DEPARTMENT OF PHYSICS
UNIVERSITY OF CAMBRIDGE

PART II PHYSICS

THEORETICAL PHYSICS II

TOPICS IN QUANTUM THEORY

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Contents

1 *Quantum Dynamics* 7

2 *Introduction to path integrals* 23

3 *Scattering theory* 37

4 *Second quantization* 59

5 *Density matrices* 81

6 *Introduction to Lie groups* 97

7 *Relativistic quantum mechanics* 113

A *Operator Kung Fu* 123

Introduction

The development of quantum theory during the 20th century led to the introduction of completely new concepts to physics. At the same time, physicists were forced – sometimes unwillingly – to adopt myriad new techniques and mathematical ideas. In this course, we'll survey some of these more advanced topics.

This course is recommended only for students who have achieved a strong performance in Mathematics as well as Physics in Part IB, or an equivalent qualification.

Outline of lectures

Topics in *italics* are non-examinable.

1. **Quantum Dynamics**

   Schrödinger, Heisenberg, interaction picture. The evolution operator and time ordering. Driven oscillator. Coherent states. A spin-$\frac{1}{2}$ in a field. The adiabatic approximation. Landau-Zener transitions. Berry's phase.

2. **Introduction to path integrals**

   The propagator and the Green's function: free particle and harmonic oscillator. The method of stationary phase, the JWKB method and the semiclassical limit.

3. **Scattering Theory**

   Scattering in one dimension. Scattering amplitude and cross section. Optical theorem. Lippmann-Schwinger equation. Born series. Partial wave analysis. Bound states.

4. **Identical Particles in Quantum Mechanics**

   Second quantisation for bosons and fermions. Single-particle density matrix and density-density correlation function. Bose-Hubbard model. Bogoliubov transformation. Interference of condensates.

5. **Density Matrices**

   Density matrix and its properties. Applications in statistical mechanics. Density operator for subsystems and entanglement. Quantum damping.

6. ***Lie Groups***

   Symmetries are groups. Lie algebra of generators. Rotations as Lie group. Representations of $SO(3)$, $SU(2)$, *Lorentz group* $SO(1,3)$ *and* $SL(2,\mathbb{C})$.

7. ***Relativistic Quantum Physics***

   Klein-Gordon equation. Antiparticles. Spinors and the Dirac equation. Relativistic covariance.

Books

A few good books at about the right level:

- JJ Sakurai, *Modern Quantum Mechanics*, 2nd edition, Addison-Wesley, 1994.
- F Schwabl, *Quantum Mechanics*, 4th edition, Springer 2007, and F Schwabl, *Advanced Quantum Mechanics*, 4th edition, Springer 2008.
- R Shankar *Principles of Quantum Mechanics*, 2nd edition, Springer 1994.
- G Baym, *Lectures on Quantum Mechanics*, W. A. Benjamin, 1969.

For more problems that you can shake a stick at, see the recently published *Exploring Quantum Mechanics* (CUP, 2013) by Galitski *et al.*. Remember that doing problems is the *only way* to cement your understanding of new concepts!

For mathematical background I'd heartily recommend Mike Stone and Paul Goldbart's *Mathematics for Physicists: A guided tour for graduate students* (CUP, 2009). This contains a lot of advanced material as well as much of what you covered in 1B Mathematics.

A great resource for just about anything you may need to know about any of the functions we meet is the NIST *Digital Library of Mathematical Functions* at `http://dlmf.nist.gov`.

Structure of these lectures

You will find problems embedded in the text. Most of these are relatively short, and often involve checking expressions, or working through omitted steps. They are therefore a vital part of the development. It's probably best to work through these immediately after (or during!) the lectures, and make a note of any points you don't understand for the examples classes.

> TANGENT Occasionally, you will see boxes of indented text like this. They indicate background material that is not on the syllabus, but which you may find interesting. You definitely don't need to know anything that appears in one of these comments (except this one). Some of these contain problems. Again, they are just for added interest. The same applies to the Appendices to Chapter 3.

You are **strongly encouraged**, however, to **immediately** work through the problems in Appendix A to improve your facility with the manipulation of operators. If you find this process excruciatingly painful, this may not be the course for you!

THIS COURSE naturally builds on the Advanced Quantum Physics course from Michaelmas, so I'll sometimes refer back to these lectures with the abbreviation **AQP**.

Course Handout

These notes were created by Austen Lamacraft, with adaptations by Andreas Nunnenkamp. Any errors or omissions are the responsibility of the present lecturer (who may well have introduced them!), so please do let me know [rjs269@cam.ac.uk] if you spot any irregularities.

1

Quantum Dynamics

In this first chapter we're going to introduce some general ideas of quantum dynamics, using the two simplest quantum systems: the harmonic oscillator and a single spin-1/2.

1.1 The Quantum Harmonic Oscillator

There's an old crack from the late quantum field theorist Sidney Coleman to the effect that

> The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction.

There's a large kernel of truth in this, for the simple reason that many systems in physics vibrate, from bridges to quantum fields, and within a certain approximation that vibration can be treated as harmonic. In this section we are going to remind ourselves about some features of quantum dynamics using this model as our basic example, as it allows most results to be expressed analytically. Along the way I'll try and point out which features generalise to more complicated systems (and which don't!).

Time independent case

The Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{1.1}$$

where the position and momentum operators satisfy

$$[x, p] = i\hbar.$$

The state of the oscillator $|\psi\rangle$ evolves in time according to the (time dependent) Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle. \tag{1.2}$$

This is a first order differential equation, and so the evolution is fixed once the initial state $|\psi(0)\rangle$ is specified. We can write the solution as

$$|\psi(t)\rangle = \exp\left(-iHt/\hbar\right)|\psi(0)\rangle \equiv U(t)|\psi(0)\rangle. \tag{1.3}$$

The operator $U(t) = e^{-iHt/\hbar}$ is called the *evolution operator*, as it evolves the state $|\psi(0)\rangle$ forward in time.

Functions of operators can be thought of as defined by their power series expansions, in this case

$$U(t) = \mathbb{1} - i\frac{Ht}{\hbar} - \frac{1}{2}\left(\frac{Ht}{\hbar}\right)^2 + \cdots. \tag{1.4}$$

Alternatively, if an operator has a complete orthonormal eigenbasis $|n\rangle$ (as quantum observables do, being Hermitian operators), we can write any such function in terms of this basis and the corresponding function of the eigenvalues E_n

$$U(t) = \sum_n e^{-iE_nt/\hbar} |n\rangle \langle n|. \tag{1.5}$$

This latter point of view then focuses attention on the eigenstates $|n\rangle$. To find these there are at least two approaches

1. *(Brute force)* Take the position representation $p = -i\hbar\frac{d}{dx}$ and study the time independent Schrödinger equation in this representation

   $$-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} + \frac{1}{2}m\omega^2x^2\psi_n = E_n\psi_n \tag{1.6}$$

   where $\langle x|n\rangle = \psi_n(x)$. The result is that the eigenfunctions have the form

   $$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \tag{1.7}$$

   with eigenvalues $E_n = \hbar\omega(n+1/2)$, where $H_n(z)$ are the Hermite polynomials

2. *(More sophisticated)* Define the hermitian conjugate pair

   $$\begin{aligned} a &= \sqrt{\frac{m\omega}{2\hbar}}\left(x + i\frac{p}{m\omega}\right) \\ a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(x - i\frac{p}{m\omega}\right), \end{aligned} \tag{1.8}$$

   which satisfy

   $$[a, a^\dagger] = 1. \tag{1.9}$$

   The Hamiltonian is expressed as

   $$H = \frac{\hbar\omega}{2}\left[a^\dagger a + aa^\dagger\right] = \hbar\omega(N + 1/2) \tag{1.10}$$

   where $N \equiv a^\dagger a$. The commutation relation Eq. (1.9) implies

   $$[N, a] = -a \qquad [N, a^\dagger] = +a^\dagger, \tag{1.11}$$

   which in turn tells us that acting with $a^\dagger$ (a) on an eigenstate $|n\rangle$of N with eigenvalue n gives another eigenstate with eigenvalue increased (decreased) by 1.

Alternatively, we can try and find $U(t)$ indirectly, from the effect it has on operators. Recall that in the *Heisenberg picture* operators acquire a time dependence

$$\mathcal{O}(t) = U^\dagger(t)\mathcal{O}U(t), \tag{1.12}$$

equivalent to the Heisenberg equation of motion

$$\frac{d\mathcal{O}(t)}{dt} = \frac{i}{\hbar}[H, \mathcal{O}(t)]. \tag{1.13}$$

Let's see what this means for the Harmonic oscillator. Evidently $H = U^\dagger(t)HU(t)$, so

$$H = U^\dagger(t)HU(t) = \frac{p(t)^2}{2m} + \frac{1}{2}m\omega^2 x(t)^2. \tag{1.14}$$

We have

$$\begin{aligned} \frac{dx(t)}{dt} &= \frac{i}{\hbar}[H, x(t)] = \frac{p(t)}{m} \\ \frac{dp(t)}{dt} &= \frac{i}{\hbar}[H, p(t)] = -m\omega^2 x(t) \end{aligned} \tag{1.15}$$

You may recognize these equations as identical to *Hamilton's equations* for the SHO

$$\begin{aligned} \frac{dx}{dt} &= \frac{\partial H}{\partial p} = \frac{p}{m} \\ \frac{dp}{dt} &= -\frac{\partial H}{\partial x} = -m\omega^2 x \end{aligned} \tag{1.16}$$

Problem 1.1

Convince yourself that the same correspondence holds for the more general Hamiltonian

$$H = T(p) + V(x) \tag{1.17}$$

The general solution is

$$\begin{aligned} x(t) &= \cos(\omega t)x(0) + \sin(\omega t)\frac{p(0)}{m\omega} \\ p(t) &= \cos(\omega t)p(0) - m\omega\sin(\omega t)x(0), \end{aligned} \tag{1.18}$$

and corresponds to a point tracing out an ellipical trajectory centred at the origin in the $x-p$ plane (*phase space*). From this point of view the operators $a, a^\dagger$ in Eq. (1.8) can be seen as complex amplitudes whose phase changes linearly in time

$$a(t) = e^{-i\omega t}a(0), \qquad a^\dagger(t) = e^{+i\omega t}a^\dagger(0). \tag{1.19}$$

Problem 1.2

Verify that Eq. (1.19) follows directly from Eq. (1.1) and the commutation relation Eq. (1.9).

