$$\phi(x) \to \pm a/\lambda$$

as $x \to \pm\infty$, and with appropriate smoothness conditions. This minimizer can be found explicitly:

$$\phi_0(x) = \frac{a}{\lambda} \tanh(ax) \tag{15.20}$$

For our second example, take

$$F(\phi) = \alpha(\cos(\phi) - 1)$$

for some $\alpha > 0$. In this case, $V(\phi)$ has a minimizer in a class of functions $\phi : \mathbb{R} \to [0, 2\pi]$ with the boundary conditions $\phi(x) \to 0$ as $x \to -\infty$ and $\phi(x) \to 2\pi/\lambda$ as $x \to \infty$, and with appropriate smoothness conditions. Again, this minimizer can be found explicitly:

$$\phi_0(x) = \frac{4}{\lambda} \tan^{-1}(e^{\sqrt{\alpha}x}). \tag{15.21}$$

Problem 15.30 *Show that (15.20) and (15.21) are critical points of the corresponding functionals $V(\phi)$.*

The boundary conditions specified above are such that

$$\phi_0(x) \to \text{ null set of } F(\phi) \text{ as } x \to \pm\infty. \tag{15.22}$$

This is needed if we want the functional $V(\phi)$ to be finite. There are three more boundary conditions satisfying (15.22) in each of the above cases. One of these boundary conditions has the minimizer $\phi_0(-x)$ while the other two have constant minimizers.

Problem 15.31 *Prove this last statement.*

The four boundary conditions split all the test functions into four topologically inequivalent sectors: functions from one of these sectors cannot be continuously deformed into functions from another sector. Thus we have a *topological conservation law* - a classical solution starting in one of the sectors stays always in the same sector (an evolution is a continuous deformation with time serving as a deformation parameter). The topological sectors can be characterized by the quantity

$$Q = \lambda(\phi(+\infty) - \phi(-\infty))$$

which is a topological invariant. It is called the *topological charge*. The solutions $\phi_0(x)$ written above have topological charges 2 and 2π respectively, while solutions $\phi_0(-x)$ have charges -2 and -2π. The solutions $\phi_0(x)$ are called *topological solitons* and the solutions $\phi_0(-x)$ are *topological anti-solitons*.

There exist topological solitons also in higher dimensions (*vortices*, *monopoles*, *instantons*, etc.), though they cannot be written explicitly. We do not describe them here, and refer the interested reader to the books [Col,Raj].

Now we return to our main subject, the quantum theory of non-trivial classical solutions. We consider a Hamiltonian of the form (15.19) which we write as

$$H = \frac{1}{2} \int : \pi^2 : + : V(\phi) : . \tag{15.23}$$

We would like to understand the spectrum of H near its bottom. This means we want to study the spectrum of H near $\inf V(\phi)$. We assume the functional $V(\phi)$ has a minimizer, ϕ_0. If ϕ_0 is trivial (i.e. $\phi_0 \equiv 0$) then since $P(\phi) = o(\phi^2)$, the correct quadratic approximation to H is just H_{KG} (as discussed above). We are interested in situations when ϕ_0 is non-trivial, such as is the case with topological solitons and other interesting objects. In what follows, we give a formal but systematic treatment of this case. For simplicity, we consider the case of non translationally-invariant functionals $V(\phi)$ (e.g. $V(\phi) = \int\{(1/2)|\nabla\phi|^2 + F(\phi, x))$ and we will make a few remarks about the translationally- invariant case at the end.

We represent the quantum field in the form

$$\phi(x) = \phi_0(x) + \xi(x)$$

where $\phi_0(x)$ is the classical minimizer of $V(\phi)$ and $\xi(x)$ represents quantum fluctuations around the classical background $\phi_0(x)$. Our goal now is to pass from the original quantum field $\phi(x)$ to the new field $\xi(x)$. Note that on the scale of λ (a small, dimensionless coupling constant), $\phi_0(x) = O(\lambda^{-1})$ and $\xi(x) = O(1)$.

The first step is to expand $V(\phi)$ around ϕ_0 to the third order:

$$V(\phi) = V(\phi_0) + \frac{1}{2} < \xi, HessV(\phi_0)\xi > + O(\lambda\xi^3).$$

We compute formally how the change of variables from ϕ to ξ affects the Gaussian measure:

$$d\mu_C(\phi) = Z^{-1}e^{-<\phi, C^{-1}\phi>/2}D\phi = Z^{-1}e^{-<\phi_0+\xi, C^{-1}(\phi_0+\xi)>/2}D\xi$$

$$= e^{-<\phi_0, C^{-1}\phi_0>/2 - <\phi_0, C^{-1}\xi>}d\mu_C(\xi).$$

Define

$$U : L^2(H^{-s}, d\mu_C(\phi)) \to L^2(H^{-s}, d\mu_C(\xi))$$

by

$$U : F(\phi) \mapsto e^{-<\phi_0, C^{-1}\phi_0>/4 - <\phi_0, C^{-1}\xi>/2}F(\phi_0 + \xi).$$

It is easily checked that U is unitary. Next, set

$$\pi_\xi^C = U\pi_\phi^C U^{-1}$$

where as before

$$\pi_\phi^C = -i\partial_\phi + \frac{i}{2}C^{-1}\phi.$$

Consequently,

$$\tilde{H} \equiv UHU^{-1} = \frac{1}{2}\int :(\pi_\xi^C)^2 + V(\phi_0+\xi):$$

on $L^2(H^{-s}, d\mu_C(\xi))$. Hence

$$\tilde{H} = \frac{1}{2}\int :((\pi_\xi^C)^2 + \xi\Lambda^2\xi + O(\lambda\xi^3)): + V(\phi_0)$$

where

$$\Lambda^2 = HessV(\phi_0) = -\Delta_x + F''(\phi_0).$$

Now we change the covariance

$$C \mapsto C_\Lambda \equiv \frac{1}{2\Lambda}.$$

Then

$$d\mu_C = \Phi d\mu_{C_\Lambda}$$

where

$$\Phi = Z_{C_\Lambda} Z_C^{-1} e^{-<\xi,(C^{-1}-C_\Lambda^{-1})\xi>/2}.$$

We define another unitary operator

$$U_1 : L^2(H^{-s}, d\mu_C) \to L^2(H^{-s}, d\mu_{C_\Lambda})$$

by $(U_1F)(\xi) = \Phi^{1/2}F(\xi)$. Then

$$U_1\pi^C U_1^{-1} = \pi_C - \frac{1}{2}(C^{-1} - C_\Lambda^{-1})\xi = \pi^{C_\Lambda} \equiv \pi.$$

Define

$$H^{new} \equiv U_1 U H U^{-1} U_1^{-1}$$

on $L^2(H^{-s}, d\mu_{C_\Lambda})$. Then

$$H^{new} = H_{quad} + \int :O(\lambda\xi^3): + V(\phi_0) \tag{15.24}$$

where

$$H_{quad} = \frac{1}{2}\int :(\pi_\xi^2 + \xi\Lambda^2\xi): . \tag{15.25}$$

Passing now to the corresponding new creation and annihilation operators, we have

$$H_{quad} = \int a^*(x)\Lambda a(x)dx. \tag{15.26}$$

Thus we have a new free theory with covariance $-1/2\Lambda$, and with the one-particle operator Λ. Λ determines entirely the spectral properties of H_{quad}.

Let us summarize the above analysis. We began with a Hamiltonian of the form (15.23), where the functional $V(\phi)$ has a minimizer ϕ_0, acting on the space $L^2(H_{-s}, d\mu_C)$. We constructed a unitarily equivalent Hamiltonian (15.24) acting on the space $L^2(H_{-s}, d\mu_{C_\Lambda})$ where the covariance is $C_\Lambda = (2\Lambda)^{-1}$ with $\Lambda = (HessV(\phi_0))^{1/2}$. Up to the additive constant $V(\phi_0)$ (the classical energy of ϕ_0), the new Hamiltonian is a perturbation of the quadratic Hamiltonian (15.25) or (15.26) by a term which is of higher order - $O(\xi^3)$ - in the new quantum field ξ. Consequently, one expects that the low-energy spectrum of the original (and new) Hamiltonian is determined by the spectrum of this quadratic Hamiltonian (15.19) or (15.23), which, in turn, is determined by the spectrum of Λ, the square root of the Hessian of $V(\phi)$ at ϕ_0.

Now we discuss briefly the translation-invariant case. First, let us back up and ask ourselves what the minimizer ϕ_0 is from a physical point of view. As a critical point of the potential functional $V(\phi)$, it is a stationary solution of the classical equations of motion for the classical Hamiltonian functional

$$H(\phi, \pi) = \int \frac{1}{2}\pi(x)^2 + V(\phi).$$

Thus ϕ_0 solves the "Newton equation"

$$\ddot{\phi} = -\partial V(\phi), \tag{15.27}$$

which is nothing else but the familiar non-linear wave equation

$$\Box\phi + P'(\phi) = 0$$

with $\Box = \partial_t^2 - \Delta_x$ the D'Alambert operator (this is the classical dynamics corresponding to the quantum dynamics given by the Schrödinger equation $i\partial\psi/\partial t = H\psi$). This equation is invariant with respect to the relativistic group of motions - the *Poincaré group*. In particular, because of translational invariance, for any $y \in \mathbb{R}^d$, $\phi_0(x - y)$ is also a stationary solution of the equation of motion (15.27). Thus we have a d-dimensional manifold

$$M_c = \{T_h\phi_0 \mid h \in \mathbb{R}^d\}$$

where T_h is the "shift operator" mapping $\phi(x)$ to $\phi(x-h)$, each point of which is a stationary solution of (15.27).

Now we expand the field $\phi(x)$ "around" the manifold M_c. In other words, we decompose any field $\phi(x)$ as

$$\phi(x) = \phi_0(x-y) + \xi(x-y)$$

where $\phi_0(x-y)$ is the projection of $\phi(x)$ onto the manifold M_c, and $\xi(x-y)$ is the projection of $\phi(x)$ in the orthogonal direction; i.e. $\xi_y \perp T_{\phi_y} M_c$ where we have used the notation $\xi_y(x) = \xi(x-y)$, $\phi_y(x) = \phi(x-y)$, etc. Note that the tangent space, $T_{\phi_y} M_c$ is spanned by the functions $\partial\phi_0(x-y)/\partial x_j$, $j = 1, \ldots, d$. Consequently, the above orthogonality condition becomes

$$\int \xi(x) \nabla \phi_0(x) dx = 0. \tag{15.28}$$

Observe that the functions $\partial\phi_0/\partial x_j$ are *zero-modes* (eigenfunctions with eigenvalue zero) of the Hessian operator $HessV(\phi_0)$. Indeed, the functions $\phi_h(x) \equiv \phi_0(x+h)$ are all critical points of the functional V:

$$\partial V(\phi_h) = 0 \qquad \forall h \in \mathbb{R}^d.$$

Differentiating this equation with respect to h_j at $h = 0$, we find

$$Hess(V(\phi_0))\partial\phi_0/\partial x_j = 0$$

which establishes our assertion. The condition (15.28) states that the fluctuations are orthogonal to the zero-modes of $HessV(\phi_0)$, and therefore lie entirely in the positive spectral subspace of $HessV(\phi_0)$.

Thus we pass from the field $\phi(x)$ to the pair $(y, \xi(x))$ where $y \in \mathbb{R}^d$ and $\xi(x)$ satisfies (15.28). That is, $y = y(\phi)$ satisfies the equation

$$\int \{\phi(x+y) - \phi_0(x)\} \nabla \phi_0(x) dx = 0$$

and

$$\xi(x) = \phi(x + y(\phi)) - \phi_0(x).$$

Conversely, the field $\phi(x)$ is reconstructed from y and $\xi(x)$ according to the equation

$$\phi(x) = \phi_0(x-y) + \xi(x-y).$$

The transformation of the momentum field, $\pi(x)$, can be found using a standard Lagrangian formalism. Then the transformations of both $\phi(x)$ and $\pi(x)$ yield a canonical transformation.

The analysis presented above for the non translation-invariant case can be extended to the translation-invariant one. We don't pursue this here.