Time dependent force

Mostly we don't leave quantum systems to get on with their own time evolution, but disturb them in some way. For example, an atom may experience an external radiation field. The prototype for this situation is the SHO subject to a time dependent force

$$H(t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - F(t)x. \tag{1.20}$$

Recall that in the Heisenberg picture the Hamiltonian remained time independent. Now it has intrinsic time dependence

How does such a system evolve? The important thing to realize is that the solution of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H(t) |\psi\rangle . \tag{1.21}$$

is *not*

$$U(t) \neq \exp\left(-iH(t)t/\hbar\right). \tag{1.22}$$

Let's consider the situation described by

$$F(t) = \begin{cases} F_1 & 0 \leq t < t_1 \\ F_2 & t_1 \leq t < t_2 \end{cases} . \tag{1.23}$$

The evolution operator is

$$U(t) = \begin{cases} U_1(t) & 0 \leq t < t_1 \\ U_2(t-t_1)U_1(t_1) & t_1 \leq t < t_2 \end{cases} \tag{1.24}$$

where $U_i(t) = e^{-iH_i t/\hbar}$ and $H_i = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - F_i x$. It's important to realize that H_1 and H_2 don't commute with each other

$$[H_1, H_2] = -i\hbar \frac{p}{m}(F_1 - F_2), \tag{1.25}$$

thus U_1 and U_2 don't commute and the product of U_1 and U_2 in Eq. (1.24) is not easily written in terms of a single exponential.

The evolution operator corresponding to a general force $F(t)$ can be understood by splitting the evolution up into many small stages

$$\begin{aligned} U(t) &= \lim_{\Delta t \to 0} e^{-iH(t-\Delta t)\Delta t/\hbar} e^{-iH(t-2\Delta t)\Delta t/\hbar} \cdots e^{-iH(\Delta t)\Delta t/\hbar} e^{-iH(0)\Delta t/\hbar}. \\ &= \lim_{\Delta t \to 0} \left(1 - \frac{iH(t-\Delta t)\Delta t}{\hbar}\right)\left(1 - \frac{iH(t-2\Delta t)\Delta t}{\hbar}\right) \cdots \left(1 - \frac{iH(0)\Delta t}{\hbar}\right) \\ &= 1 - \frac{i}{\hbar}\int_0^t dt_1\, H(t_1) - \frac{1}{\hbar^2}\int_0^t dt_2 \int_0^{t_2} dt_1\, H(t_2)H(t_1) + \ldots . \end{aligned} \tag{1.26}$$

Note that the time arguments of $H(t)$ are increasing from right to left. The final expression for $U(t)$ can be written in a dangerously compact fashion by using the notation

$$\mathcal{T}[H(t_1)H(t_2)] = \begin{cases} H(t_1)H(t_2) & t_1 \geq t_2 \\ H(t_2)H(t_1) & t_2 > t_1 \end{cases} , \tag{1.27}$$

and so on. The operation denoted by $\mathcal{T}$ is usually called *time ordering*. We have

$$U(t) = 1 - \frac{i}{\hbar}\int_0^t dt_1\, H(t_1) - \frac{1}{2\hbar^2}\int_0^t dt_2 \int_0^t dt_1\, \mathcal{T}[H(t_1)H(t_2)] + \ldots . \tag{1.28}$$

Allowing the integrals to range over $0 < t_i < t$ instead of ordering them necessitates the introduction of a factor $\frac{1}{n!}$ at the n^{th} order. This allows us to write

$$U(t) = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_0^t dt'\, H(t')\right) \tag{1.29}$$

This expression should be handled with extreme care! It evidently reduces to $e^{-iHt/\hbar}$ in the case of a time-independent Hamiltonian. In the general case, it is only really useful in the form of the expansion Eq. (1.28).

To make progress in the case of the driven oscillator, it's useful to once again consider the Heisenberg equations of motion

$$\begin{aligned}\frac{dx(t)}{dt} &= \frac{i}{\hbar}[H, x(t)] = \frac{p(t)}{m} \\ \frac{dp(t)}{dt} &= \frac{i}{\hbar}[H, p(t)] = -m\omega^2 x(t) + F(t).\end{aligned} \tag{1.30}$$

In terms of a and $a^\dagger$

$$H(t) = \frac{\hbar\omega}{2}\left(a^\dagger a + a a^\dagger\right) - F(t)\sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \tag{1.31}$$

and we have

$$\frac{da}{dt} = -i\omega a + iF(t)\sqrt{\frac{1}{2m\hbar\omega}}. \tag{1.32}$$

If we define $\tilde{a}(t) = e^{i\omega t}a(t)$, we get

$$\frac{d\tilde{a}}{dt} = +i\frac{F(t)e^{i\omega t}}{\sqrt{2m\hbar\omega}}, \tag{1.33}$$

with general solution

$$\tilde{a}(t) = \tilde{a}(0) + \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega t'}dt', \tag{1.34}$$

and similarly

$$\tilde{a}^\dagger(t) = \tilde{a}^\dagger(0) - \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{-i\omega t'}dt'. \tag{1.35}$$

Problem 1.3

Satisfy yourself that this corresponds to the classical solution of a forced oscillator.

What can we do with this solution? Suppose we start from the ground state, which satisfies

$$a|0\rangle = 0. \tag{1.36}$$

Since $a(t) = U^\dagger(t)aU(t)$ we have $aU(t) = U(t)a(t)$ and thus

$$aU(t)|0\rangle = \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}dt'U(t)|0\rangle, \tag{1.37}$$

we have that $U(t)|0\rangle$ is an eigenstate of $\tilde{a}(0) = a$ with eigenvalue

$$\frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}dt', \tag{1.38}$$

in other words, it is a *coherent state*. Recall from **AQP** that a coherent state $|\alpha\rangle$ is defined as an eigenstate of a with eigenvalue α (generally complex, as a is not Hermitian)

$$a|\alpha\rangle = \alpha|\alpha\rangle. \tag{1.39}$$

The explicit form of a normalized coherent state is

$$|\alpha\rangle = e^{-|\alpha|^2/2}e^{\alpha a^\dagger}|0\rangle, \tag{1.40}$$

where both the property Eq. (1.39) and the normalization follow from the fundamental commutator $[a, a^\dagger] = 1$.

Problem 1.4

Prove this.

Note that the ground state $|0\rangle$ is a coherent state with $\alpha = 0$.

Problem 1.5

Show that if we start in a coherent state $|\alpha\rangle$, then after time t we are in the state

$$U(t)\,|\alpha\rangle = e^{i\phi(t)}\,|\alpha'\rangle \tag{1.41}$$

where

$$\alpha' = \alpha e^{-i\omega t} + \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}dt'. \tag{1.42}$$

Find the form of the phase $\phi(t)$.

Problem 1.6

Verify that the result Eq. (1.38) is consistent with first order time dependent perturbation theory for the amplitude to transition to the first excited state.

1.2 *A Spin in a Field*

Two state systems abound in physics. Or rather, many physical situations can be approximated by considering only two states. Some important examples are the spin states of the electron, a pair of atomic states coupled by external radiation, and the two equivalent positions of the Nitrogen atom in the trigonal pyramid structure of Ammonia (NH_4). Quantum two state systems are central to the field of **quantum computing**, where they replace the classical bit of information and are often known as **qubits**.

The simplest quantum system we can write down consists of just two states. The Hilbert space is then two dimensional, and any operator can be thought of as a 2×2 matrix. In this section, we'll see that there is a lot to be learnt from this seemingly elementary problem.

It's convenient to describe such a system using the language of spin-1/2, even though the two states may have nothing to do with real spin. The most general time dependent Hamiltonian can then be written using the spin-1/2 operators $S_i = \frac{1}{2}\sigma_i$ as

$$H(t) = \mathbf{H}(t)\cdot\mathbf{S}, \tag{1.43}$$

in terms of a time dependent 'magnetic field' $\mathbf{H}(t)$ (that again may have nothing to do with a real magnetic field). Using the Pauli matrices, we have the explicit form

$$H(t) = \frac{1}{2}\begin{pmatrix} H_z(t) & H_x(t) - iH_y(t) \\ H_x(t) + iH_y(t) & -H_z(t) \end{pmatrix}. \tag{1.44}$$

The Schrödinger equation corresponding to Eq. (1.43) is

$$i\hbar\frac{d\,|\Psi\rangle}{dt} = H(t)\,|\Psi\rangle \tag{1.45}$$

where $|\Psi\rangle = \begin{pmatrix}\psi_\uparrow \\ \psi_\downarrow\end{pmatrix}$.

As before, the formal solution to Eq. (1.45) can be written as

$$|\Psi(t)\rangle = U(t,t')\,|\Psi(t')\rangle\,, \tag{1.46}$$

In the present case, $U(t,t')$ is a 2×2 unitary matrix. It's perhaps a bit surprising that, for this most basic of all possible problems of quantum dynamics, there is no simple relationship between $H(t)$ and $U(t,t')$. If we think of $U(t,t')$ as representing a kind of rotation in Hilbert space, $H(t)$ corresponds to an instantaneous 'angular velocity' describing an infinitesimal rotation. Because these rotations do not commute at different times, the relationship between the infinitesimal rotations and the finite rotation that results is complicated.

The same picture emerges if we look at the Heisenberg equation of motion for $\mathbf{S}(t) = U^\dagger(t,t')\mathbf{S}(t')U(t,t')$, which take the form

$$\begin{aligned}\frac{d\mathbf{S}}{dt} &= \frac{i}{\hbar}\left[H(t),\mathbf{S}\right] \\ &= \hbar^{-1}\mathbf{H}(t)\times\mathbf{S},\end{aligned} \tag{1.47}$$

by virtue of the spin commutation relations $\left[S_i, S_j\right] = i\varepsilon_{ijk}S_k$. Thus $\mathbf{S}$ precesses about $\mathbf{H}(t)$, which corresponds to the instantaneous angular velocity. Differential equations involving operators may make you uncomfortable, but this one is linear and first order, so the solution must be expressible in the form of a matrix connecting the initial and final operators

The usual $\hbar$ is missing because we defined $\mathbf{S} = \frac{1}{2}\sigma$

I'll try to stick to the convention of denoting matrices by sans serif fonts like THIS.

$$\mathbf{S}(t) = \mathsf{R}(t,t')\mathbf{S}(t'). \tag{1.48}$$

R is a 3×3 matrix describing the rotation of the spin from time t' to time t. The formal expression for $\mathsf{R}(t,t')$ is

$$\mathsf{R}(t,t') = \mathcal{T}\exp\left(\int_{t'}^{t}\Omega(t_i)\,dt_i\right). \tag{1.49}$$

where the matrix $\Omega(t)$ describing infinitesimal rotations has elements $\Omega_{jk}(t) = -(1/\hbar)H_i(t)\varepsilon_{ijk}$ i.e.

$$\Omega(t) = \hbar^{-1}\begin{pmatrix} 0 & -H_z(t) & H_y(t) \\ H_z(t) & 0 & -H_x(t) \\ -H_y(t) & H_x(t) & 0\end{pmatrix}. \tag{1.50}$$

$U(t,t')$ and $\mathsf{R}(t,t')$ contain the same information, of course. We'll return to the relationship between these two in Chapter 6 on Lie Groups.

Problem 1.7

Find the explicit form of $U(t,t')$ and $\mathsf{R}(t,t')$ when $\mathbf{H} = H\hat{\mathbf{z}}$, corresponding to uniform precession about the z-axis.

Rabi oscillations

One time dependent situation that we can describe exactly is the rotating field

$$\mathbf{H}(t) = \begin{pmatrix} H_{\mathrm{R}}\cos(\omega t) \\ H_{\mathrm{R}}\sin(\omega t) \\ H_0\end{pmatrix}, \tag{1.51}$$

corresponding to the Hamiltonian

$$H(t) = H_0 S_z + \frac{H_{\mathrm{R}}}{2}\left(S_+e^{-i\omega t} + S_-e^{i\omega t}\right), \tag{1.52}$$

where $S_\pm = S_x \pm iS_y$. The key to solving the problem is to transform the Schrödinger equation Eq. (1.45) by multiplying by $\exp\left(i\omega t S_z\right)$. Define

$$\left|\Psi_{\mathrm{R}}(t)\right\rangle \equiv \exp\left(i\omega t S_z\right)\left|\Psi(t)\right\rangle. \tag{1.53}$$

This transformed state satisfies

$$\begin{aligned} i\hbar\frac{d}{dt}\left|\Psi_{\mathrm{R}}\right\rangle &= i\hbar e^{i\omega t S_z}\frac{d}{dt}\left|\Psi\right\rangle - \hbar\omega S_z\left|\Psi_{\mathrm{R}}\right\rangle \\ &= e^{i\omega t S_z}H(t)\left|\Psi\right\rangle - \hbar\omega S_z\left|\Psi_{\mathrm{R}}\right\rangle \\ &= e^{i\omega t S_z}H(t)e^{-i\omega t S_z}\left|\Psi_{\mathrm{R}}\right\rangle - \hbar\omega S_z\left|\Psi_{\mathrm{R}}\right\rangle \\ &= H_{\mathrm{Rabi}}\left|\Psi_{\mathrm{R}}\right\rangle \end{aligned} \tag{1.54}$$

In the last line we defined

$$H_{\mathrm{Rabi}} \equiv e^{i\omega t S_z}H(t)e^{-i\omega t S_z} - \hbar\omega S_z = \left(H_0 - \hbar\omega\right)S_z + H_R S_x. \tag{1.55}$$

To get the last equality you have to transform the Hamiltonian. You can use Eq. (A.2), or, since everything is a 2×2 matrix, you can multiply the matrices explicitly.

Physically, this corresponds to viewing things in a frame rotating with the field, so the Hamiltonian is now time independent. In this new frame the system precesses about a fixed axis $(H_{\mathrm{R}}, 0, H_0 - \hbar\omega)$ at the **Rabi frequency**

$$\omega_{\mathrm{R}} = \hbar^{-1}\sqrt{\left(H_0 - \hbar\omega\right)^2 + H_{\mathrm{R}}^2}. \tag{1.56}$$

The amplitude of the oscillations in S_z due to this precession is maximal when $H_0 = \hbar\omega$. In this case the rotation frequency of the field matches the frequency of precession about the z-axis that would occur if $H_{\mathrm{R}} = 0$.

1.3 *The adiabatic approximation*

The idea of **separation of scales**, be they in length, time, or energy, is endemic in science. If we are interested in studying processes on one scale (such as the weather, say) we hope that they don't depend on the details of processes at another (the motion of molecules). Rather, we hope that these latter processes can be described in an average way, involving only a few parameters and dynamical quantities (density, local velocity).

The **Born–Oppenheimer approximation** is another example.

The adiabatic approximation is a special case of this idea. Let's suppose that in our two level system, the field $\mathbf{H}(t)$ is changing very slowly (we'll make this idea precise in a moment). If this motion is truly glacial, we'd expect to be able to forget about it altogether, and just solve the problem by finding the energy eigenstates and eigenvalues in the present epoch

$$H(t)\left|\pm_t\right\rangle = E_\pm(t)\left|\pm_t\right\rangle. \tag{1.57}$$

We put the t in a subscript on the states to emphasise that they depend on time as a *parameter*. We refer to the $\left|\pm_t\right\rangle$ as the **instantaneous energy eigenstates**. Although we can always define these states for any $H(t)$, we have no reason in general to expect that this t-dependence has anything to do with the other kind of t-dependence that arises by solving the time dependent Schrödinger equation.

The **adiabatic theorem** is roughly the statement that these two t dependences *do* in fact coincide, in the limit that $H(t)$ changes very slowly. To make this more precise, let's expand the state of the system, evolving in time *according to the Schrödinger equation*, in the instantaneous eigenbasis

$$|\Psi(t)\rangle = c_+(t)\,|+_t\rangle + c_-(t)\,|-_t\rangle\,. \tag{1.58}$$

Thus, some of the t dependence is 'carried' by the $|\pm_t\rangle$, and by substituting into the Schrödinger equation we are going to find the time dependence of the $c_\pm(t)$. This involves finding $d\,|\pm_t\rangle\,/dt$.

It's a bit like the interaction representation in time dependent perturbation theory

Now the following idea you may find a bit odd. Since the time dependence of $|\pm_t\rangle$ is parametric, we can view the problem of calculating $d\,|\pm_t\rangle\,/dt$ as an exercise in *time independent* perturbation theory. Going from t to $t+\delta t$ changes the Hamiltonian by an amount

$$\delta H(t) = \frac{dH(t)}{dt}\delta t. \tag{1.59}$$

Treating this as a perturbation, the state $|+_t\rangle$ changes by an amount

$$\delta\,|+_t\rangle = \frac{\langle -_t|\delta H(t)|+_t\rangle}{E_+(t)-E_-(t)}\,|-_t\rangle\,, \tag{1.60}$$

so that

$$\frac{d\,|+_t\rangle}{dt} = \frac{\langle -_t|\dot{H}(t)|+_t\rangle}{E_+(t)-E_-(t)}\,|-_t\rangle\,. \tag{1.61}$$

Using Eq. (1.61) and the corresponding result for $d\,|-_t\rangle\,/dt$, we find that the Schrödinger equation gives the following pair of equations for the $c_\pm(t)$

$$i\hbar\frac{d}{dt}\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} E_+(t) & i\hbar\frac{\langle +_t|\dot{H}|-_t\rangle}{E_+-E_-} \\ i\hbar\frac{\langle -_t|\dot{H}|+_t\rangle}{E_--E_+} & E_-(t) \end{pmatrix}\begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}. \tag{1.62}$$

If $H(t)$ is changing slowly enough, the off-diagonal terms can be neglected and the solution is

Note the resemblance to the WKB wavefunction, with energy and time taking the roles of momentum and position. WKB is a kind of adiabatic approximation in space.

$$c_\pm(t) = \exp\left(-\frac{i}{\hbar}\int_0^t E_\pm(t')\,dt'\right)c_\pm(0). \tag{1.63}$$

Thus the amplitudes evolve independently, and there are no transitions between the instantaneous eigenstates. The phase factor is a generalization of the familiar $e^{-iE_\pm t/\hbar}$ for stationary states, which accounts for the slowing varying instantaneous eigenenergy.

When is this approximation valid? The off-diagonal matrix element in Eq. (1.62) must be small compared to $E_1(t)-E_2(t)$, which corresponds to the condition

$$\hbar|\langle -_t|\dot{H}|+_t\rangle| \ll [E_+(t)-E_-(t)]^2\,. \tag{1.64}$$

- *Degeneracy* must be avoided, because the eigenbasis becomes undefined within the degenerate subspace. You can't remain in an eigenstate if you don't know what it is.

- The approximation is a *semiclassical* one, meaning that it improves at smaller $\hbar$.

TANGENT

Adiabatic is a peculiar term that appears in two related contexts in physics, both referring to slow changes to a system. In thermodynamics, it describes changes without a change in entropy. For reversible changes, this corresponds to no flow of heat, which is the origin of the name (from the Greek for ‘impassable’).

Later, the idea entered mechanics when it was realized that a mechanical system with one degree of freedom undergoing periodic motion, and subject to slow changes, has an **adiabatic invariant**. This turns out to be the **action**

$$S = \oint p\,dx$$

($\oint$ indicates that we integrate for one period of the motion) Largely due to the work of Paul Ehrenfest (1880-1933), the invariant played a major role in the ‘old’ quantum theory that predated Schrödinger, Heisenberg, *et al.*. If the motion of a system is quantized, slow changes to the system’s parameters presumably do not lead to sudden jumps. Thus the quantity that comes in quanta must be an adiabatic invariant – and conveniently Planck’s constant has the right units. This line of reasoning eventually gave rise to the **Bohr–Sommerfeld quantization condition**

$$\oint p\,dx = nh, \qquad n \text{ integer.}$$

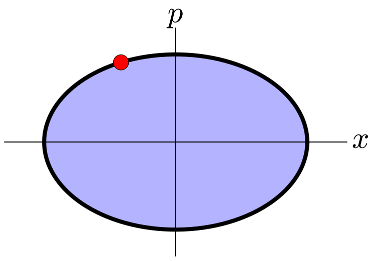


Figure 1.1: The action of a periodic trajectory is equal to the area enclosed in the phase plane. For a simple harmonic oscillator the curve is an ellipse and the action is the product of the energy and the period. If the period of the oscillator is altered slowly (by changing the length of a pendulum, say) the ellipse will distort but the area will remain fixed.