15.8.1 Discussion

1. **Quantization:** Physically, we can re-interpret what we have done above as quantization of the classical solution $\phi_0(x)$ in the first case, or the manifold of solutions $\phi_0(x-y)$ in the second. Indeed, we can arrive at the results above by first doing the canonical transformation

$$\phi(x) \mapsto \xi(x) = \phi(x) - \phi_0(x) \quad \text{and} \quad \pi(x) \mapsto \pi(x) \tag{15.29}$$

and then performing canonical quantization.

In the translation invariant case, we have to quantize in the presence of a symmetry group. Have we encountered such a problem before? In fact we have, in quantizing the Maxwell equations. There we had to deal with gauge symmetries. As a result, we quantize the electromagnetic field in the direction transverse to the orbits of the gauge group. Passing to the field ξ in (15.29) can be considered as quantization in the direction transverse to the group of translations.

2. **Relativistic invariance**. Classical equation (15.27) is invariant with respect to the relativistic group of motions - the *Lorentz group*. Therefore any stationary solution, ϕ_0, of this equation can be "boosted" by a Lorentz transformation into a traveling wave:

$$\phi_v(x,t) = \phi_0(\frac{x - vt - x_0}{\sqrt{1-v^2}}) \tag{15.30}$$

.

Problem 15.32 *Check by direct calculation that the function ϕ_v satisfies (15.27) provided ϕ_0 is a critical point of $V(\phi)$.*

Thus in the translationally invariant case, a single stationary solution leads to an entire $2d$-dimensional manifold of solutions. These solutions are traveling waves, or *solitons* (in physics terminology). They are parameterized by their initial positions, x_0 and their velocities, v. They can be represented as lines on the manifold M_c.

3. **Momentum conservation**. The physical quantity which is conserved due to translation invariance is the field momentum. In the classical case, the latter is given by

$$P(\phi,\pi) = \int \pi(x)\nabla\phi(x)dx.$$

The quantum field momentum, P, is obtained by quantizing $P(\phi, \pi)$ in the standard way.

Problem 15.33 *Show that in the translation-invariant case, $P(\phi, \pi)$, and its quantum counterpart, P, are conserved - i.e.*

$$\{P(\phi, \pi), H(\phi, \pi)\} = 0 \qquad \textit{and} \qquad \frac{1}{\hbar}[P, H] = 0.$$

Suppose $d = 1$. For the soliton (15.30), the energy $E_{sol} = H(\phi_v, \pi_v)$, and the momentum $P_{sol} = P(\phi_v, \pi_v)$, satisfy the relativistic relation

$$E_{sol} = P_{sol}^2 + M_{sol}^2 \tag{15.31}$$

where $M_{sol} = H(\phi_0, \pi_0)$ is the mass of the soliton (i.e. its rest energy).

Problem 15.34 *(a) Derive the* virial relation

$$\int |\nabla \phi_0|^2 = \lambda^{-2} \int F(\lambda \phi_0) \tag{15.32}$$

for the soliton. To derive this, consider the family $\phi_s(x) \equiv \phi_0(sx)$. Since ϕ_0 is a critical point of the functional $V(\phi)$, we have

$$\frac{d}{ds} V(\phi_s)|_{s=1} = 0.$$

The latter implies (15.32).

(b) Use the virial relation to prove the relativistic formula (15.31).

The quantum momentum P leads to the soliton center momentum q conjugate to the soliton center coordinate.

Chapter 16

Quantum electrodynamics of non-relativistic particles: the theory of radiation

In this chapter we describe the theory of the phenomenon of emission and absorption of electromagnetic radiation by systems of non-relativistic particles such as atoms and molecules. Attempts to create such a theory at the end of the last century and the beginning of this one led to the birth of quantum physics, and were a driving force in the development of quantum field theory. The upshot of these attempts is the theory of quantization of matter and radiation described in the previous chapters. Only by assuming the matter and the radiation to be quantum, can one give a consistent description of the phenomenon in question. Thus, our starting point should be a Schrödinger operator describing quantum particles interacting between themselves, and with quantum radiation. In mathematical terms, the question we address is how the bound state structure of the particle system is modified by the interaction with radiation. One expects that the ground state of the particle system survives, while the excited states turn into resonances. The real parts of the resonances - the resonance energies - produce the *Lamb shift*, first experimentally measured by Lamb and Retherford (Lamb was awarded the Nobel prize for this discovery). The imaginary parts of the resonances - the decay probabilities - are given by the *Fermi Golden Rule* (see, eg, [HuS]). This picture was established rigorously in [BFS1]-[BFS4], whose results we describe here.

16.1 The Hamiltonian

Recall from Section 15.4.4 that the quantized electromagnetic field is described by two canonical fields: the quantized vector potential (quantized connection) $A'(x)$ and quantized electric field $E(x)$ acting on the Fock space $\mathcal{H}_f \equiv \mathcal{F}$. They satisfy the standard commutation relations

$$i[E(x), A'(y)] = C(x-y) \cdot \mathbf{1},$$

etc., where $C(x-y)$ is the integral kernel of the projection operator from the vector-fields on $\mathbb{R}^3$ to the divergence-free (transverse) vector fields. The quantum Hamiltonian governing the evolution is given by

$$H'_f \equiv \frac{1}{2} \int \, : \, E(x)^2 + \big(\operatorname{curl} A(x)\big)^2 \, : \, d^3x,$$

which is just a quantization of the classical Hamiltonian functional. In terms of the creation and annihilation operators these objects are written as follows

$$A'(x) = \int \big(e^{ik\cdot x} a(k) + \text{h.c.}\big) g'(k) d^3k,$$

where $g'(k) \equiv c\sqrt{\hbar}(2\pi)^{-3}\big(2\omega'(k)\big)^{-1/2}$, $\omega'(k) = c|k|$, and h.c. stands for the "hermitian conjugate", and

$$H'_f = \int \hbar\omega'(k) a^*(k) a(k) d^3k.$$

A system of quantum matter (atom, molecule, etc. with fixed nuclei) is defined by the Schrödinger operator

$$H_{\text{part}} = \sum_{j=1}^{N} \frac{1}{2m} p_j^2 + e^2 V_{\text{coul}}(\underline{x}, \underline{R})$$

acting on $\mathcal{H}_{\text{part}} \ \big(= L^2(\mathbb{R}^{3N})\big)$ (or a subspace of this of a definite symmetry type). Here N is the number of electrons involved, and m, x_j and $p_j = -i\hbar\nabla_{x_j}$ are the mass, coordinate and momentum, respectively, of the j-th electron. Furthermore, e is the absolute value of the electron charge, $\underline{x} = (x_1, \ldots, x_N)$, $\underline{R} = (R_1, \ldots, R_M)$, and $V_{\text{coul}}(\underline{x}, \underline{R})$ is the total Coulomb potential for N electrons and M nuclei located at the positions $x_1, \ldots, x_N$, and at $R_1, \ldots, R_M$, respectively, divided by $-e$.

Radiation interacts with matter via the minimal coupling mechanism (see section 8.7). An equivalent way to arrive at it (which is couched in purely mathematical

terms) is to remember that $A'(x)$ is the quantum connection, so we replace the usual derivatives by the covariant ones:

$$p \longrightarrow p_{A'} \equiv p - \frac{e}{c}A'(x) \ . \tag{16.1}$$

Thus to obtain the full, interacting Hamiltonian we replace the particle momenta, p_j, in H_{part} by the covariant momenta $p_{A',j} = p_j - \frac{e}{c}A'(x_j)$ and add to the result the field Hamiltonian H'_f responsible for dynamics of $A'(x)$. However, the operator we obtain in this way is ill-defined: it has an empty domain of definition. The problem is that $A'(x)$ is too rough an operator-function. To remedy it we institute an *ultraviolet cut-off*. Namely we replace $A'(x)$ in (16.1) by an operator $A_\chi(x)$:

$$A'(x) \to A_\chi(x) \equiv \check{\chi} * A'(x)$$

where $\check{\chi}$ is a smoothed-out δ-function. In fact, the specific shape of χ is not important for us. All we need at the beginning will be encoded in an estimate below.

As a result we arrive at the standard Hamiltonian of non-relativistic matter interacting with radiation

$$H(e) = \sum_{j=1}^{N} \frac{1}{2m}(p_{eA,j})^2 + e^2 V_{\text{coul}}(\underline{x}, \underline{R}) + H_f$$

acting on $\mathcal{H}_{\text{part}} \otimes \mathcal{H}_f$, where $p_{eA,j} = p_j - eA(x_j)$, $p_j = -i\nabla_{x_j}$, and

$$H_f = \int \omega(k) a^*(k) a(k) d^3k,$$

with $\omega(k) = |k|$. One can show that $H(e)$ is well defined under some mild restrictions on χ.

Now we pass to dimensionless variables as follows

$$x \to \frac{\hbar^2}{me^2}\, x \ , \qquad k \to \frac{e^2}{\hbar c}\frac{me^2}{\hbar^2} k \ ,$$

i.e., the electron coordinates are measured in units of the Bohr radius $r_{\text{bohr}} = \frac{\hbar^2}{me^2}$. Then the Hamiltonian $H(e)$ is mapped into the Hamiltonian $\frac{me^4}{\hbar^2}H(\varepsilon)$, where

$$H(\varepsilon) = \sum_{j=1}^{N} \frac{1}{2} p^2_{\varepsilon A,j} + V(\underline{x}) + H_f \, ,$$

where $\varepsilon = \left(\frac{e^2}{\hbar c}\right)^{3/2} K^{1/2}$, $A(x) = K^{-1/2} A_\chi\left(\frac{e^2}{\hbar c}x\right)$ with $\chi(k)$ replaced by $\chi\left(\frac{e^2}{\hbar c}\frac{me^2}{\hbar^2}k\right)$, and $V(\underline{x}) = V_{\rm coul}\left(\underline{x}, \frac{me^2}{\hbar^2}\underline{R}\right)$. Thus the energy is measured in the units of $\frac{me^4}{\hbar^2} = mc^2\left(\frac{e^2}{\hbar c}\right)^2 = 2$ Rydberg. Note that $\alpha \equiv \frac{e^2}{\hbar c}$ is the fine-structure constant. Its physical value is $\approx \frac{1}{137}$, however in this work it is considered as a small, dimensionless parameter.

The Hamiltonian $H(\varepsilon)$ is, of course, equivalent to our original Hamiltonian $H(e)$. Understanding the spectral composition of $H(\varepsilon)$ is the object of this chapter.

To simplify notation we only consider the case $N = 1$:

$$H(\varepsilon) = \frac{1}{2} p_{\varepsilon A}^2 + V(x) + H_f \ , \tag{16.2}$$

where $x \in \mathbb{R}^3$ and $p_{\varepsilon A} = p - \varepsilon A(x)$ with $p = -i\nabla_x$. Now $H_{\rm part} = \frac{1}{2}p^2 + V(x)$.

The operator $A(x)$ has the same form as $A'(x)$:

$$A(x) = \int (e^{ik\cdot x} a(k) + h.c.) g(k) d^3k$$

but with the new coupling function $g(k) = \chi(k) g'(k)$. We assume that g is real and satisfies

$$\int \frac{|g|^2}{\omega} < \infty. \tag{16.3}$$

Thus $H(\varepsilon)$ depends also on the (coupling) function (or form factor) $g(k)$.