Landau–Zener tunnelling

The picture of adiabatic evolution described above is extremely simple, and it’s natural to ask how it breaks down when the condition Eq. (1.64) is not satisfied. Let’s consider time evolution with the Hamiltonian

$$H(t) = \begin{pmatrix} \beta t & \Delta \\ \Delta & -\beta t \end{pmatrix}. \tag{1.65}$$

The instantaneous eigenvalues are

$$E_\pm(t) = \pm\sqrt{(\beta t)^2 + \Delta^2}. \tag{1.66}$$

We denote the corresponding eigenvalues $|\pm_t\rangle$. As a function of t, the eigenvalues show an **avoided crossing**. The adiabatic theorem tells us that if we start in the state corresponding to the lower energy $E_-(t)$, and β is sufficiently small, the state at time t is

$$\exp\left(-\frac{i}{\hbar}\int_0^t E_-(t')dt'\right)|-_t\rangle\,, \tag{1.67}$$

where $|-_t\rangle$ is the corresponding eigenstate. We’re integrating from $t = 0$ because the integral diverges at $-\infty$ as the phase whizzes faster and faster.

How small should β be? We use the condition Eq. (1.64), and the fact that the minimum splitting of the energy levels is 2Δ to arrive at the requirement

$$\frac{\hbar\beta}{\Delta^2} \ll 1. \tag{1.68}$$

We are interested in the situation where this is not the case.

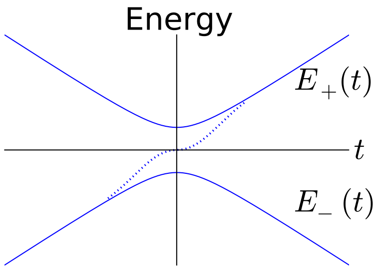


Figure 1.2: Instantaneous eigenvalues of the Landau–Zener problem. The dotted line schematically illustrates what happens when we pass over the branch point.

Problem 1.8

When $\frac{\hbar\beta}{\Delta^2} \gg 1$, we expect a system that starts out at in the lower state at large negative times to end up in the upper state, with only a small probability of remaining in the lower state. This limit can be treated using time-dependent perturbation theory in the splitting Δ. Since the unperturbed levels pass through each other, staying in the lower state corresponds to making a *transition* between the unperturbed states.

Show that the corresponding probability is

$$P(|-_{t=-\infty}\rangle \to |-_{t=\infty}\rangle) = \frac{\pi\Delta^2}{\hbar\beta} \tag{1.69}$$

TANGENT

In fact, we can do better than this, via an ingenious excursion into the complex plane. The functions $E_\pm(t)$ have branch cuts starting at $t = \pm i\Delta/\beta$. We can think of adiabaticity failing because the branch points are too close to the real axis.

But who said t had to be real? There is nothing to stop us integrating the Schrödinger equation along an arbitrary contour. Then we can be as far away from the branch points as we like (Fig. 1.3), and the adiabatic approximation should be valid once more. We can use Eq. (1.67): the exponent now acquires a real part, which describes the decay of the amplitude.

Having made the adiabatic approximation, we can deform the contour of integration in Eq. (1.67). The real part of the exponent arising during evolution from $t = -\infty$ to $t = +\infty$ can then be written

$$\frac{2i}{\hbar}\int_0^{i\Delta/\beta} \sqrt{(\beta t)^2 + \Delta^2}\, dt = -\frac{\pi\Delta^2}{2\hbar\beta}, \tag{1.70}$$

giving the modulus of the amplitude

$$|c_-(-\infty \to +\infty)| = \exp\left(-\frac{\pi\Delta^2}{2\hbar\beta}\right). \tag{1.71}$$

Note, however, that our state is now evolving with an instantaneous energy $E_+(t)$, because we passed onto the other sheet of the Riemann surface. We are now in the *upper* state $|+_t\rangle$, see Fig. 1.2.

Thus the square of Eq. (1.71) actually gives the probability to make the transition to the upper state. The probability to remain in the lower state is therefore

$$P_{\text{ground}} = 1 - \exp\left(-\frac{\pi\Delta^2}{\hbar\beta}\right). \tag{1.72}$$

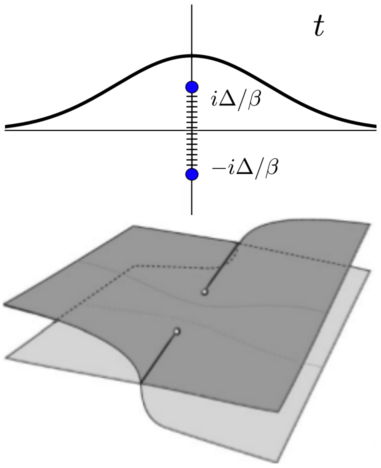


Figure 1.3: (Top) Branch cut and contour of time evolution in the complex t plane. (Bottom) Riemann surface of $\sqrt{(\beta t)^2 + \Delta^2}$ (real part).

Problem 1.9

Find the eigenvectors of Eq. (1.65) explicitly and verify that going around the branch point as shown in Fig. 1.3 takes us from $|-_t\rangle$ to $|+_t\rangle$

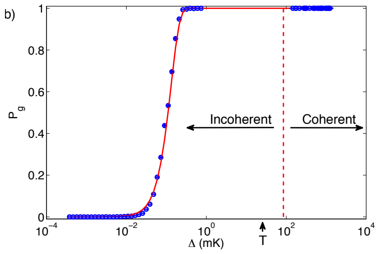


Figure 1.4: Comparison of Eq. (1.72) with the probability of a superconducting qubit to remain in the ground state. The two states correspond to different values of the magnetic flux trapped in a superconducting ring, and the bias is provided by ramping another flux (**?**).

The original paper (**?**) is a model of clarity and highly recommended.

1.4 *Berry's phase*

There is a surprise lurking in our derivation of the adiabatic theorem, one that remained hidden until 1984. We found the change in the instantaneous eigenstates in a small interval δt to be

$$\delta\,|+_t\rangle = \frac{\langle -_t|\delta H(t)|+_t\rangle}{E_+(t) - E_-(t)}\,|-_t\rangle\,. \tag{1.60}$$

This change is in the direction of $|-_t\rangle$ i.e. *orthgonal* to $|+_t\rangle$. The usual justification for this in the context of perturbation theory is that any change parallel to $|+_t\rangle$ is no change at all, amounting only to a modification of the magnitude or phase of the state, neither or which is physically meaningful. For example, a small change in the phase of $|+_t\rangle$ gives

$$|+_t\rangle \to e^{i\delta\theta}\,|+_t\rangle \sim (1 + i\delta\theta)\,|+_t\rangle\,. \tag{1.73}$$

Suppose now that $H(t)$ is subject to some adiabatic *cyclic* change around some closed path γ in the space of matrices. If after time T we have $H(T) = H(0)$, then after evolving $|+_t\rangle$ according to Eq. (1.60) it would be natural to expect that it will return to its original value. That is,

$$|+_T\rangle \overset{?}{=} |+_0\rangle\,. \tag{1.74}$$

Berry's remarkable discovery was that *this does not happen*. Rather,

$$|+_T\rangle = e^{i\theta_{\rm B}[\gamma]}\,|+_0\rangle\,, \tag{1.75}$$

where the phase $\theta_{\rm B}[\gamma]$ that now bears his name is a functional of the path γ.

To get a better grip on this slippery concept, recall that the Hamiltonian of our two state system (Eq. (1.43)) is parametrized in terms of the field $\mathbf{H}(t)$. Suppose we fix the states $|\mathbf{H}, \pm\rangle$ for each value of the field at the outset. That is, there is no ambiguity in the phase as in Eq. (1.75). We can then use these states to write the state of the system in the instantaneous eigenbasis (c.f. Eq. (1.58))

$$|\Psi(t)\rangle = c_+(t)\,|\mathbf{H}(t), +\rangle + c_-(t)\,|\mathbf{H}(t), -\rangle\,. \tag{1.76}$$

If $|\mathbf{H}, +\rangle$ changes smoothly as $\mathbf{H}$ changes, we will see that Eq. (1.60) *cannot* be obeyed: there is always some contribution in the direction of $|\mathbf{H}, +\rangle$ corresponding to a change of phase. This defines a vector field in the space of $\mathbf{H}$ by

$$\mathbf{A}_+(\mathbf{H}) \equiv -i\,\langle\mathbf{H}, +|\,(\nabla_{\mathbf{H}}\,|\mathbf{H}, +\rangle)\,, \tag{1.77}$$

and likewise for $|\mathbf{H}, -\rangle$.

Problem 1.10

Show that using normalized states guarantees that $\mathbf{A}_+(\mathbf{H})$ is real.

Things become a lot clearer with a concrete example. Let's write $\mathbf{H} = H_0\mathbf{n}$, with $\mathbf{n}$ a unit vector. Introducing spherical polar coordinates in the usual way

$$\mathbf{n} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}, \tag{1.78}$$

The Hamiltonian $H = \mathbf{H}\cdot\mathbf{S}$ takes the form

$$H = \frac{H_0}{2}\begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta. \end{pmatrix} \tag{1.79}$$

You can then easily check that the eigenstate $|\mathbf{H}, +\rangle$ is

$$|\mathbf{H}, +\rangle = \begin{pmatrix} \cos(\theta/2)\, e^{-i\phi/2} \\ \sin(\theta/2)\, e^{i\phi/2} \end{pmatrix}. \tag{1.80}$$

Computing $\mathbf{A}_+(\mathbf{H})$ defined by Eq. (1.77) gives

$$\mathbf{A}_+(\mathbf{H}) = -\hat{\boldsymbol{\phi}}\frac{\cot\theta}{2H_0}. \tag{1.81}$$

The gradient operator in spherical polars is $\nabla = \hat{\mathbf{r}}\,\partial_r + \frac{\hat{\boldsymbol{\theta}}}{r}\partial_\theta + \frac{\hat{\boldsymbol{\phi}}}{r\sin\theta}\partial_\phi$. We'll often use the notation $\partial_x = \frac{\partial}{\partial x}$, $\partial_x^2 = \frac{\partial^2}{\partial x^2}$, etc. in these notes.

Problem 1.11

By finding $|\mathbf{H},-\rangle$, convince yourself that

$$\mathbf{A}_-(\mathbf{H}) = +\hat{\boldsymbol{\phi}}\frac{\cot\theta}{2H_0}. \tag{1.82}$$

We now use Eq. (1.76) in the derivation of the adiabatic theorem as before. Instead of Eq. (1.60) we get

$$\delta\,|\mathbf{H},+\rangle = \frac{\langle \mathbf{H},-|\delta H|\mathbf{H},+\rangle}{H_0}\,|\mathbf{H},-\rangle + i\mathbf{A}_+(\mathbf{H})\cdot\delta\mathbf{H}\,|\mathbf{H},+\rangle\,, \tag{1.83}$$

where we have used $E_+ - E_- = H_0$. After making the adiabatic assumption we get

$$i\hbar\frac{d}{dt}\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} E_+(t) + \hbar\mathbf{A}_+(\mathbf{H})\cdot\dot{\mathbf{H}} & 0 \\ 0 & E_-(t) + \hbar\mathbf{A}_-(\mathbf{H})\cdot\dot{\mathbf{H}} \end{pmatrix}\begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}, \tag{1.84}$$

and the solution is now

$$c_\pm(t) = \exp\left(-\frac{i}{\hbar}\int_0^t \left[E_\pm(t') + \hbar\mathbf{A}_\pm(\mathbf{H})\cdot\dot{\mathbf{H}}\right]\,dt'\right)c_\pm(0). \tag{1.85}$$

Moving around a closed loop, we see that the states acquires an additional phase

$$\theta_{\mathrm{B},\pm}[\gamma] = -\oint_\gamma \mathbf{A}_\pm(\mathbf{H})\cdot d\mathbf{H}, \tag{1.86}$$

which depends only on the path, and not on the way it is traversed (i.e. the parametrization $\mathbf{H}(t)$).

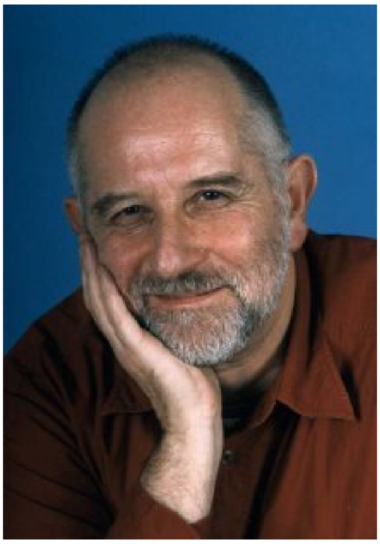


Figure 1.5: Sir Michael Berry may be best known to the general public as the winner of the 2000 IgNobel prize for physics, for his work on levitating frogs. He shared the prize with Andre Geim, who went on to be the first person to win both the IgNobel and Nobel prizes (the latter in 20010 for the discovery of Graphene). Many predict that Berry will be the next.

CLEARLY, $\mathbf{A}_\pm$ depends on how we chose our states $|\mathbf{H},\pm\rangle$ in the first place. So you could be forgiven for thinking that $\theta_{\mathrm{B},\pm}$ does too. However, any other choice can be obtained by multiplying $|\mathbf{H},\pm\rangle$ by some $\mathbf{H}$ dependent phase factor. Then

$$\begin{aligned} |\mathbf{H},\pm\rangle &\to \exp\left(i\Lambda_\pm(\mathbf{H})\right)|\mathbf{H},\pm\rangle \\ \mathbf{A}_\pm(\mathbf{H}) &\to \mathbf{A}_\pm + \nabla_{\mathbf{H}}\Lambda_\pm(\mathbf{H}), \end{aligned} \tag{1.87}$$

and the line integral in Eq. (1.86) is unchanged. Thus $\theta_{B,\alpha}$ is a property of the path γ in the $\mathbf{H}$ space, not of how the phases of the eigenstates are chosen.

You should recognize Eq. (1.87) as a *gauge transformation*, with $\mathbf{A}_\pm(\mathbf{H})$ playing the role of the vector potential (sometimes called the **Berry potential**). We have just shown that $\theta_{\mathrm{B},\pm}$ is a gauge invariant quantity.

To get to the geometric meaning of $\theta_{\mathrm{B},\pm}$, we compute the 'magnetic field' associated with $\mathbf{A}_\pm$

$$\mathbf{B}_\pm(\mathbf{H}) \equiv \nabla_{\mathbf{H}}\times\mathbf{A}_\pm(\mathbf{H}) = \pm\frac{\mathbf{n}}{2H_0^2}. \tag{1.88}$$

which corresponds to a **magnetic monopole** of charge $\pm\frac{1}{2}$ at the origin. This field is a gauge invariant quantity, which provides another way of seeing the gauge invariance of $\theta_{\mathrm{B},\pm}$. Using Stokes' theorem to convert the loop integral in Eq. (1.86) into a surface integral over a surface Σ bounded by γ gives

While there is an ambiguity of $\Omega \leftrightarrow 4\pi - \Omega$ in the solid angle enclosed by a curve, this is harmless because (accounting for the change in the sense of the curve) it amounts to a change of the phase by 2π.

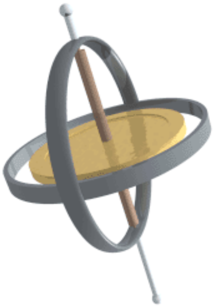
$$\theta_{B,\pm}[\gamma] = -\int_\Sigma \mathbf{B}_\pm \cdot d\mathbf{S} = \mp\frac{\Omega}{2}, \tag{1.89}$$

where Ω is the solid angle enclosed by Σ.

Note that the singularities appearing the gauge field in Eq. (1.81) at the north and south poles have no physical meaning. It is better to focus on the field $\mathbf{B}_\pm$ which is well behaved there.

TANGENT A beautiful *classical* analogue of Berry's phase can be demonstrated using a gyroscope. Imagine holding one end of its axle, and moving it around so that a unit vector parallel to the axle traces out a closed curve on the unit sphere. When you return the axle to its original orientation, you will find – provided the bearings are nice and smooth – that the wheel has rotated! Remarkably, the angle of rotation turns out to be the solid angle enclosed within the curve traced out on the unit sphere.

Other discussions of this effect can be found in (**?**) and (**?**).



It sounds like this must be connected to Berry's phase, and indeed it is. Though the physics of this situation is very different, the mathematics is almost identical. To deal with the physics first: the key point is that, by holding the gyroscope by the axle, we never apply any torque parallel to the axle. Thus the angular momentum in this direction is fixed (to zero, say). However, this direction is changing in time.

Let's denote by θ the angular orientation of the wheel on the axle. Imagine marking out the angle in degree increments on the axle, and measuring θ using some mark on the wheel. It's natural to write the condition of vanishing angular momentum as

$$L_{\text{axle}} \overset{?}{=} I\dot{\theta} = 0. \tag{1.90}$$

Actually, this won't quite do, because the whole point is that the axle itself is going to move. Imagine twisting the axle back and forth, keeping it pointing in the same direction. The wheel will not move, though the angle θ will be going up and down because the axle is moving.

To include this effect, imagine defining an orthonormal triad of vectors $(\mathbf{a}, \mathbf{b}, \mathbf{n})$, where $\mathbf{n}$ is parallel to the axle, and $\mathbf{a} \times \mathbf{b} = \mathbf{n}$. The motion we just described corresponds to a rotation in the $\mathbf{a} - \mathbf{b}$ plane. Rotating the axle by ϕ corresponds to

$$\begin{aligned} \mathbf{a} &\to \cos\phi\mathbf{a} + \sin\phi\mathbf{b} \\ \mathbf{b} &\to \cos\phi\mathbf{b} - \sin\phi\mathbf{a}. \end{aligned} \tag{1.91}$$

Now notice that

$$d\phi = -\mathbf{a}\cdot d\mathbf{b} = \mathbf{b}\cdot d\mathbf{a} \tag{1.92}$$

Thus Eq. (1.90) should really be

$$\dot{\theta} + \dot{\phi} = \dot{\theta} + \frac{1}{2}\left[\mathbf{b}\cdot\dot{\mathbf{a}} - \mathbf{a}\cdot\dot{\mathbf{b}}\right] = 0. \tag{1.93}$$

To make the connection to Berry's phase, we introduce the *complex* vector $\boldsymbol{\psi} = (\mathbf{a} + i\mathbf{b})/\sqrt{2}$. Then Eq. (1.93) can be written

$$\dot{\theta} + i\boldsymbol{\psi}^\dagger \frac{d\boldsymbol{\psi}}{dt} = 0. \tag{1.94}$$

Now for each direction $\mathbf{n}$, fix $\mathbf{a}$ and $\mathbf{b}$. We have some freedom here, as we can always choose them differently by rotating in the plane normal to $\mathbf{n}$ as in Eq. (1.91). This is entirely analogous to the freedom to choose a gauge that we had in the quantum problem. Once we have done this, we can find the angle of rotation by

$$\Delta\theta = \int \dot{\theta}\, dt = \int -i\boldsymbol{\psi}^\dagger \frac{d\boldsymbol{\psi}}{dt}\, dt = \int \mathbf{A}_{\mathbf{n}} \cdot d\mathbf{n}, \tag{1.95}$$

where we defined $\mathbf{A}_{\mathbf{n}} = -i\boldsymbol{\psi}^\dagger \nabla_{\mathbf{n}} \boldsymbol{\psi}$. Just as with Berry's phase, this angle is independent of the arbitrary choice we just made.

Now we just have to compute it. We first fix an explicit form for the triad

$$\begin{aligned}\mathbf{a} &= (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) \\ \mathbf{b} &= (-\sin\phi, \cos\phi, 0) \\ \mathbf{n} &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta),\end{aligned} \tag{1.96}$$

and then compute

$$\mathbf{A_n} = -\cos\theta\nabla_{\mathbf{n}}\phi. \tag{1.97}$$

We get

$$\Delta\theta = \oint \mathbf{A_n}\cdot d\mathbf{n} = \int (\nabla_{\mathbf{n}}\times\mathbf{A_n})\cdot d\mathbf{S} = \int \sin\theta\, d\theta\, d\phi = \Omega, \tag{1.98}$$

which is the result stated above.