At this point we forget about the origin of the potential $V(x)$, but rather assume it to be a general real function satisfying standard assumptions, say

$$\min\big(V(x), 0\big) \in L^2 + L^\infty \quad \text{and} \quad \max\big(V(x), 0\big) \in L^2_{\rm loc} \tag{16.4}$$

(see [RSII]). Certainly, the Coulomb potential satisfies this assumption. One can show that under conditions (16.3-16.4), the operator $H(\varepsilon)$ is essentially self-adjoint on the domain $D(H(0))$,

16.2 Perturbation set-up

We would like first to examine a system consisting of matter and radiation not coupled to each other. Such a system is described by the Hamiltonian

$$H(0) = H_{\rm part} \otimes \mathbf{1}_f + \mathbf{1}_{\rm part} \otimes H_f \, , \tag{16.5}$$

which is obtained by setting the parameter ε in (16.2), to zero: $\varepsilon = 0$. Using the separation of variables, we obtain

$$\sigma\big(H(0)\big) = \sigma(H_{\rm part}) + \sigma(H_f)$$
$$\sigma_p\big(H(0)\big) = \sigma_p(H_{\rm part}) + \sigma_p(H_f)$$
$$\sigma_{\rm cont}\big(H(0)\big) = \sigma_1 \cup \sigma_2 \cup \sigma_3$$

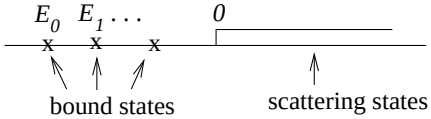
where

$$\sigma_1 = \sigma_p(H_{\rm part}) + \sigma_{\rm cont}(H_f)$$
$$\sigma_2 = \sigma_{\rm cont}(H_{\rm part}) + \sigma_p(H_f)$$
$$\sigma_3 = \sigma_{\rm cont}(H_{\rm part}) + \sigma_{\rm cont}(H_f).$$

Recall the spectral structure of the Schrödinger operator $H_{\rm part}$. Typically, we have

$$\sigma(H_{\rm part}) = \{\text{negative EV's } E_j\} \cup \{\text{ continuum } [0,\infty)\} \tag{16.6}$$

Here $j = 0, 1, \ldots$ and we assume $E_0 \leq E_1 \leq \ldots$. The eigenfunction, $\psi_0^{\rm part}$, corresponding to E_0 is called the *ground state*, while the eigenfunctions $\psi_j^{\rm part}$ for E_j with $j \geq 1$, are called the *excited states*. The generalized functions of the continuous spectrum are identified with the scattering states.



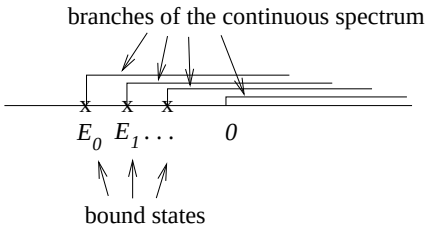
(16.7)

Spectrum of $H_{\rm part}$

For the field, $\sigma_{\rm cont}(H_f) = [0,\infty)$ and $\sigma_p(H_f) = \{0\}$. The eigenvalue 0 corresponds to the vacuum vector: $H_f\Omega = 0$. Thus we have

$$\sigma\big(H(0)\big) = \{\text{EV's } E_j\} \bigcup_{j=0}^{\infty} \{\text{continuum branch } [E_j,\infty)\}\ , \tag{16.8}$$

where $E_\infty = 0$. The obtained spectrum is pictured below.



(16.9)

Spectrum of $H(0)$

The eigenfunctions of $H(0)$ corresponding to the eigenvalues E_j are

$$\psi_j^{\rm part} \otimes \Omega \ . \tag{16.10}$$

The generalized eigenfunctions corresponding to the branch $[E_j, \infty)$ of its continuous spectrum are

$$\psi_j^{\rm part} \otimes \prod_{i=1}^{n} a^*(k_i)\Omega \tag{16.11}$$

for various $n \geq 1$ and $k_1, \ldots, k_n$. (The corresponding spectral points are $E_j(k) = E_j + \sum_{i=1}^{n} \omega(k_i)$.) The solutions of the time-dependent Schrödinger equation

$$i\frac{\partial \psi}{\partial t} = H(0)\psi \tag{16.12}$$

with the initial conditions (16.10) and (16.11) are given by

$$e^{-iE_j t}(\psi_j^{\rm part} \otimes \Omega)$$

and

$$e^{-iE_j(k)}\big(\psi_j^{\rm part} \otimes \prod_{i=1}^{n} a^*(k_i)\Omega\big) \ ,$$

respectively. The first of these states describes the particle system in the state $\psi_j^{\rm part}$ with no photons around, while the second one corresponds to the system in the state $\psi_j^{\rm part}$ and n photons with the momenta $k_1, \ldots, k_n$. Both states are stationary in time. In the absence of coupling between matter and radiation the system of matter and radiation placed in one of these states remains in the same state forever. Radiation is neither absorbed nor emitted by this system.

This picture is expected to change as the interaction between the matter and radiation is switched on. Understanding how this picture changes is the main problem of the mathematical theory of radiation.

16.3 Results

The rigorous answer to the question posed above is given in the theorem below. This theorem refers to the notion of resonance described in [BFS1]-[BFS2] (see

also section 14.2) and, for various statements, uses subsets of the following set of conditions we now formulate. We begin with the condition on the coupling function $g = g(k)$, besides condition (16.3) which is assumed throughout the chapter without further mention:

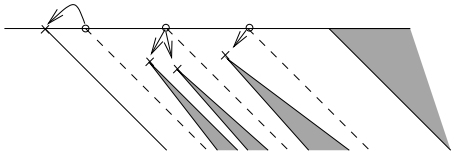
(A) $g_\theta(k) \equiv e^{-3\theta/2} g(e^{-\theta}k)$, as an $L^2\big(\omega^{-1}d^3k\big)$-function of k, and $V(e^\theta x)$, as a multiplication operator from $D(\Delta_x)$ to $\mathcal{H}_{\rm part}$, have analytic continuations in θ from $\mathbb{R}$ into a complex neighbourhood of $\theta = 0$.

Finally, we formulate a condition we use in the proof of one of the results

(B) $\exists\, R, \alpha > 0$ s.t. $V(x) \geq \alpha|x|^2$ for $|x| \geq R$.

Theorem 16.1 *Let Condition (A) hold, and let $\varepsilon \neq 0$ be sufficiently small. Then (i) $H(\varepsilon)$ has a unique ground state. This state descends from $\psi_0^{\rm part} \otimes \Omega$, and is exponentially localized in the particle coordinates. (ii) $H(\varepsilon)$ has no other bound states. In particular, the excited states of $H_{\rm part}$ (i.e. $\psi_j^{\rm part} \otimes \Omega$, $j \geq 1$) are unstable. Let, in addition, Condition (B) hold. Then (iii) the excited states of $H_{\rm part}$ turn into resonances of $H(\varepsilon)$, $\varepsilon \neq 0$ (see Fig.16.13).*

Statement (ii) assumes Condition (A), and statement (iii) assumes Conditions (A) and (B).



(16.13)

Bifurcation of eigenvalues of $H(0)$ (the second Riemann sheet)

A complete proof of statements (i)-(iii) can be found in [BFS2]-[BFS4]. We will describe the proof of (i) in Chapter 17. The proofs of (ii) and (iii) are similar.

This theorem gives mathematical content to formal calculations performed in physics with the help of perturbation theory. The purpose of this theorem, as well as of the calculations mentioned, is to explain theoretically the following fundamental physical phenomena: a system of matter, say an atom or a molecule, in its lowest energy state is stable and well localized in space, while the same system placed in the vacuum in the excited state, e.g. in $\psi_j^{\rm part} \otimes \Omega$, $j \geq 1$, emits radiation and descends to its lowest energy state. The mathematical manifestation of the first statement is that $H(\varepsilon)$ has a ground state, which is well localized in the particle coordinates,

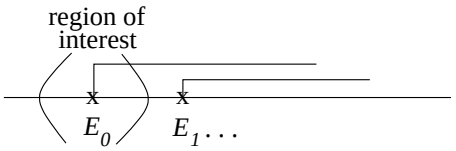
– statement (i) of the theorem – while statement (ii), rendered in mathematical terms, says that the system in question has no stable states in a neighbourhood of the excited states of the particle system. Moreover, statement (iii) says that the excited states, $\psi_j^{\text{part}} \otimes \Omega$, $j \geq 1$, of the particles in the vacuum lead to metastable states, i.e., solutions of the time-dependent Schrödinger equation (16.12) which are localized for long intervals of time, but eventually disintegrate. A metastable state is another term for a resonance. These metastable states are responsible for the phenomena of emission and absorption of radiation and their life-times tell us how long in average we have to wait until a particle system emits (or absorbs) radiation.

A proof of Theorem 16.1 is outlined in Chapter 17, where the basic technique - the *renormalization group* - is introduced. We will close out the present chapter with a brief discussion of this approach.

For simplicity, consider just the ground state. Our goal is to understand the low energy spectrum of $H(\varepsilon)$ for ε sufficiently small. Namely, we address the questions:

- Does $H(\varepsilon)$ have a ground state?
- What is the structure of the spectrum of $H(\varepsilon)$ near its infimum?

Look first at the spectrum of $H(\varepsilon = 0)$, i.e., when the interaction is turned off:



(16.14)

Region of interest w.r.t. spec$H(0)$

This picture suggests that only the ground state ψ_0^{part} of H_{part} and the low energy states of H_f are essential. The key idea here is to *project out the inessential parts* of the spectrum without distorting the essential ones. But how to do this? Let us try the first idea that comes to mind:

$$H \to P_\rho H P_\rho \ , \tag{16.15}$$

where P_ρ is the spectral projection for $H(0)$ associated with the interval $[E_0, E_0 + \rho]$. We can write it out as

$$P_\rho = P_0^{\text{part}} \otimes E_{[0,\rho]}(H_f) \ . \tag{16.16}$$

Here P_0^{part} is the orthogonal projection onto ψ_0^{part} and $E_{[0,\rho]}(H_f)$ is the spectral projection for H_f for the interval $[0, \rho]$. The latter "cuts-off" the energy states of H_f with energy above ρ.

The operator $P_\rho H(\varepsilon) P_\rho$ acts on states of the form

$$\psi_0^{\text{part}} \otimes \phi \ , \ \phi \in \text{Ran} E_{[0,\rho]}(H_f) \ .$$

This is exactly what we want. However, the low energy spectrum of $P_\rho H(\varepsilon) P_\rho$ is different from that of $H(\varepsilon)$. So we have lost the spectral information we are after. In Section 17.1 we learn how to project the operators to smaller subspaces without losing the spectral information of interest. But there is a trade-off involved as usual. While the map (16.15) on operators H is linear, the new map we introduce is not. This new map is called the *decimation map* (or *Feshbach map*).

In Section 17.3, the decimation map is applied to our (shifted) Hamiltonian $H(\varepsilon) - z\mathbf{1}$ to obtain a new family of operators, $H_0(\varepsilon, z)$, which act only on the low-energy part of the field space $\mathcal{H}_f$ (and not on the particle component of the state space). Furthermore, for z near the particle ground-state energy, E_0, $H_0(\varepsilon, z)$ has the same spectrum near 0 as $H(\varepsilon)$ does near E_0. This process is referred to as *elimination of the particle and high photon energy degrees of freedom*. To study the spectrum of $H(\varepsilon)$ near E_0, then, it suffices to study the spectrum of $H_0(\varepsilon, z)$ around 0, for z near E_0.

In order to analyze the spectrum of $H_0(\varepsilon, z)$, we change our viewpoint, and think of the operators $H_0(\varepsilon, z)$ as single elements of a whole space of operators (a Banach space, in fact - see Section 17.6). On this space, we define the *renormalization map*

$$\mathcal{R}_\rho = S_\rho \circ D_\rho$$

where D_ρ is another application of the decimation map, and S_ρ is a simple rescaling map (see Sections 17.7 and 17.8). D_ρ maps operators which act on states with photon energies ≤ 1 to operators which act on states with photon energies $\leq \rho$. The rescaling S_ρ restores the operators to ones that act on states with photon energies ≤ 1 again. By design, the renormalization map $\mathcal{R}_\rho$ is *isospectral* in the sense that near 0, K and $\mathcal{R}_\rho(K)$ have the same spectrum. The effect of $\mathcal{R}_\rho$ when we apply it to $H_0(\varepsilon, z)$, is to focus in on a neighbourhood of the spectrum of $H_0(\varepsilon, z)$ near 0. The smaller ρ is, the smaller this neighbourhood is.

The renormalization map, which obeys a semi-group law ($\mathcal{R}_{\rho_1} \circ \mathcal{R}_{\rho_2} = \mathcal{R}_{\rho_1 \rho_2}$), thus gives rise to an isospectral semi-flow on our Banach space of operators. We will see that under this flow, $H_0(\varepsilon, z)$ tends toward the operator ωH_f (for some $\omega \in \mathbb{C}$) as $\rho \to 0$. In fact, $\mathbb{C} H_f$ is a line of fixed points of the flow ($\mathcal{R}_\rho(\omega H_f) = \omega H_f$). By

studying the behaviour of the flow near this line of fixed points, we can relate the spectrum of $H_0(\varepsilon, z)$ near 0 (and hence of $H(\varepsilon)$ near E_0) to that of H_f, which we know well. This is the basic idea behind the proof of Theorem 16.1. This program, which is described somewhat vaguely here, will be studied in detail in Chapter 17.

Chapter 17

Renormalization group

In this chapter we describe the operator version of the powerful method of *renormalization group* due to [BFS1]-[BFS4]. We demonstrate how this method works by applying it to the problem of radiation (see Chapter 16). In particular, we continue our study of the Hamiltonian $H(\varepsilon)$ (introduced in the previous chapter) which describes quantum particles coupled to a quantized EM field. We prove Theorem 16.1 (i) stating the existence of the ground state of the operator $H(\varepsilon)$ for sufficiently small $|\varepsilon|$. The problems of instability of the excited states and existence of the resonances - statements (ii) and (iii) of Theorem 16.1 - can be treated in the same way.

17.1 Decimation map

In this section we realize the first step in our analysis of the Hamiltonian $H(\varepsilon)$. Our goal is to pass from the family $H(\varepsilon) - z \cdot \mathbf{1}$ to a family $H_0(\varepsilon, z)$ of operators acting effectively on the space $\mathrm{Ran}\, \chi_{H_f \leq \rho} \subset \mathcal{F}$ and which has spectrum of the same nature at 0. The family $H_0(\varepsilon, z)$ will turn out to be more accessible to spectral analysis. Passing from $H(\varepsilon) - z \cdot \mathbf{1}$ to $H_0(\varepsilon, z)$ will be referred to as *elimination of the particle and high photon energy* (actually, the photon energy $\geq \rho$) *degrees of freedom.*

In this section we study maps between sets of operators which are *isospectral* in the sense specified below.

Let P and $\bar{P}$ be bounded operators on a separable Banach space X, satisfying $P + \bar{P} = \mathbf{1}$. Denote by C_P the set of all closed operators, H, on X whose domains have dense (in $\mathrm{Ran}\, P$) intersections with $\mathrm{Ran}\, P$ and which satisfy

$$\|R_{\bar{P}}\| < \infty \,, \tag{17.1}$$

$$\|PHR_{\bar{P}}\| < \infty \quad \text{and} \quad \|R_{\bar{P}}HP\| < \infty \ . \tag{17.2}$$

Here $H_P = PHP \restriction \mathrm{Ran}P$, etc. and $R_{\bar{P}} = \bar{P}H_{\bar{P}}^{-1}\bar{P}$. We define the map

$$D_P \ : \ C_P \to (\text{Closed operators on Ran}\, P)$$

by

$$D_P(H) = P(H - HR_{\bar{P}}H)P \restriction_{\mathrm{Ran}\, P} \ . \tag{17.3}$$

We call D_P the *decimation map.*

The following operators play an important role in our analysis:

$$Q \equiv Q(H) \equiv P - R_{\bar{P}}HP \tag{17.4}$$

and

$$Q^{\#} \equiv Q^{\#}(H) \equiv P - PHR_{\bar{P}} \tag{17.5}$$

We have $Q^{\#}(H) = Q(H^*)^*$, but we do not use this property.

The operators P, Q, and $Q^{\#}$, have the following properties

$$\mathrm{Null}Q \cap \mathrm{Null}H' = \{0\} \quad \text{and} \quad \mathrm{Null}P \cap \mathrm{Null}H = \{0\} \tag{17.6}$$

and

$$HQ = PH' \quad \text{and} \quad Q^{\#}H = H'P \ , \tag{17.7}$$

where $H' = D_P(H)$. These relations are proved below.

The main result of this section is the following

Theorem 17.1 *Assume (17.1)-(17.2) hold, i.e. H is in the domain of the map D_P. Then the operators H and $D_P(H)$ are isospectral at 0, in the sense that*

$$(a) 0 \in \sigma(H) \leftrightarrow 0 \in \sigma(D_P(H))$$

and

$$(b) H\psi = 0 \leftrightarrow D_P(H)\phi = 0$$

where ψ and ϕ are related by $\phi = P\psi$ and $\psi = Q\phi$.

Proof: We begin with a general statement:

Proposition 17.2 *Assume conditions (17.1) and (17.2) are satisfied. Then (17.6)-(17.7) imply that $0 \in \sigma(H) \Rightarrow 0 \in \sigma(H')$ (the crucial part for us of property (a)). Moreover, we have always that $\mathrm{Null}P \cap \mathrm{Null}H = \{0\}$.*

Proof. Let $0 \in \rho(H')$. Then we can solve the equation $H'P = Q^{\#}H$ for P to obtain

$$P = H'^{-1}Q^{\#}H \ . \tag{17.8}$$

The equation $P + \bar{P} = \mathbf{1}$ and the definition $H_{\bar{P}} = \bar{P}H\bar{P}$ implies

$$\bar{P} = \bar{P}H_{\bar{P}}^{-1}\bar{P}H\bar{P} \cdot \bar{P} = \bar{P}H_{\bar{P}}^{-1}(\bar{P}H - \bar{P}HP) \ . \tag{17.9}$$

Substituting expression (17.8) for P into the r.h.s., we find

$$\bar{P} = \bar{P}H_{\bar{P}}^{-1}(\bar{P} - \bar{P}HPH'^{-1}Q^{\#})H \ .$$

Adding this to Eqn (17.8) multiplied from the left by P yields

$$\mathbf{1} = \left[\bar{P}H_{\bar{P}}^{-1}\bar{P} - \bar{P}H_{\bar{P}}^{-1}\bar{P}HPH'^{-1}Q^{\#} + PH'^{-1}Q^{\#}\right] H$$

Since by our conditions $\bar{P}H_{\bar{P}}^{-1}\bar{P}HP$ is bounded, the expression in the square brackets represents a bounded operator. Hence H has a bounded inverse. So $0 \in \rho(H)$.

The second statement follows from the relation

$$\mathbf{1} = QP + R_{\bar{P}}H \ , \tag{17.10}$$

which, in turn, is implied by Eqn (17.9) and the relation $P + \bar{P} = \mathbf{1}$. □

Next we prove relations (17.6)-(17.7). The second relation in (17.6) is shown in Proposition 17.2, while the first one follows from the inequality $\|Qu\|^2 = \|Pu\|^2 + \|\bar{R}HPu\|^2 \geq \|Pu\|^2$.

Now we prove relations (17.7). Using the definition of $Q(H)$, we transform

$$HQ \equiv HP - H\bar{P}H_{\bar{P}}^{-1}\bar{P}HP \tag{17.11}$$

$$= PHP + \bar{P}HP - PH\bar{P}H_{\bar{P}}^{-1}\bar{P}HP$$

$$-\bar{P}H\bar{P}H_{\bar{P}}^{-1}\bar{P}HP$$

$$= PHP - PH\bar{P}H_{\bar{P}}^{-1}\bar{P}HP \equiv P \cdot D_P(H).$$

Next, we have

$$Q^{\#}H \equiv PH - PH\bar{P}H_{\bar{P}}^{-1}\bar{P}H$$

$$= PHP + PH\bar{P} - PH\bar{P}H_{\bar{P}}^{-1}\bar{P}HP - PH\bar{P}H_{\bar{P}}^{-1}H\bar{P}$$

$$= PHP - PH\bar{P}H_{\bar{P}}^{-1}\bar{P}HP \equiv D_P(H)P.$$

Statement (b) of Theorem 17.1 follows from relations (17.6)-(17.7). A part of statement (a) was shown in Proposition 17.2. We now prove the remaining part of statement (a). Proposition 17.2 implies that $0 \in \rho(H)$ if $0 \in \rho(H')$, where $H' \equiv D_P(H)$.

Now let, conversely, $0 \in \rho(H)$ and show that $0 \in \rho(H')$. To simplify notation we do it only in the case when P is a projection. Then this statement follows from the relation

$$H'^{-1} = PH^{-1}P \tag{17.12}$$

which we set out to prove now. We have by the definition

$$H'PH^{-1}P = PHPH^{-1} - PH\bar{P}H_{\bar{P}}^{-1}\bar{P}HPH^{-1}P$$

$$= P - PH\bar{P}H^{-1}P - PH\bar{P}H_{\bar{P}}^{-1}\bar{P}H(\mathbf{1}-\bar{P})H^{-1}P = P \ .$$

Similarly one shows that $PH^{-1}PH' = P$. Hence H' has the bounded inverse $PH^{-1}P$.

Thus we have shown that $0 \in \rho(H) \leftrightarrow 0 \in \rho(D_P(H))$, which is equivalent to $0 \in \sigma(H) \leftrightarrow 0 \in \sigma(D_P(H))$. □

The *decimation* (or *Feshbach*) *map*, $D_P(H)$, maps operators on X into operators on $\mathrm{Ran}\, P$ in such a way that $H - z \cdot \mathbf{1}$ and $D_P(H - z \cdot \mathbf{1})$ are isospectral at 0 on the set $\rho(H_{\bar{P}})$.

Proposition 17.3 *(semigroup property)* $D_{P_1} \circ D_{P_2} = D_{P_1 P_2}$ *provided* P_1 *and* P_2 *are commuting projections.*

Proof. Assume for simplicity that H and $D_{P_1}(H)$ are invertible. Then the statement follows by applying Eqn (17.12) twice. □

17.2 Relative Bounds

Before proceeding with the first application of the decimation map constructed above, we prove a key relative bound on the quantized vector potential $A(x)$ used in this application. In this section $\|\cdot\|_{\mathcal{F}}$ stands for the norm in the Fock space $\mathcal{F}$.

Theorem 17.4 *We have*

$$\|A(x)\psi\|_{\mathcal{F}} \leq 2\left(\int \frac{|g|^2}{\omega}\right)^{1/2} \|H_f^{1/2}\psi\|_{\mathcal{F}} + \left(\int |g|^2\right)^{1/2} \|\psi\|_{\mathcal{F}} \ . \tag{17.13}$$

A proof of this theorem follows readily from Lemma 17.5 below.

Discussion. The estimate above depends crucially on the ultraviolet cut-off we instituted in $A(x)$. To get a feeling about this estimate it is useful to write $A(x)$ as

$$A(x) = \check{\chi} * A'(x)$$

where, recall, $A'(x)$ is the original quantized vector potential, given by the same equation as before

$$A'(x) = \int (e^{ik\cdot x}a(k) + h.c.)g'(k)d^3k$$

with $g'(k) = (2\pi)^{-3}(2\omega(k))^{-1/2}$, and $\chi(k) = g(k)g'(k)^{-1}$, the ultraviolet cut-off. Then

$$\begin{aligned} |\check{\chi} * A'(x)| &\leq \|(-\Delta)^{-1/2}\check{\chi}\|\|(-\Delta)^{1/2}A'\| \\ &= \left(\int \frac{|\chi|^2}{\omega^2}\right)^{1/2} \left(\int |\mathrm{curl}A'|^2\right)^{1/2}. \end{aligned}$$

Of course, because of the Wick ordering in the definition of H_f, $(\int |\mathrm{curl}A'|^2)^{1/2}$ is not bounded by $H_f^{1/2}$. So the argument above does not lead to a rigorous proof, but it gives us an idea about what is going on here.

Lemma 17.5 *(relative bounds on $a^\#$)*

$$\|a(f)\psi\|_{\mathcal{F}}^2 \leq \int \frac{|f|^2}{\omega}\|H_f^{1/2}\psi\|_{\mathcal{F}}^2 \tag{17.14}$$

and

$$\|a^*(f)\psi\|_{\mathcal{F}}^2 \leq \int \frac{|f|^2}{\omega}\|H_f^{1/2}\psi\|_{\mathcal{F}}^2 + \int |f|^2\|\psi\|_{\mathcal{F}}^2. \tag{17.15}$$

Proof. (Drop the subscript $\mathcal{F}$.) By the Schwarz inequality

$$\begin{aligned} \|a(f)\psi\| &\leq \int |f|\|a\psi\| \\ &\leq \left(\int \frac{|f|^2}{\omega}\right)^{1/2} \left(\int \omega\|a\psi\|^2\right)^{1/2}. \end{aligned}$$

Since

$$\int \omega\|a\psi\|^2 = \langle\psi, H_f\psi\rangle,$$

the first inequality follows.