$\nabla_{\mathbf{n}} \times \mathbf{A_n}$ can be found in a slicker way without introducing an explicit parametrization of the triad. To evaluate the antisymmetric tensor

$$\partial_i\mathbf{a}\cdot\partial_j\mathbf{b} - \partial_j\mathbf{a}\cdot\partial_i\mathbf{b}, \tag{1.99}$$

we first notice that $\partial_i\mathbf{a}$ must lie in the $\mathbf{b}-\mathbf{n}$ plane (to preserve normalization) and likewise $\partial_j\mathbf{b}$ must lie in the $\mathbf{a}-\mathbf{n}$ plane. Thus Eq. (1.99) can be written

$$\partial_i\mathbf{a}\cdot\partial_j\mathbf{b} - \partial_j\mathbf{a}\cdot\partial_i\mathbf{b} = (\mathbf{n}\cdot\partial_i\mathbf{a})\left(\mathbf{n}\cdot\partial_j\mathbf{b}\right) - \left(\mathbf{n}\cdot\partial_j\mathbf{a}\right)(\mathbf{n}\cdot\partial_i\mathbf{b}). \tag{1.100}$$

Now using the property $\mathbf{n}\cdot\partial_i\mathbf{a} = -\mathbf{a}\cdot\partial_i\mathbf{n}$, which follows from preserving the orthogonality of the triad under differentiation, we have

$$\begin{aligned}(\mathbf{n}\cdot\partial_i\mathbf{a})\left(\mathbf{n}\cdot\partial_j\mathbf{b}\right) - \left(\mathbf{n}\cdot\partial_j\mathbf{a}\right)(\mathbf{n}\cdot\partial_i\mathbf{b}) &= (\mathbf{a}\cdot\partial_i\mathbf{n})\left(\mathbf{b}\cdot\partial_j\mathbf{n}\right) - \left(\mathbf{a}\cdot\partial_j\mathbf{n}\right)(\mathbf{b}\cdot\partial_i\mathbf{n}) \\ &= (\mathbf{a}\times\mathbf{b})\cdot\left(\partial_i\mathbf{n}\times\partial_j\mathbf{n}\right) \\ &= \mathbf{n}\cdot\left(\partial_i\mathbf{n}\times\partial_j\mathbf{n}\right).\end{aligned} \tag{1.101}$$

In polar coordinates

$$\mathbf{n}\cdot\left(\partial_i\mathbf{n}\times\partial_j\mathbf{n}\right) = \sin\theta\,\partial_i\theta\,\partial_j\phi, \tag{1.102}$$

which is just what we found before.

2

Introduction to path integrals

My machines came from too far away.

Richard Feynman

2.1 The languages of quantum theory

From the outset, quantum mechanics was written in two apparently different languages. Schrödinger's equation, published in 1926, describes the time evolution of the wave function $\Psi(\mathbf{r}, t)$ of the system

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right]\Psi(\mathbf{r}, t). \tag{2.1}$$

It is historically the *second* formulation of modern quantum theory, the first having been given a year earlier by Heisenberg. In Heisenberg's version it is the matrix elements of observables that evolve in time: hence this way of doing things is sometimes known as *matrix mechanics*. Schrödinger quickly proved the equivalence of the two approaches, and in Dirac's formulation of operators acting in Hilbert space, this equivalence is rather evident. The evolution of a state can be written using the unitary operator of time evolution $U(t) \equiv e^{-iHt/\hbar}$, where H is the Hamiltonian, as

$$|\Psi(t)\rangle = U(t)\,|\Psi(0)\rangle\,. \tag{2.2}$$

For any operator $\mathcal{O}$ and pair of states $|\Phi\rangle$, $|\Psi\rangle$, we then have

$$\langle\Psi(t)|\mathcal{O}|\Phi(t)\rangle = \langle\Psi(0)|\mathcal{O}(t)|\Phi(0)\rangle \tag{2.3}$$

where $\mathcal{O}(t) \equiv e^{iHt/\hbar}\mathcal{O}e^{-iHt/\hbar}$ defines the time evolution of $\mathcal{O}$. To put it another way, $\mathcal{O}(t)$ obeys the *Heisenberg equation of motion*

$$\frac{d\mathcal{O}}{dt} = \frac{i}{\hbar}\left[H, \mathcal{O}\right]. \tag{2.4}$$

Dirac's book *The Principles of Quantum Mechanics* (**?**), published in 1930, is worth opening to marvel at how little the formalism has changed from that day to this. To get some idea of the speed with which these rather abstract notions had entered physics, bear in mind that Heisenberg's mentor Max Born had to point out to him that the novel rule Heisenberg had found for composing matrix elements was nothing but matrix multiplication, little used by physicists of the day!

In contrast to the Schrödinger equation, which allowed physicists trained to solve the partial differential equations of classical physics to go to work on the problems of the atom, Heisenberg's formulation is practically useless. It took the genius of Wolfgang Pauli to solve the Hydrogen atom using matrix mechanics, a calculation we will discuss in Chapter 6

The original reference is (**?**). Coincidentally, around the same time a *fourth* formulation of quantum theory was given by Groenewold and Moyal. This **phase space formulation** makes contact with classical mechanics through the Hamiltonian, rather than Lagrangian, viewpoint. We'll meet it briefly in Chapter 5.

Eq. (2.1) and Eq. (2.4) embody a radical departure from classical ideas. In particular, the notion of a trajectory $\mathbf{r}(t)$ of a particle in time is nowhere to be seen. It is surprising, then, that there is a way to describe quantum mechanics in terms of trajectories, and more surprising still that it did not emerge until more than 20 years after the above formulations. This is **Feynman's path integral**.

2.2 *The propagator*

The path integral is a tool for calculating the **propagator**. Since this is an idea of wider utility, we'll take a moment to get acquainted. In fact, we already have, for the propagator is just a representation of the time evolution operator

The weird notation $K(\mathbf{r},t|\mathbf{r}',t)$ is to emphasize that $\mathbf{r}'$ and t' are to be treated as parameters. In particular, when we apply the Hamiltonian, it will operate on the $\mathbf{r}$ variable only.

$$K(\mathbf{r},t|\mathbf{r}',t') \equiv \theta(t-t')\left\langle \mathbf{r}|U(t-t')|\mathbf{r}'\right\rangle, \tag{2.5}$$

where $|\mathbf{r}\rangle$ denotes a position eigenstate. $\theta(t)$ is the step function

$$\theta(t) \equiv \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases}. \tag{2.6}$$

As the name implies, $K(\mathbf{r},t|\mathbf{r}',t')$ is used to propagate the state of a system forward in time. Thus Eq. (2.2) may be written, for $t > t'$

$$\begin{aligned} \Psi(\mathbf{r},t) = \langle \mathbf{r}|\Psi(t)\rangle &= \langle \mathbf{r}|U(t-t')|\Psi(t')\rangle \\ &= \int d\mathbf{r}' \, \langle \mathbf{r}|U(t-t')|\mathbf{r}'\rangle \, \langle \mathbf{r}'|\Psi(t')\rangle \\ &= \int d\mathbf{r}' \, K(\mathbf{r},t|\mathbf{r}',t')\Psi(\mathbf{r}',t'), \end{aligned} \tag{2.7}$$

where in the second line we inserted a complete set of states. Equivalently, $K(\mathbf{r},t|\mathbf{r}',t')$ is the *fundamental solution* of the time dependent Schrödinger equation, which means that it satisfies

$$\begin{gathered} \left[i\hbar\frac{\partial}{\partial t} - H\right] K(\mathbf{r},t|\mathbf{r}',t') = i\hbar\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \text{ and} \\ K(\mathbf{r},t|\mathbf{r}',t') = 0 \text{ for } t < t' \end{gathered} \tag{2.8}$$

Problem 2.1

Explain why these two definitions are equivalent. *Hint*: integrate Eq. (2.8) through a small interval $t' - \epsilon < t < t' + \epsilon$ to find $K(\mathbf{r},t'+\epsilon|\mathbf{r}',t')$.

The idea of representing the solution of a partial differential equation (PDE) should be familiar to you from your study of Green's functions. Indeed, 'Green's function' and 'propagator' are often used interchangeably.

The fact that the wavefunction at later times can be expressed in terms of $\Psi(\mathbf{r},0)$ is a consequence of the Schrödinger equation being first order in time (and linearity naturally implies the relationship is a linear one). To see the generality of the idea, let us first discuss how it works for the heat equation, another PDE first order in time. The fundamental solution satisfies

$$\begin{gathered} \left[\frac{\partial}{\partial t} - D\nabla_{\mathbf{r}}^2\right] K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \\ K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t') = 0 \text{ for } t < t' \end{gathered} \tag{2.9}$$

Problem 2.2

Show (i.e. verify – if you have the answer already that's perfectly acceptable!) that the fundamental solution of the heat equation is

$$K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t') = \frac{\theta(t-t')}{(4\pi D(t-t'))^{3/2}} \exp\left[-\frac{(\mathbf{r}-\mathbf{r}')^2}{4D(t-t')}\right] \tag{2.10}$$

Thus if $\Theta(\mathbf{r},0)$ describes the initial temperature distribution within a uniform medium with thermal diffusivity D, then at some later time we have

$$\Theta(\mathbf{r},t) = \int d\mathbf{r}'\, K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',0)\Theta(\mathbf{r}',0). \tag{2.11}$$

Eq. (2.10) and Eq. (2.11) have the following meaning. We can represent the initial continuous temperature distribution as an array of hot spots of varying temperatures. The evolution of a hot spot is found by solving Eq. (2.10), with the right hand side representing a unit amount of heat injected into the system at point $\mathbf{r}'$ and time t'. As time progresses, each hot spot diffuses outwards with a Gaussian profile of width $\sqrt{D(t-t')}$, independently of the others by virtue of the linearity of the equation.

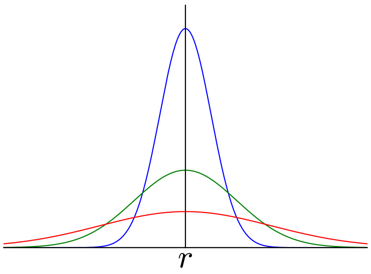


Figure 2.1: Spreading of a hot spot.

Problem 2.3

What can be accomplished in one time step can equally well be done in two. The propagator must have the property

$$K(\mathbf{r},t|\mathbf{r}',t') = \int d\mathbf{r}''\, K(\mathbf{r},t|\mathbf{r}'',t'')K(\mathbf{r}'',t''|\mathbf{r}',t'). \tag{2.12}$$

Verify that this holds for $K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t')$.

With this in hand, it's a small leap to find the propagator for the free particle Schrödinger equation. The Hamiltonian is $H = -\frac{\hbar^2\nabla^2}{2m}$, so by taking $D \to \frac{\hbar}{2m}$ and $t \to it$, we get

In d dimensions the $3/2$ power in the prefactor becomes $d/2$.

$$K_{\text{free}}(\mathbf{r},t|\mathbf{r}',t') = \theta(t-t')\left(\frac{m}{2i\pi\hbar(t-t')}\right)^{3/2} \exp\left[-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')}\right] \tag{2.13}$$

The propagator in momentum space

We originally defined the propagator in Eq. (2.5) as a real space representation of the time evolution operator. We could just as well choose to take matrix elements in another basis. Since the free particle Hamiltonian $H = -\frac{\hbar^2\nabla^2}{2m}$ is diagonal in momentum space, it makes sense to look at

$$\begin{aligned} K_{\text{free}}(\mathbf{p},t|\mathbf{p}',t') &= \theta(t-t')\,\langle\mathbf{p}|U(t-t')|\mathbf{p}'\rangle \\ &= \theta(t-t')\exp\left(-i\frac{\mathbf{p}^2}{2m}\frac{t-t'}{\hbar}\right)\delta(\mathbf{p}-\mathbf{p}') \end{aligned} \tag{2.14}$$

Don't forget that with the normalization used here, $|\mathbf{r}\rangle$ has units of $[\text{Length}]^{-d/2}$, while $|\mathbf{p}\rangle$ has units $[\text{Momentum}]^{-d/2}$. A δ-function $\delta(\mathbf{x})$ in d-dimensions has units of $[x]^{-d}$.