The second inequality follows from the first and the relation

$$\|a(f)^*\psi\|^2 = \langle\psi, a(f)a(f)^*\psi\rangle = \|a(f)\psi\|^2 + \int |f|^2\|\psi\|^2. \square$$

17.3 Elimination of particle and high photon energy degrees of freedom

This is the first application of the decimation map. Our task is to map (particles + fields) into fields. We consider only the ground state. Excited states are treated similarly once $H(\varepsilon)$ is suitably prepared.

Since we are looking at a vicinity of the ground state energy of $H(\varepsilon)$, the degrees of freedom connected to the excited particle states and to high photon energies should *not be relevant.* So we eliminate them isospectrally using the decimation map.

Recall $\chi_{H_f\leq\rho} = E_{(-\infty,\rho)}(H_f)$ denotes the spectral projection for the operator H_f onto energies $\leq \rho$ (and similarly for $\chi_{H_f\geq\rho}$, etc.). Let $P_\rho = P_0^{\rm part} \otimes \chi_{H_f\leq\rho}$, where, recall,

$$P_0^{\rm part} = P_{\psi_0^{\rm part}} = \text{projection onto the ground state } \psi_0^{\rm part} \text{ of } H_{\rm part}.$$

We want to apply the map D_{P_ρ} to the operators $H(\varepsilon) - z\cdot\mathbf{1}$ for z in a neighbourhood of the ground state energy E_0.

Recall that the decimation map D_P is defined on operators H, s.t. $D(H)\cap{\rm Ran}P$ is dense in $D(H)$, provided $0\in\rho(H_{\bar P})$ and

$$\|PHR_{\bar P}\| < \infty \quad \text{and} \quad \|R_{\bar P}HP\| < \infty\ ,$$

where $R_{\bar P} = \bar P(H_{\bar P})^{-1}\bar P$. In what follows E_0 and E_1 are the ground state energy and the first excited state of $H_{\rm part}$, and $\Delta E = E_1 - E_0$.

Theorem 17.1 and Proposition 17.13 of the Appendix (Section 17.11) imply

Theorem 17.6 *Let $|\varepsilon| \ll \Delta E$. Then D_{P_ρ} is defined on operators of the form $H(\varepsilon) - w\cdot\mathbf{1}$, where $w\in\{z \mid {\rm Re}\, z \leq E_0 + \frac{1}{2}\Delta E\}$, and is isospectral.*

Since we are interested in the part $\{z \mid {\rm Re}\, z \leq E_0 + \frac{1}{2}\Delta E\}$ of the spectrum, we can study $D_{P_\rho}(H(\varepsilon) - z)$ instead of $H(\varepsilon)$.

Observe that if the projection $P_0^{\rm part}$ has rank 1, then the operator $D_{P_\rho}(H(\varepsilon) - z)$ is of the form

$$D_{P_\rho}(H(\varepsilon) - z) = P_0^{\rm part} \otimes \chi_{H_f\leq\rho} H_0(\varepsilon, z)\chi_{H_f\leq\rho}\ ,$$

where the operator $H_0(\varepsilon, z)$, defined by this relation, acts on ${\rm Ran}\chi_{H_f\leq\rho}$. Thus we passed from the operator $H(\varepsilon)$ acting on $\mathcal{H}_{\rm part}\otimes\mathcal{F}$ to the operator $H_0(\varepsilon, z)$ acting on the much smaller space ${\rm Ran}\chi_{H_f\leq\rho}$, which is isospectral to $H(\varepsilon) - z\cdot\mathbf{1}$ in the set

$$\{z \mid {\rm Re}\, z \leq E_0 + \frac{1}{2}\Delta E\}$$

in the sense of Theorem 17.1. We eliminated, in an isospectral way, the degrees of freedom corresponding to the particles and to the photon energies $\geq \rho$, i.e. we projected out the part $\mathrm{Ran}\,(\mathbf{1} - P_0^{\mathrm{part}})$ of the particle space $\mathcal{H}_{\mathrm{part}}$ and the part $\mathrm{Ran}\,\chi_{H_f \geq \rho}$ of the Fock space $\mathcal{F}$. ρ is called the *photon energy scale.*

Though the operator $H_0(\varepsilon, z)$ looks rather complicated we will show in the next section that the complicated part of it gives a very small contribution, so it is of the form

$$H_0(\varepsilon, z) = \Delta_0 E + H_f + \text{ small terms } ,$$

where $\Delta_0 E$ is a computable energy shift of the order $O(\varepsilon^2)$.

If we ignore the small terms, then

$$\mathrm{spec}\, H(\varepsilon) \text{ in } (-\infty, E_0 + \Delta_0 E) \approx \mathrm{spec}\, H_f + E_0 + \Delta_0 E.$$

Now note that $H_f + E_0 + \Delta_0 E$ has the eigenvalue $E_0 + \Delta_0 E$, with the eigenfunction Ω, and the continuum $[E_0 + \Delta_0 E, \infty)$ with the generalized eigenfunctions $\psi_0^{\mathrm{part}} \otimes \Pi a^*(k_j)\Omega$. Hence $Q_{\bar{P}_p}(H(\varepsilon) - z)\Omega$ gives an approximate eigenfunction of $H(\varepsilon)$ with an approximate eigenvalue $E_0 + \Delta_0 E$ and similarly for the continuum. In fact, we will find energies $E^{(n)} = E_0 + O(\varepsilon^2)$ and numbers $w^{(n)} = 1 + O(\varepsilon^2)$ s.t. for $\rho = 0(\varepsilon) \ll 1$ and any $n \geq 1$ $H(\varepsilon)$ is isospectral to $E^{(n)} + w^{(n)} H_f + O(\rho^n)$ in the disk $D(E^{(n)}, \rho^n)$. This is called *infrared asymptotic freedom.*

17.4 Generalized Wick Representation

Though the operator $H_0(\varepsilon, z)$ looks much more complicated than $H(\varepsilon)$, in fact the complicated terms can be easily estimated and shown to give a relatively small contribution. These estimates are based on a presentation of the operator $H_0(\varepsilon, z)$ in the *generalized Wick (or normal) form.*

The operator $H_0(\varepsilon, z)$ we are interested in has no Wick representation. However, it can be expressed in a closely related form which serves the same purpose as the Wick one, but covers a much wider class of operators. We call this form, the *generalized Wick representation.* To describe this representation we introduction first some abbreviations:

$$(a^\#)^n = \prod_{j=1}^{n} a^\#(k_j) \quad \text{and} \quad d^n k = d^3k_1 \ldots d^3k_n \ ,$$

where $a^\#$ stands either for a^* or for a and is the same throughout the product. The short-hand

$$\int (a^*)^r h_{rs}(H_f) a^s \quad \text{or sometimes} \quad \int (a^*)^r h_{rs} a^s \tag{17.16}$$

stands for the operator

$$\int \prod_{j=1}^{r} a^*(k_j) h_{rs}(H_f, k_1 \dots k_{r+s}) \prod_{i=r+1}^{r+s} a(k_i) d^{r+s}k \ .$$

Here $h_{rs}(\mu, \underline{k})$, $\underline{k} = (k_1 \dots k_{r+s})$, are measurable functions on $[0,1] \times \mathbb{C}^{3(r+s)}$, uniformly Lipschitz in μ, called the *coupling functions*. Their behaviour in $\underline{k}$ will be specified later.

We say that an operator H on $\operatorname{Ran} \chi_{H_f \le \rho}$ is in the *generalized Wick form* if it can be written as

$$H = \sum_{r,s \ge 0} \int (a^*)^r h_{rs}(H_f) a^s \ .$$

Operators of the form (17.16) will be called (rs)-monomials. So far these definitions are purely formal since we do not describe a class of coupling functions h_{rs} for which the corresponding operators are, say, densely defined or bounded. This will be done later. For now we mention only that though H_f can be expressed in the standard Wick form

$$H_f = \int \omega a^* a \ ,$$

the corresponding coupling function, $\omega(k_1)\delta(k_1 - k_2)$, is more singular than we allow. But even if this coupling function was smooth, to find the Wick form of operators like $\chi_{H_f \le \rho}$, of which h_{rs} are composed in our case, is not an easy matter.

In what follows we manipulate the operators $a^*(k)$, $a(k)$ and H_f as if they were independent. We use only the commutation relations between these operators:

$$[a(k), H_f] = \omega(k) a(k) \ , \qquad \text{etc.}$$

The point here is that though we do not take expectations of operators in the vacuum state or, what is equivalent, do not sandwich operators by projections onto the vacuum, we do sandwich them by projections, $\chi_{H_f \le \rho}$, onto the low lying spectrum states of the free Hamiltonian, H_f. As a result we show that terms containing at least one creation or annihilation operator give a relatively small contribution and the contribution is smaller, the greater the number of creation and annihilation operators these terms contain.

17.5 Hamiltonian $H_0(\varepsilon, z)$

Our goal now is to show that the operator $H_0(\varepsilon, z)$, defined by the relation

$$H_0(\varepsilon, z) \equiv \langle \psi_0^{\text{part}} \ , \ D_\rho^{(0)} \big(H(\varepsilon) - z \cdot \mathbf{1} \big) \psi_0^{\text{part}} \rangle_{\mathcal{H}_{\text{part}}} \tag{17.17}$$

for $z \in \Omega$, can be represented in the generalized Wick form

$$H_0(\varepsilon, z) = \sum_{r,s \geq 0} \int (a^*)^r h_{0,rs}(H_f) a^s \tag{17.18}$$

and to estimate its coupling functions $h_{0,rs}(\mu, \underline{k})$. Our results are summed up in the following

Theorem 17.7 *Assume Condition (A) holds. Let $\varepsilon \ll \delta \equiv \min(\Delta E, \rho)$ (ρ is the scale parameter entering the definition of $H_0(\varepsilon, z)$). The operator $H_0(\varepsilon, z)$ has a generalized Wick representation, Eqn (17.18), with coupling functions, $h_{0,rs}$, analytic in $z \in \Omega$ and satisfying the estimates*

$$\begin{aligned} &|h_{0,rs}(\mu, \underline{k})| + |\partial_\mu h_{0,rs}(\mu, \underline{k})| \\ &\leq \text{const} \prod_{j=1}^{r+s} (\text{const} \cdot \varepsilon \cdot \delta^{-1} \cdot \omega(k_j)^{-1/2}) \ , \end{aligned} \tag{17.19}$$

where the product is absent in the case $r = s = 0$, and

$$|\partial_\mu h_{0,00}(\mu) - 1| \leq \text{const} \cdot \varepsilon^2/\delta^2 \ . \tag{17.20}$$

The proof of this theorem is simple but lengthy. We omit it.

17.6 Banach space of operators

Instead of looking at the single Hamiltonian, $H_0(\varepsilon, z)$, we now consider an entire space of Hamiltonians of which $H_0(\varepsilon, z)$ is just one point (or complex curve depending on the parameter z). Our aim is to establish an isospectral flow on *this space* which takes $H_0(\varepsilon, z)$ to a simple operator.

From now on we use the shorthand $\chi_{\leq \rho} \equiv \chi_{H_f \leq \rho}$ and $\chi_{> \rho} \equiv \chi_{H_f > \rho}$ for our smoothed out characteristic functions.