Problem 2.4

Confirm that Eq. (2.13) and Eq. (2.14) are related by a change of basis (Fourier transform) using

$$\langle \mathbf{r}|\mathbf{p}\rangle = \frac{\exp(i\mathbf{p}\cdot\mathbf{r}/\hbar)}{(2\pi\hbar)^{3/2}}.$$

Notice that the reproducing property (Problem 2.3) is trivial in this basis.

This idea generalises to any time independent Hamiltonian with a complete set of energy eigenfunctions $\{\varphi_\alpha(\mathbf{r})\}$ and eigenvalues $\{E_\alpha\}$

$$K(\mathbf{r},t|\mathbf{r}',t') = \theta(t-t')\sum_\alpha \varphi_\alpha(\mathbf{r})\varphi^*_\alpha(\mathbf{r}')e^{-iE_\alpha(t-t')/\hbar}. \qquad (2.15)$$

For a time dependent Hamiltonian, we have the complication that the time evolution operator must be thought of as a function of two variables – the initial and final times, say – rather than just the *duration* of evolution.

$$|\Psi(t)\rangle = U(t,t')\,|\Psi(t')\rangle\,. \qquad (2.16)$$

Nevertheless, the propagator $K(\mathbf{r},t|\mathbf{r}',t') = \theta(t-t')\,\langle\mathbf{r}|U(t,t')|\mathbf{r}'\rangle$ obeys the same basic equation Eq. (2.8).

In terms of the Hamiltonian $H(t)$, $U(t,t')$ has the deceptively simple form

$$U(t,t') = \mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_i\, H(t_i)\right],$$

where $\mathcal{T}$ denotes the time ordering operator. The time ordering is essential because the commutator of the Hamiltonian evaluated at two different times is in general nonzero.

2.3 *The path integral*

By using the reproducing property of the kernel (Problem 2.3) we can subdivide the evolution from time t_i to t_f into N smaller intervals of length $\Delta t = (t_\mathrm{f}-t_\mathrm{i})/N$, each characterized by its own propagator

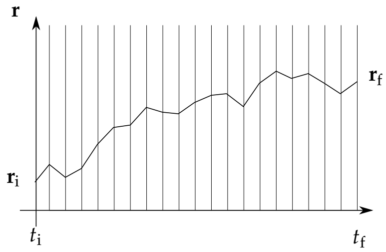


Figure 2.2: Slicing the propagation time into many small intervals.

$$K(\mathbf{r}_\mathrm{f},t_\mathrm{f}|\mathbf{r}_\mathrm{i},t_\mathrm{i}) = \int d\mathbf{r}_1\cdots d\mathbf{r}_{N-1}\; K(\mathbf{r}_\mathrm{f},t_\mathrm{f}|\mathbf{r}_{N-1},t_{N-1})\cdots K(\mathbf{r}_1,t_1|\mathbf{r}_\mathrm{i},t_\mathrm{i}). \qquad (2.17)$$

This is not totally perverse: as we will see shortly the apparent increase in complexity is countered by the simplification of the propagator for small propagation intervals. The idea is that in the limit[1] the integration over the variables $\{\mathbf{r}_i\}$ becomes an *integral over paths* $\mathbf{r}(t)$, with a continuous index – time – rather than a discrete one. This is the path integral.

So what is the integrand? A clue is provided by the observation that in the presence of a constant potential $V(\mathbf{r}) = V_0$, the propagator is a simple modification of Eq. (2.13)

$$K_\mathrm{free}(\mathbf{r},t|\mathbf{r}',t') = \theta(t-t')\left(\frac{m}{2i\pi\hbar(t-t')}\right)^{3/2}\exp\left[-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')} - i\frac{V_0(t-t')}{\hbar}\right], \qquad (2.18)$$

as may be verified by direct substitution into the Schrödinger equation. Now as the propagation time $t-t'$ goes to zero, we know that the propagator is going to approach a δ-function. Therefore, Eq. (2.18) should still hold if we take V_0 to be the value of the potential at the midpoint $\frac{\mathbf{r}+\mathbf{r}'}{2}$ (say)[2].

Putting this into Eq. (2.17), for $N\to\infty$, $(\mathbf{r}_{i+1}-\mathbf{r}_i)^2/(t_{i+1}-t_i)\to\dot{\mathbf{r}}^2\Delta t$,

$$K(\mathbf{r}_\mathrm{f},t_\mathrm{f}|\mathbf{r}_\mathrm{i},t_\mathrm{i}) = \int_{\substack{\mathbf{r}(t_\mathrm{f})=\mathbf{r}_\mathrm{f}\\ \mathbf{r}(t_\mathrm{i})=\mathbf{r}_\mathrm{i}}} \mathcal{D}\mathbf{r}(t)\,\exp\left(\frac{i}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\left[\frac{m\dot{\mathbf{r}}^2}{2} - V(\mathbf{r}(t))\right]dt\right). \qquad (2.19)$$

---

[1] These three words are terribly glib. Spare a thought for the mathematicians who had to try and make something respectable out of this!

[2] The particular choice is unimportant here, but the midpoint prescription turns out to be vital when a vector potential is included. See (?), Chapter 4.

The symbol $\mathcal{D}\mathbf{r}(t)$, which corresponds to a 'volume element' in the space of paths, is presumed to contain the appropriate normalization, including a horribly divergent factor $\left(\frac{m}{2i\pi\hbar\Delta t}\right)^{3N/2}$. The subscript on the $\int \mathcal{D}\mathbf{r}(t)$ integral indicates that all paths must begin at $\mathbf{r}_{\mathrm{i}}$ and end at $\mathbf{r}_{\mathrm{f}}$.

One may wonder how Eq. (2.19), beset by such mathematical vagaries, can be of any use at all. One thing we have going for us is that all of these difficulties have nothing to do with $V(\mathbf{r})$, and are therefore unchanged in going from the free particle case to something more interesting. We can therefore use the free particle result to provide the normalization, and calculate the effect of introducing $V(\mathbf{r})$ relative to this.

Enter the Lagrangian

It's a historical oddity that the Hamiltonian is one of the last things you meet in classical mechanics and one of the first in quantum mechanics. Eq. (2.19) represents the first appearance in quantum mechanics of the *Lagrangian*

$$L(\mathbf{r}, \dot{\mathbf{r}}) \equiv \frac{m\dot{\mathbf{r}}^2}{2} - V(\mathbf{r}), \tag{2.20}$$

and its time integral, the *action*

$$S[\mathbf{r}(t)] \equiv \int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}} L(\mathbf{r}(t), \dot{\mathbf{r}}(t))\, dt \tag{2.21}$$

The square brackets are used to indicate that S is a *functional* of the path. A functional is a machine that takes a function and produces a number.

As you know very well, variations of the path $\mathbf{r}(t)$ with fixed endpoints (i.e $\mathbf{r}(t_{\mathrm{i}}) = \mathbf{r}_{\mathrm{i}}$, $\mathbf{r}(t_{\mathrm{f}}) = \mathbf{r}_{\mathrm{f}}$) leave the action unchanged to first order if (and only if) the *Euler–Lagrange equations* are satisfied

$$\frac{\partial L}{\partial \mathbf{r}} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{r}}}\right) = 0. \tag{2.22}$$

As we'll see shortly, the path integral provides a natural explanation of how these equations and the action principle arise in the classical limit.

2.4 *Path integral for the harmonic oscillator*

To show that this all works we at least have to be able to solve the harmonic oscillator. Confining ourselves to one dimension, the Lagrangian is

$$L_{\mathrm{SHO}}(x, \dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2. \tag{2.23}$$

The propagator is therefore expressed as the path integral

$$K_{\mathrm{SHO}}(x_{\mathrm{f}}, t_{\mathrm{f}}|x_{\mathrm{i}}, t_{\mathrm{i}}) = \int_{\substack{x(t_{\mathrm{f}})=x_{\mathrm{f}} \\ x(t_{\mathrm{i}})=x_{\mathrm{i}}}} \mathcal{D}x(t)\, \exp\left(\frac{i}{\hbar} \overbrace{\int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}} \left[\frac{m\dot{x}^2}{2} - \frac{m\omega^2 x^2}{2}\right] dt}^{S_{\mathrm{SHO}}[x(t)]}\right). \tag{2.24}$$

This form is reminiscent of a Gaussian integral. Before we can use this insight, we first have to deal with the feature that the paths $x(t)$ satisfy the boundary conditions $x(t_{\mathrm{i}}) = x_{\mathrm{i}}$, $x(t_{\mathrm{f}}) = x_{\mathrm{f}}$. We can make things simpler by substituting $x(t) = x_0(t) + \eta(t)$, where $x_0(t)$ is some function satisfying these same conditions. Then $\eta(t)$, the new integration variable, satisfies $\eta(t_{\mathrm{i}}) = \eta(t_{\mathrm{f}}) = 0$.