Consider a positive function J on $\mathbb{R}^3$ satisfying

$$\int_{\omega \leq 1} J^2 + \int_{\omega \leq 1} \frac{J^2}{\omega} < \infty.$$

Define the Banach space, $\mathcal{B}_J$, of formal expressions of the form $H = \sum_{r+s \geq 0} H_{rs}$, where

$$H_{rs} = \int (a^*)^r h_{rs}(H_f) a^s.$$

As before, the r.h.s. here is a shorthand for the expression

$$\int \prod_{j=1}^{r} a^*(k_j) h_{rs}(H_f, k_1 \dots k_{r+s}) \prod_{j=r+1}^{r+s} a(k_j) d^{r+s}k.$$

The coupling functions, $h_{rs}(\mu, \underline{k})$, are assumed to satisfy the estimates

$$\|h_{rs}\|_J \equiv \sum_{n=0}^{1} \|h_{rs}\|_{J,n} < \infty \ , \tag{17.21}$$

where

$$\|h_{rs}\|_{J,n} \equiv \sup_{\mu,k} [J^{-1 \otimes (r+s)} |\partial_\mu^n h_{rs}|] < \infty \ . \tag{17.22}$$

Here we used the notation

$$J^{\otimes n} = \prod_{j=1}^{n} J(k_j) \ . \tag{17.23}$$

We set $\|H_{rs}\|_{J,n} \equiv \|h_{rs}\|_{J,n}$, $\|H_{rs}\|_J \equiv \|h_{rs}\|_J$ and

$$\|H\|_J = \max_{rs} \|H_{rs}\|_J \ . \tag{17.24}$$

We identify expressions H with operators $\chi_{\leq 1} H \chi_{\leq 1}$ (via an obvious one-to-one correspondence). The latter are bounded operators on $\mathcal{F}$ as follows from

Proposition 17.8 *(a key bound)*

$$\|\chi_{\leq 1} H_{rs} \chi_{\leq 1}\| \leq \left(\int_{\sum \omega(k_j) \leq 1} \frac{|h_{rs}|^2}{\prod_1^{r+s} \omega(k_j)} d^{r+s}k \right)^{1/2}$$

$$\leq \lambda(J,1)^{r+s} \|H_{rs}\|_{J,0} \ , \tag{17.25}$$

where

$$\lambda(J,1) = \left(\int_{\omega \leq 1} \frac{J^2}{\omega} \right)^{1/2} .$$

Thus $\chi_{\leq 1} H \chi_{\leq 1} = \Sigma \chi_{\leq 1} H_{rs} \chi_{\leq 1}$ *converges in norm, provided*

$$\int_{\omega \leq 1} \frac{J^2}{\omega} < 1.$$

Proof. We have by an operator norm inequality

$$\|\chi_{\leq 1} H_{rs} \chi_{\leq 1}\| \leq \int \int \|a^r \chi_{\leq 1}\| \|h_{rs}\| \|a^s \chi_{\leq 1}\| \ . \tag{17.26}$$

A technical estimate (which can be found in [BFS1], cf also the $n = 1$ case with 17.14) implies that the following estimate holds

$$\int h \|a^n \chi_{\leq 1}\| \leq \left(\int\limits_{\sum \omega_j \leq 1} \frac{|h|^2}{\prod\limits_1^n \omega_j} \right)^{1/2} \ ,$$

where $\omega_j = \omega(k_j)$, which completes the proof of the first part of (17.25). The proof of the second inequality in (17.25) follows from the relations $\|h_{rs}\| \leq \|h_{rs}\|_J \cdot J^{\otimes(r+s)}$ and

$$\int\limits_{\sum\limits_1^n \omega_j \leq 1} \left(\frac{J^2}{\omega} \right)^{\otimes n} \leq \lambda(J,1)^n \ . \qquad \square$$

In what follows we think about H as an operator restricted to the subspace $\mathrm{Ran}\chi_{\leq 1}$. Moreover, we take J to be of the form $J = \xi \cdot \omega^{-\nu}$ where $\xi > 0$ and $\nu \leq \frac{1}{2}$. The cases important for us are $\nu = \frac{1}{2}$, if Condition (B) is not assumed, and $\nu = -\frac{1}{2}$ otherwise.

$\mathcal{B}_J$ is our basic Banach space of operators. For $\nu < \frac{1}{2}$ it is sufficient for our purposes. For $\nu = \frac{1}{2}$ it is not. To treat the latter case we introduce, in an appropriate place, a more refined Banach space.

17.7 Rescaling

We want to map our operators into operators on a fixed, *ρ-independent* space. To this end we rescale them as follows. Define a unitary group, $U(\theta)$, by

$$U(\theta) \prod a^*(f_j)\Omega = \prod a^*(U_\theta f_j)\Omega \tag{17.27}$$

where U_θ is the rescaling transformation acting on $L^2(\mathbb{R}^3)$, given by

$$(U_\theta f)(k) = e^{-3\theta/2} f(e^{-\theta} k). \tag{17.28}$$

In particular, $U(\theta)\Omega = \Omega$. Moreover, we have the following relations

$$U(\theta)a^{\#}(k)U(\theta)^{-1} = e^{3\theta/2}a^{\#}(e^{\theta}k) \tag{17.29}$$

$$U(\theta)H_f U(\theta)^{-1} = e^{-\theta}H_f. \tag{17.30}$$

The last equation implies

$$U(-\ln(\rho)) : \ \mathrm{Ran}\,\chi_{H_f\leq\rho} \to \mathrm{Ran}\,\chi_{H_f\leq 1}. \tag{17.31}$$

Now we define the rescaling transformation on operators as

$$S_\rho(H) = e^{\theta}U(\theta)HU(\theta)^{-1}, \qquad \theta = -\ln\,\rho. \tag{17.32}$$

Note $S_\rho(H_f) = H_f$. By (17.31), if an operator H acts on $\mathrm{Ran}\,\chi_{\leq\rho}$, then $S_\rho(H)$ acts on $\mathrm{Ran}\,\chi_{\leq 1}$, a ρ-independent space.

Observe that we can define S_ρ directly as $S_\rho = \frac{1}{\rho}S(\rho)$, where the one-parameter group $S(\rho)$ is defined by the properties

1. $S(\rho)(A\cdot B) = S(\rho)(A)\cdot S(\rho)(B)$,
2. $S(\rho)a^{\#}(f) = a^{\#}(U_\theta f)$, $\theta = -\ln\rho$.

Scaling dimension. If we rescale $H_{rs} = \int (a^*)^r h_{rs} a^s$, we obtain

$$S_\rho(H_{rs}) = \int (a^*)^r h^{(\rho)}_{rs} a^s, \tag{17.33}$$

where

$$h^{(\rho)}_{rs}(H_f, k) = \rho^{3/2(r+s)-1}h_{rs}(\rho H_f, \rho k)\ . \tag{17.34}$$

We take $J = \xi\omega^{-\nu}$. If $H_{rs}\in\mathcal{B}_J$, then h_{rs} behaves for small $|k_j|$'s as $\prod_{j=1}^{r+s}\omega(k_j)^{-\nu}$. So

$$S_\rho(H_{rs}) \sim \rho^{(3/2-\nu)(r+s)-1}H_{rs}\ .$$

The important term here is $\underline{r+s-1}$. If $r+s\geq 2$, then $\|S_\rho(H_{rs})\|_J \to 0$ as $\rho\to 0$ for $\nu < 1$!

The physics terminology (for $\nu = \frac{1}{2}$) is as follows:

$$r+s = 1 \ \leftrightarrow\ \text{marginal terms}$$

$$r+s \geq 2 \ \leftrightarrow\ \text{irrelevant terms.}$$

We record also the action of the group S_ρ on the Banach space $\mathcal{B}_J$ (remember that $J = \xi\omega^{-\nu}$). The following equation follows from Eqns (17.33)-(17.34):

$$\|S_\rho(H_{rs})\|_J = \rho^{(3/2-\nu)(r+s)-1}\|H_{rs}\|_J = \rho^{-1}\|H_{rs}\|_{\rho^{\nu-3/2}J} \ . \tag{17.35}$$

Applying these equalities to operators of the form $H = \sum_{r+s\geq 0} H_{rs}$ and $H_1 = \sum_{r+s\geq 1} H_{rs}$, we find

$$\|S_\rho(H)\|_J = \rho^{-1}\|H\|_{\rho^{\nu-3/2}J} \ ,$$

$$\|S_\rho(H_1)\|_J \leq \|H_1\|_{\rho^{\nu-\frac{1}{2}}J} \leq \rho^{1/2-\nu}\|H_1\|_J \quad \text{for } \nu \leq \frac{1}{2} \ . \tag{17.36}$$

17.8 Renormalization map

Let $D_\rho := D_{P_\rho}$, where $P_\rho = \chi_{H_f\leq\rho}$, and D_P is the decimation map which is defined in (17.3). We define the renormalization map by

$$\mathcal{R}_\rho = S_\rho \circ D_\rho \ . \tag{17.37}$$

It is shown in [BFS4] that $\mathcal{R}_\rho$ is defined on a small neighbourhood in B_J of the set $\mathbb{C}\cdot H_f$. Given that, we discuss briefly properties of $\mathcal{R}_\rho$. The statements of the theorem below are either obvious or follow from results above.

Theorem 17.9 *The renormalization map $\mathcal{R}_\rho$ has the following properties:*

1. *$\mathcal{R}_\rho$ is isospectral in the sense that $\rho\cdot\mathcal{R}_\rho(H)$ and H are isospectral at 0,*
2. *$\mathcal{R}_\rho$ is a semigroup: $\mathcal{R}_{\rho_2}\circ\mathcal{R}_{\rho_1} = \mathcal{R}_{\rho_2\rho_1}$ and $\mathcal{R}_1 = \mathbf{1}$, provided $\chi_{\lambda\leq\rho_2}\chi_{\lambda\leq\rho_1} = \chi_{\lambda\leq\rho_2}$,*
3. *$\mathcal{R}_\rho(wH_f + z\mathbf{1}) = wH_f + \frac{1}{\rho}z\mathbf{1}\ \forall w,z\in\mathbb{C}$. In particular, $\mathbb{C}H_f$ is a complex line of fixed points of $\mathcal{R}_\rho$: $\mathcal{R}_\rho(wH_f) = wH_f\ \forall w\in\mathbb{C}$, and $\mathbb{C}\cdot\mathbf{1}$ is (a part of) the unstable manifold.*

Denote $\mathcal{M}_{fp} \equiv \mathbb{C}\cdot H_f$. We want to understand the dynamics of $\mathcal{R}_\rho$ as $\rho\to 0$ in a vicinity of the fixed point manifold $\mathcal{M}_{fp}$. We will use the following definitions for local stable and unstable manifolds:

$$\mathcal{M}_s = \{H\in U\big|\mathcal{R}_\rho(H)\to\mathcal{M}_{fp} \text{ as } \ \rho\to 0\}$$

and

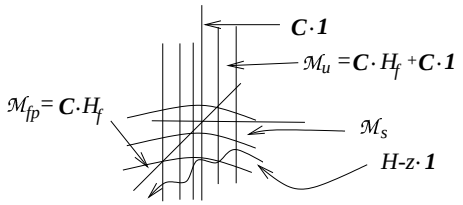
$$\mathcal{M}_u = \{H\in U\big|\mathcal{R}_\rho(H)\to\mathcal{M}_{fp} \text{ as } \ \rho\to\infty\} \ , \tag{17.38}$$

where U is an appropriate neighbourhood of $\mathcal{M}_{fp}$ in $\mathcal{B}_J$. Statement 3 above shows that the subspace $\mathbb{C} \cdot H_f + \mathbb{C} \cdot \mathbf{1}$ is a part of the local unstable manifold $\mathcal{M}_u$.

We will show later that the local stable manifold, $\mathcal{M}_s$, has complex co-dimension 1. More precisely we show that for every operator H in U there is a function $E : \{H \in U | \langle H \rangle_\Omega = 0\} \to \mathbb{R}$, such that

$$\mathcal{M}_s = \{H \in U | \langle H \rangle_\Omega = E(H^T)\} \tag{17.39}$$

where we have used the notation $H^T \equiv H - \langle H \rangle_\Omega \cdot \mathbf{1}$ (so that $\langle H^T \rangle_\Omega = 0$), i.e. $\mathcal{M}_s$ is the graph of E.



(17.40)

RG flow

The set U is such that Theorem 17.7, proven above, implies that for ε sufficiently small

$$H^{(0)}(\varepsilon, z) \equiv S_{\rho_0}(H_0(\varepsilon, z)) \in U \ . \tag{17.41}$$

Recall that the operator $\rho_0 \cdot H^{(0)}(\varepsilon, z)$ is isospectral to $H(\varepsilon) - z \cdot \mathbf{1}$ in the set

$$\Omega \equiv \{z \in \mathbb{C} | \mathrm{Re}\ z \leq E_0 + \frac{1}{2}\Delta E\} \ . \tag{17.42}$$

Moreover, $\rho \cdot \mathcal{R}_\rho(H^{(0)}(\varepsilon, z))$ is isospectral to $\rho_0 \cdot H^{(0)}(\varepsilon, z)$ in the set Ω_ρ defined by

$$\Omega_\rho \equiv \{z \in \Omega | |\langle \mathcal{R}_\rho(H^{(0)}(\varepsilon, z)) \rangle_\Omega| \leq \frac{1}{2}\rho\} \ .$$

We will show that this set contains an interval of size $\frac{1}{2}\rho \|H_1\|_J$ and is contained in an interval of size $2\rho\|H_1\|_J$, both centered at some E_ρ. As a result $H(\varepsilon) - z \cdot \mathbf{1}$ is isospectral to $\rho\mathcal{R}_\rho(H^{(0)}(\varepsilon, z))$ in Ω_ρ. On the other hand, for ρ small, $\mathcal{R}_\rho(H^{(0)}(\varepsilon))$ is close to a fixed point:

$$\mathcal{R}_\rho(H^{(0)}(\varepsilon)) \approx w_\rho \cdot H_f$$

for the same $w_\rho \in \mathbb{C}$. Thus in Ω_ρ, $H(\varepsilon)$ has the same spectral characteristics as the operator $E_\rho + w_\rho \cdot H_f$. This is the core idea of our analysis.

17.9 Linearized flow

Consider the linearized maps, $\partial\mathcal{R}_\rho(w\cdot H_f)$, for $\mathcal{R}_\rho$ at the fixed points $w\cdot H_f$, $w\in\mathbb{C}$. A straightforward computation gives

$$\partial\mathcal{R}_\rho(w\cdot H_f)\xi = S_\rho(\xi)\ .$$

Thus $\partial\mathcal{R}_\rho(w\cdot H_f)$ is independent of $w\in\mathbb{C}$ and can be identified with the rescaling map S_ρ.

Since the linearized operator $\Lambda\equiv\partial\mathcal{R}_\rho(w\cdot H_f)$ is independent of $w\cdot H_f\in\mathbb{C}\cdot H_f$, then so are its unstable, central and stable subspaces, V_u, V_c and V_s, which we identify now.

The subspaces V_u, V_c and V_s are defined by the conditions that they span the entire space $\mathcal{B}_J$, that they overlap only at $\{0\}$ and that they verify

$$\|\Lambda\restriction V_s\|<1\ ,\quad \|\Lambda^{-1}\restriction V_u\|<1$$

and

$$\Lambda\restriction V_c = \mathbf{1}_{V_c}\ ,$$

where $\Lambda\equiv\partial\mathcal{R}_\rho(wH_f)=S_\rho$.

Consider a generalized Wick monomial H_{rs} with a coupling function h_{rs} which is homogeneous of degree $-\alpha$ in each variable k; and homogeneous of degree β in μ. Then, due to (17.34) and (17.36), we have that

$$S_\rho(H_{rs}) = \rho^{(3/2-\alpha)(r+s)+\beta-1}H_{rs}\ ,$$

i.e. H_{rs} is an eigenvector of S_ρ with the eigenvalue $\rho^{(3/2-\alpha)(r+s)+\beta-1}$. For $H_{rs}\in\mathcal{B}_J$ with $J=\xi\omega^{-\nu}$ the worst case scenario is $\alpha=\nu$ and $\beta=0$ for $r+s\geq 1$. In the case $r=s=0$, the coupling function h_{00} is independent of the k_j's and can be written as

$$h_{00}(\mu) = E + w\cdot\mu + h_1(\mu) \tag{17.43}$$

with $E=h_{00}(0)$, $w=h'_{00}(0)$ and $h_1(\mu)=h_{00}(\mu)-h_{00}(0)-h'_{00}(0)\mu$. The first term on the r.h.s is of the type $(\alpha=0,\beta=0)$, the second, of the type $(\alpha=0,\beta=1)$, while the third is of the type $(\alpha=0,\beta=2)$. Thus the spectrum of $\partial\mathcal{R}_\rho(w\cdot H_f)$ on $\mathcal{B}_J$ is the union of the sets

$$\{\rho^{-1}\}\ ,\quad \{\rho^{m-1}\},\ m\geq 1\quad\text{and}\quad \{\rho^{(3/2-\alpha)n-1}\big|\operatorname{Re}\alpha\leq\nu\}\ ,n\geq 1\ , \tag{17.44}$$

with the spectral subspaces

$$\mathbb{C}\cdot\mathbf{1}\ ,\mathbb{C}\cdot H_f^m,\ m\geq 1\quad \text{and}\ \{\sum_{r+s=n} H_{rs}\big|H_{rs}\in\mathcal{B}_J\}\ ,n\geq 1\ . \tag{17.45}$$

(Here we ignored the fact that for $H_{rs}\in\mathcal{B}_J$ the coupling functions h_{rs} are, in general, not homogeneous in μ. However, it is easy to account for this discrepancy.)

Decomposition (17.43) suggests that we should introduce the subspace

$$\mathcal{T}=\{T=T(H_f)|T(\cdot):[0,1]\to\mathbb{C}\ \text{is}\ C^2\ \text{with}\ \ T(0)=T'(0)=0\}\ . \tag{17.46}$$

The result above leads to an identification of stable, central and unstable subspaces, V_s, V_c and V_u, of the linearized renormalization group map at $\mathcal{M}_{fp}$.

These subspaces V_s, V_c and V_u depend on the parameter ν entering the definition of the Banach space $\mathcal{B}_J$, $J=\xi w^{-\nu}$. We consider several ranges of this parameter.

$\underline{\nu<\frac{1}{2}}$:

$$V_u=\mathbb{C}\cdot\mathbf{1}\ ,\ V_c=\mathbb{C}\cdot H_f \tag{17.47}$$

and

$$V_s=\{\sum_{r+s\geq 1} H_{rs}|H_{rs}\in\mathcal{B}_J\}+\mathcal{T} \tag{17.48}$$

$\underline{\nu=\frac{1}{2}}$.

$$V_u=\mathbb{C}\cdot\mathbf{1}\ ,\ V_c=\mathbb{C}\cdot H_f+\{\sum_{r+s=1} H_{rs}|H_{rs}\in\mathcal{B}_J\}$$

and

$$V_s=\{\sum_{r+s\geq 2} H_{rs}|H_{rs}\in\mathcal{B}_J\}+\mathcal{T}$$

$\underline{\frac{1}{2}<\nu<1}$.

$$V_u=\mathbb{C}\cdot\mathbf{1}+\{\sum_{r+s=1} H_{rs}|H_{rs}\in\mathcal{B}_J\},$$

$$V_c=\mathbb{C}\cdot H_f$$

and

$$V_s=\{\sum_{r+s\geq 2} H_{rs}|H_{rs}\in\mathcal{B}_J\}+\mathcal{T}$$

and so forth. When proceeding to $\nu\geq 1$ one has to remember that the original operator $H(\varepsilon)$ is not bounded below if g behaves as $\omega^{-\nu}$ with $\nu\geq 1$, as $|k|\to 0$.

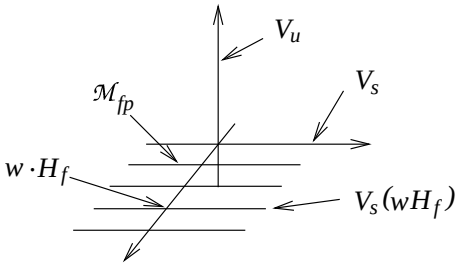
The decompositions into stable, central and unstable subspaces mentioned above can be modified if one notices that the subspace $\mathcal{T}$ is invariant under the full non-linear flow, $\mathcal{R}_\rho$, as well as the linearized one, $\partial\mathcal{R}_\rho(wH_f)$:

$$\mathcal{R}_\rho(T) = \partial\mathcal{R}_\rho(w \cdot H_f)T = S_\rho(T) = T_\rho \ ,$$

where $T_\rho = T_\rho(H_f)$ with $T_\rho(\mu) = \rho^{-1}T(\rho\mu)$. Thus we could have added $\mathcal{T}$ to the central subspace V_c (cf. [BFS2]). We do not do this here.

We are interested in the cases $\nu < \frac{1}{2}$ (more precisely $\nu = -\frac{1}{2}$) and $\nu = \frac{1}{2}$. We arrive at the first case, if Condition (B) (the confinement condition) is satisfied, by performing a *Pauli-Fierz transform* (see [BFS2,BFS4]). In the absence of Condition (B) we stick with the original standard Hamiltonian (16.2) which leads via Theorem 17.7 to the second case, $\nu = \frac{1}{2}$. Note that in both cases $V_u = \mathbb{C} \cdot \mathbf{1}$ and is, in fact, the unstable manifold, $\mathcal{M}_u$, for the entire flow. Now we comment on the peculiarities of the cases $\nu < \frac{1}{2}$ and $\nu = \frac{1}{2}$.

In the case $\nu < \frac{1}{2}$, the central subspace, $V_c = \mathbb{C} \cdot H_f$, is also the central manifold, $\mathcal{M}_c$, for $\mathcal{R}_\rho$. It consists of fixed points of $\mathcal{R}_\rho$ and is denoted also by $\mathcal{M}_{fp}$. Moreover, the stable affine subspaces $V_s(wH_f) \equiv w \cdot H_f + V_s$ for fixed points $w \cdot H_f$, $w \in \mathbb{C}$, foliate the subspace $V_u^\perp$ (see Fig. 17.49).



(17.49)

Stable, central and unstable subspaces

These circumstances allow for a complete analysis of the flow $\mathcal{R}_\rho$ near the fixed point manifold $\mathcal{M}_{fp}$ (see Section 17.10).

Note also that in the case $\nu < \frac{1}{2}$

$$\|\Lambda_u\| = \|\Lambda_u^{-1}\|^{-1} = \rho^{-1} \quad \text{and} \quad \|\Lambda_s\| = \rho^{1/2-\nu} < \|\Lambda_u^{-1}\| \ ,$$

where $\Lambda_u = \Lambda \restriction V_u$ and $\Lambda_s = \Lambda \restriction V_s$. We have used here that $1 \geq \frac{1}{2} - \nu$ for $\nu \geq -\frac{1}{2}$.

The case $\nu = \frac{1}{2}$ is more subtle. The main problem here is that the central manifold is larger than the manifold of fixed points. Our task in the remainder of

this section is to isolate the smallest possible central subspace – the central subspace for $\nu = \frac{1}{2}$ considered above is too large, a big piece of it could, in fact, be taken into the stable subspace. To do this we have to use a more refined Banach space instead of $\mathcal{B}_J$. We do not pursue this case any further here, but refer the interested reader to [BFS4].

17.10 Central-stable manifold for RG and spectra of Hamiltonians

In this section we give a construction of the stable manifold $\mathcal{M}_s$ in the cases $\nu < \frac{1}{2}$ and $\nu = \frac{1}{2}$. We use an abstract central-stable manifold theorem whose proof can be found in [BFS4].

We begin with the case $\nu < \frac{1}{2}$. Let $U_\varepsilon = \{H \in \mathcal{B}_J \big| \|H - w \cdot H_f\|_J \leq |w| \cdot \varepsilon$, for some $w \neq 0\}$. It follows from technical estimates which can be found in [BFS4] (see also [BFS2]), that $\mathcal{R}_\rho$ maps U_ε into $\mathcal{B}_J$, provided $\varepsilon \leq \frac{1}{8}$, $\int\limits_{\omega \leq 1} \frac{J^2}{\omega} \leq \frac{1}{16}$ and $4\varepsilon \leq \rho$. We define $U_\varepsilon^T \equiv \{H \in U_\varepsilon | \langle H \rangle_\Omega = 0\}$, the truncated disc. Our first result is

Theorem 17.10 *Let $\nu < \frac{1}{2}$. There is a function $f : U_\varepsilon^T \to \mathbb{C}$ s.t. $\mathcal{M}_s \equiv \operatorname{graph} f$ is invariant under $\mathcal{R}_\rho$ and*

$$\forall H \in \mathcal{M}_s \; \exists\, w \cdot H_f \in \mathcal{M}_{fp} : \mathcal{R}_\rho^n(H) \to w \cdot H_f$$

as $n \to \infty$ in the topology of $\mathcal{B}_J$ and therefore in the norm topology. Here graph$f$ *is identified with the set $\{H^T + f(H^T) | H^T \in U_\varepsilon^T\}$.*

We reinterpret Theorem 17.10, which looks like a stable manifold theorem, but could also be called central-stable one. Indeed, $\mathcal{M}_s$ is a stable manifold, $\mathcal{M}_s(\mathcal{M}_{fp})$, for the invariant manifold

$$\mathcal{M}_{fp} = \mathbb{C} \cdot H_f \; . \tag{17.50}$$

However, $\mathcal{M}_{fp}$ is a manifold of fixed points which can be identified with the central manifold (which is equal to the central subspace) for each of its fixed points: $\mathcal{M}_{fp} = \mathcal{M}_c(w \cdot H_f) = V_c \; \forall\, w \cdot H_f \in M_{fp}$. The tangent space of $\mathcal{M}_s$ at any $w \cdot H_f \in M_{fp}$ is

$$V_c + V_s =: V_{cs} \; . \tag{17.51}$$

Consequently, $\mathcal{M}_s$ is also the central-stable manifold, $\mathcal{M}_{cs}(w \cdot H_f)$, for any fixed point $w \cdot H_f \in \mathcal{M}_{fp}$. Furthermore, U_ε^T is nothing but $U_\varepsilon \cap V_{cs}$ and $\mathbb{C}$ can be

identified with the unstable subspace $V_u = \mathbb{C} \cdot \mathbf{1}$, so that

$$f : U_\varepsilon \cap V_{sc} \to V_u \tag{17.52}$$

for any fixed point $w \cdot H_f \in \mathcal{M}_{fp}$. Recall that the identification of the unstable, central and stable subspaces is based on the formula

$$\partial \mathcal{R}_\rho(w \cdot H_f) = S_\rho \ , \tag{17.53}$$

where S_ρ is the rescaling map, valid for any $w \cdot H_f \in \mathcal{M}_{fp}$.

To prove Theorem 17.10 we apply an abstract stable manifold theorem. To this end we should ascertain that $\mathcal{R}_\rho$ is Frechét differentiable at least $1+\varepsilon$ times. In fact we have

Theorem 17.11 *The map $\mathcal{R}_\rho$ is analytic on U_ε.*

Proof: Let $P \equiv \chi_{H_f \leq \rho}$. By the definition of $\mathcal{R}_\rho$, and equation (17.36), it suffices to show that $\bar{R}(H) \equiv H_f \bar{P}(\bar{P}H\bar{P})^{-1}\bar{P}H_f$, where $\bar{P} = \mathbf{1} - P$, is analytic as a map from U_ε to the Banach space $B_{4\rho^{-1/2}J}$. Let $H \in U_\varepsilon$ and assume $\|\delta H\| \leq \varepsilon$, where $\delta H = H - H_f$, i.e. we take $r = 1$ here. We rewrite $\bar{R}(H)$ as

$$\bar{R} = H_f^{1/2}\bar{P}[\mathbf{1} + K]^{-1}\bar{P}H_f^{1/2} \ ,$$

where $K = H_f^{-1/2}(\delta H)_{\bar{P}}H_f^{-1/2}$. Since $\lambda(J,1) \equiv \left(\int\limits_{\omega \leq 1} \frac{J^2}{\omega} \right)^{1/2} \leq \frac{1}{4}$, equation (17.25) implies that

$$\|K\| \leq 4\|\delta H\|_J \ .$$

Thus for $\|\delta H\|_J < \frac{1}{4}$, $[\mathbf{1} + K]^{-1}$ can be expanded in a Neumann series. Now Proposition 15.1 of [BFS4] implies that

$$\|H_f^{1/2}K^nH_f^{1/2}\|_{4\rho^{-1/2}J} \leq 2\rho(2\rho^{-1/2}\|\delta H\|_J)^n \ .$$

Thus the series $H_f^{1/2} \sum\limits_{n=1}^{\infty} (-K)^n H_f^{1/2}$ converges in the Banach space $\mathcal{B}_{4\rho^{-1/2}J}$. Since $K = H_f^{-1/2}\bar{P}\delta H\bar{P}H_f^{-1/2}$ the claim follows. □

Now we rephrase in our notation an abstract result proven in [BFS4].

Theorem 17.12 *Let $\nu < \frac{1}{2}$. For any $w \cdot H_f \in \mathcal{M}_{fp}$ with $w \geq \delta > 0$ there a map $f_s : V_s \to V_{cu} \equiv V_c + V_u$, s.t. the manifold $\mathcal{M}_s(wH) \equiv \mathrm{graph} f_s$ is invariant under $\mathcal{R}_\rho$ and*

(i) $\forall\, H \in \mathcal{M}_s(w \cdot H_f) \Rightarrow \mathcal{R}_\rho(H) \to w \cdot H_f$ *as* $\rho \to 0$

(ii) the manifold $\mathcal{M}_s \equiv \bigcup_{w \cdot H_f \in \mathcal{M}_{fp}, |w| \geq \delta} \mathcal{M}_s(w \cdot H_f)$ *has all the properties stated in Theorem 17.10.*

Clearly, Theorem 17.10 follows from Theorem 17.12.

17.11 Appendix

Proposition 17.13 *Let* $\Delta E = \min(E_1 - E_0, \rho)$. *Assume* $|\varepsilon| \ll \Delta E$ *and let*

$$\Omega \equiv \{z \in \mathbb{C} | \mathrm{Re} z \leq E_0 + \frac{1}{2}\Delta E\} \tag{17.54}$$

Then (i) $\Omega \subset \rho(H_{\bar{P}}(\varepsilon))$ *and (ii) for* $z \in \Omega$,

$$\|P_\rho H(\varepsilon) \bar{P}_\rho (H_{\bar{P}_\rho}(\varepsilon) - z)^{-1}\| \leq C|\varepsilon| \Big/ \Delta E \ . \tag{17.55}$$

Proof. In order to simplify the exposition somewhat in a couple of places below, we use also the condition $\int |g(k)|^2 d^3k < \infty$. However, using more careful estimates this condition can be avoided.

Since $\mathrm{div}\, A(x) = 0$, we obtain by expanding $\big(p - \varepsilon A(x)\big)^2$:

$$H(\varepsilon) = H(0) + \varepsilon \cdot I(\varepsilon),$$

where $I(\varepsilon)$ is the interaction energy

$$I(\varepsilon) = -p \cdot A(x) + \frac{1}{2}\varepsilon A(x)^2.$$

Write for $P = P_\rho$ and $I = I(\varepsilon)$

$$H_{\bar{P}}(\varepsilon) = H_{\bar{P}}(0) + \varepsilon I_{\bar{P}}, \text{ where}$$

$$H_{\bar{P}}(0) = H_{\mathrm{part}} \bar{P}_0^{\mathrm{part}} \otimes \mathbf{1}_f + \mathbf{1}_{\mathrm{part}} \otimes H_f \chi_{H_f \geq \rho} \ .$$

Then

$$(H_{\bar{P}}(\varepsilon) - z) = (H_{\bar{P}}(0) - z)^{1/2}[\mathbf{1} + \varepsilon K](H_{\bar{P}}(0) - z)^{1/2}, \tag{17.56}$$

$$K = (H_{\bar{P}}(0) - z)^{-1/2} I_{\bar{P}} (H_{\bar{P}}(0) - z)^{-1/2}.$$

Using the definition of I, we find

$$\|K\| \leq \|p(H_{\bar{P}}(0)-z)^{-1/2}\|\|A(x)\bar{P}(H_{\bar{P}}(0)-z)^{-1/2}\|$$
$$+\frac{\varepsilon}{2}\|(H_{\bar{P}}(0)-z)^{-1}\bar{P}A(x)\|\|A(x)\bar{P}(H_{\bar{P}}(0)-z)^{-1/2}\| \ .$$

The relative bound on $A(x)$ proven above implies that

$$\|A(x)\bar{P}(H_{\bar{P}}(0)-z)^{-1/2}\| \leq 2\left(\int \frac{|g|^2}{\omega}\right)^{1/2} \|H_f^{1/2}(H_{\bar{P}}(0)-z)^{-1/2}\bar{P}\|$$
$$+\left(\int |g|^2\right)^{1/2} \|(H_{\bar{P}}(0)-z)^{-1/2}\bar{P}\| \ . \tag{17.57}$$

Now assume for the moment that spec $H_{\rm part}$ is discrete. Then

$$H_f^{1/2}(H_{\bar{P}}(0)-z)^{-1/2}\bar{P} = \sum_{j\geq 1} P_j^{\rm part} \otimes H_f^{1/2}\big(H_f-(z-E_j)\big)^{-1/2}$$
$$+P_0^{\rm part}\otimes H_f^{1/2}(H_f-(z-E_0))^{-1}\chi_{H_f\geq\rho} \ ,$$

where $P_j^{\rm part}$ is the orthogonal projection onto the state $\psi_j^{\rm part}$. Hence for $\mathrm{Re}\, z < E_1$, $E_0+\rho$ and $\Sigma \equiv \{(E,s)|$ either $E\in\sigma(H_{\rm part})\backslash\{E_0\}$ and $s\geq 0$ or $E\in\sigma(H_{\rm part})$ and $s\geq\rho\}$ we have

$$\|H_f^{1/2}(H_{\bar{P}}(0)-z)^{-1/2}\bar{P}\| \leq \sup_{\Sigma}\frac{s^{1/2}}{|s-(z-E)|^{1/2}} \leq 1 \ . \tag{17.58}$$

In fact, this estimate holds for a general $H_{\rm part}$. We accept this without a proof. Similarly,

$$\|(H_{\bar{P}}(0)-z)^{-1/2}\bar{P}\| \leq \sup_{\Sigma}|s-(z-E)|^{-1/2} \leq (\Delta E)^{-1/2} \ . \tag{17.59}$$

These estimates, together with (17.57) imply that

$$\|A(x)\bar{P}(H_{\bar{P}}(0)-z)^{-1/2}\| \leq 2\left(\int\frac{|g|^2}{\omega}\right)^{1/2}+\left(\int|g|^2\right)^{1/2}/(\Delta E)^{1/2} \ . \tag{17.60}$$

Since $\sigma(H_{\bar{P}}(0)) = [\bar{E},\infty)$, where, $\bar{E}=\min(E_1,E_0+\rho)$, we have that $\|p(H_{\bar{P}}(0)-z)^{-1/2}\| \leq C\mathrm{dist}(z,[\bar{E},\infty))^{-1/2}$. Thus $\|K\|\leq C|z-\bar{E}|^{-1}$ for $\mathrm{Re}\, z<E_1$ and therefore

$$\|K\| \leq C(\Delta E)^{-1} \ , \tag{17.61}$$

if $z \in \Omega$. Pick now $|\varepsilon| \leq C\Delta E/2$. Then $\|\varepsilon K\| \leq 1/2$ and therefore the r.h.s. of (17.56) is invertible. Hence

$$\{z \mid \mathrm{Re}\, z \leq E_0 + 1/2\Delta E\} \ \subset \ \rho(H_{\bar{P}}(\varepsilon)),$$

provided $|\varepsilon| \ll \Delta E$.

Moreover, since $PH(\varepsilon)(H_{\bar{P}}(\varepsilon) - z)^{-1} = \varepsilon PI(H_{\bar{P}}(\varepsilon) - z)^{-1}$, we estimate

$$\|PH(\varepsilon)(H_{\bar{P}}(\varepsilon) - z)^{-1}\bar{P}\| \leq \left(\varepsilon\|P \cdot p\| + \frac{\varepsilon^2}{2}\|PA(x)\|\right)$$

$$\times \|A(x)(H_{\bar{P}}(\varepsilon) - z)^{-1}\bar{P}\| \ .$$

Now Eqns (17.56), (17.59) and (17.60) imply then

$$\|A(x)(H_{\bar{P}}(\varepsilon) - z)^{-1}\bar{P}\| \leq C|z - \bar{E}|^{-1} \ .$$

Next since p is bounded relative to H_{part} we have that

$$\|P \cdot p\| \leq C \ .$$

Finally, bound (17.13) implies that

$$\|PA(x)\| \leq C(\rho^{-1/2} + 1) \ .$$

Collecting, the last four estimates and using that $\mathrm{Re}\, z \leq E_0 + \Delta E$, we arrive at (17.55). □

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