What should we take for $x_0(t)$? Making the substitution in the action gives

$$S_{\text{SHO}}[x_0(t)+\eta(t)] = S_{\text{SHO}}[x_0(t)] + S_{\text{SHO}}[\eta(t)] + \int_{t_{\text{i}}}^{t_{\text{f}}} \left[m\dot{x}_0(t)\dot{\eta}(t) - m\omega^2 x_0(t)\eta(t)\right] dt. \quad (2.25)$$

Integrating the last term by parts, and bearing in mind that $\eta(t)$ vanishes at the endpoints, puts it in the form

$$-\int_{t_{\text{i}}}^{t_{\text{f}}} \left[m\ddot{x}_0(t) + m\omega^2 x_0(t)\right] \eta(t)\, dt. \quad (2.26)$$

We recognize the quantity in square brackets as the equation of motion of the simple harmonic oscillator. Thus if we choose $x_0(t)$ to satisfy this equation, the cross term in Eq. (2.25) vanishes and the propagator takes the form

$$K_{\text{SHO}}(x_{\text{f}}, t_{\text{f}}|x_{\text{i}}, t_{\text{i}}) = \exp\left(\frac{i}{\hbar} S_{\text{SHO}}[x_0(t)]\right) \times \int_{\eta(t_{\text{f}})=\eta(t_{\text{i}})=0} \mathcal{D}\eta(t) \, \exp\left(\frac{i}{\hbar}\int_{t_{\text{i}}}^{t_{\text{f}}} \left[\frac{m\dot{\eta}^2}{2} - \frac{m\omega^2\eta^2}{2}\right] dt\right). \quad (2.27)$$

Choosing $x_0(t)$ to be the classical trajectory eliminates the linear term in η in general. This is after all exactly what the action principle tells us that classical trajectories do (note the condition of fixed endpoints, vital in the derivation of the Euler–Lagrange equations, arises naturally here). The action for $\eta(t)$ will not be independent of $x_0(t)$ for more complicated – i.e. non-quadratic – Lagrangians, however.

Problem 2.5

Show that the classical action is

$$S_{\text{SHO}}[x_0(t)] = \frac{m\omega}{2\sin\left[\omega\left(t_{\text{f}} - t_{\text{i}}\right)\right]} \left[\left(x_{\text{i}}^2 + x_{\text{f}}^2\right)\cos\left[\omega\left(t_{\text{f}} - t_{\text{i}}\right)\right] - 2x_{\text{i}}x_{\text{f}}\right] \quad (2.28)$$

Now we turn our attention to the η path integral in Eq. (2.27). Because the action for $\eta(t)$ is independent of time, and $\eta(t)$ vanishes at the endpoints, it cries out to be expanded in a Fourier series

$$\eta(t) = \sum_{n=1}^{\infty} \eta_n \sin\left[\frac{\pi n\left(t - t_{\text{i}}\right)}{t_{\text{f}} - t_{\text{i}}}\right]. \quad (2.29)$$

In terms of the Fourier coefficients $\{\eta_n\}$ the action takes the form

$$S_{\text{SHO}}[\eta(t)] = \frac{m\left(t_{\text{f}} - t_{\text{i}}\right)}{4} \sum_{n=1}^{\infty} \left[\frac{\pi^2 n^2}{(t_{\text{f}} - t_{\text{i}})^2} - \omega^2\right] \eta_n^2. \quad (2.30)$$

The η integral now begins to look like a product of Gaussian integrals, provided that we are free to interpret $\mathcal{D}\eta(t) = \prod_i^\infty d\eta_n$ (we are).

The Gaussian integral we can do

$$\int_{-\infty}^{\infty} dx\, e^{-bx^2/2} = \sqrt{\frac{2\pi}{b}}. \quad (2.31)$$

So we take a wild guess and write

$$K_{\text{SHO}}(x_{\text{f}}, t_{\text{f}}|x_{\text{i}}, t_{\text{i}}) \overset{?}{=} \exp\left(\frac{i}{\hbar} S_{\text{SHO}}[x_0(t)]\right) \times \prod_{n=1}^{\infty} \sqrt{\frac{4\pi i\hbar}{m} \frac{(t_{\text{f}} - t_{\text{i}})}{\pi^2 n^2 - \omega^2 (t_{\text{f}} - t_{\text{i}})^2}}. \quad (2.32)$$

Does it work? No. But then we didn't expect it to, because of the difficulties in defining the path integral in the first place. However, as we noted in the previous section, the fudge factor required is independent of the potential, so the overall normalization can be deduced from the free particle result that must apply when $\omega = 0$. Adapting the result Eq. (2.13) to one dimension, we find

$$K_{\mathrm{SHO}}(x_{\mathrm{f}}, t_{\mathrm{f}}|x_{\mathrm{i}}, t_{\mathrm{i}}) = \left(\frac{m}{2i\pi\hbar(t_{\mathrm{f}} - t_{\mathrm{i}})}\right)^{1/2} \exp\left(\frac{i}{\hbar} S_{\mathrm{SHO}}[x_0(t)]\right) \times \prod_{n=1}^{\infty}\left(1 - \frac{\omega^2(t_{\mathrm{f}} - t_{\mathrm{i}})^2}{\pi^2 n^2}\right)^{-1/2}. \tag{2.33}$$

The infinite product was found by Leonhard Euler (1707-1783)

$$\prod_{n=1}^{\infty}\left(1 - \frac{\omega^2(t_{\mathrm{f}} - t_{\mathrm{i}})^2}{\pi^2 n^2}\right) = \frac{\sin\omega(t_{\mathrm{f}} - t_{\mathrm{i}})}{\omega(t_{\mathrm{f}} - t_{\mathrm{i}})}. \tag{2.34}$$

We arrive at the final result

$$K_{\mathrm{SHO}}(x_{\mathrm{f}}, t_{\mathrm{f}}|x_{\mathrm{i}}, t_{\mathrm{i}}) = \left(\frac{m\omega}{2i\pi\hbar\sin\omega(t_{\mathrm{f}} - t_{\mathrm{i}})}\right)^{1/2} \exp\left(\frac{i}{\hbar} S_{\mathrm{SHO}}[x_0(t)]\right). \tag{2.35}$$

Problem 2.6

Show that this is correct. *Hint*: You only need to show that this solves the appropriate Schrödinger equation, as the short time behaviour (when $\omega(t_{\mathrm{f}} - t_{\mathrm{i}}) \ll 1$) is the same as for the free particle.

What can you actually do with a path integral?

- Gaussian integrals (like the simple harmonic oscillator).
- Err...
- That's it.

Bear in mind, however, that the number of problems that can be solved exactly by the other formulations of quantum mechanics is also rather limited. Apart from the harmonic oscillator, the other Hamiltonian you all know how to solve exactly is the Hydrogen atom. Can it be done with a path integral? The answer is yes[3]. Furthermore, the special features of the Hydrogen atom that make it amenable to exact solution – we'll discuss them in Chapter 6 – are precisely the same features that make it possible to calculate the path integral.

The value of the path integral is firstly to provide a new language for quantum theory, one that has given rise to many new insights. New effects can arise when the *topology* of paths is important, e.g. the Aharonov–Bohm effect.

A new formulation can also suggest new approximate methods to solve problems that have no exact solution. The most obvious approach is to expand the integrand in the path integral in powers of the potential $V(\mathbf{r})$. This

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[3] This illustrates the principle of *conservation of troubles*, according to which a problem is no easier or harder in a different language; the difficulties are just moved around (and sometimes out of sight!).

turns out to be equivalent to time-dependent perturbation theory, as you can easily check.

A more useful line of attack is to try to evaluate the path integral *numerically*, using the same discretization of time that we used to derive it. For Eq. (2.19) this is in fact a terrible idea, as the integrand is complex, and oscillates wildly, leading to very poor convergence. However, as we'll see in Chapter 5, it is possible to formulate the *partition function* of quantum statistical mechanics as a path integral in *imaginary* time. We've already seen the form of the propagator in imaginary time, when we discussed the heat equation (Eq. (2.10)). Notice that it is real and positive, so we can think of it as a probability distribution. Evaluating the partition function by sampling the probability distribution of paths is the basis of the **path integral Monte Carlo** method.

2.5 *Semiclassics and the method of stationary phase*

The other great insight provided by the path integral concerns the emergence of classical mechanics from quantum mechanics. The appearance of the Lagrangian and action in the integrand should already have us asking what role the condition of stationary action plays in quantum theory. A clue is provided by a method of approximating ordinary integrals that goes by the names **steepest descent**, **stationary phase**, **saddle point**, or occasionally **Laplace's method**.

In order to illustrate an application of the method of stationary phase, we depart from the consideration of the propagator – evaluated by the path integral – and discuss the semiclassical method for solving for energy eigenstates of the Schrödinger equation.

JWKB method

The JWKB (Jeffreys, Wentzel, Kramers, Brillouin) method is a semiclassical technique for obtaining approximate solutions to the one-dimensional Schrödinger equation. It is mainly used in calculating bound-state energies and tunnelling rates through potential barriers, and is valid in the semiclassical limit $\lambda = \frac{h}{p} = \frac{h}{mv} \to 0$ or $\hbar \to 0$ or $m \to \infty$ where m is the mass of the particle, p its momentum etc.

The key idea is as follows. Imagine a particle of energy E moving through a region where the potential $V(x)$ is *constant*. If $E > V$, the wave function is of the form

$$\begin{aligned} \psi(x) &= A\, e^{\pm ikx} \\ k &= \frac{\sqrt{2m(E-V)}}{\hbar}. \end{aligned}$$

The plus sign indicates particles travelling to the right etc. The wave function is oscillatory, with constant wavelength $\lambda = 2\pi/k$, and has constant amplitude, A. Consider now the case where $V(x)$ is not a constant but varies rather slowly in comparison to λ (so that in a region containing many wavelengths the potentially is essentially constant). Then it is reasonable to suppose that ψ remains practically sinusoidal except that the wavelength and the amplitude change slowly with x. This is the central theme of the JWKB method: rapid oscillations are modulated by gradual variation in amplitude and wavelength.

Similarly, if $E < V$ (with V a constant), then ψ is exponential:

$$\begin{aligned} \psi(x) &= A\, e^{\pm Kx} \\ K &= \frac{\sqrt{2m(V-E)}}{\hbar} \end{aligned}$$

Now, if $V(x)$ is not constant but again varies slowly in comparison to $1/K$, the solution remains practically exponential except that A and K are now slowly varying functions of x.

There are of course places where this idea breaks down, e.g. in the vicinity of a classical turning point where $E \approx V$. Here, λ (or $1/K$) goes to infinity and $V(x)$ can hardly be said to vary "slowly"! Proper handling of this is the most difficult aspect of the JWKB approximation but the final results are simple and easy to implement.

Derivation

We seek to solve

$$\begin{aligned} \frac{d^2\psi}{dx^2} + k^2(x)\psi(x) = 0 \\ k^2(x) = \frac{2m}{\hbar^2}(E - V(x)) \end{aligned} \tag{2.36}$$

The semiclassical limit corresponds to k large. If k were constant, then of course the solutions would just be $e^{\pm ikx}$. This suggests that we try $\psi(x) = e^{iS(x)}$, where in general $S(x)$ is a complex function. Then,

$$\begin{aligned} \frac{d\psi}{dx} &= iS'e^{iS} \\ \frac{d^2\psi}{dx^2} &= (iS'' - S'^2)e^{iS} \end{aligned} \tag{2.37}$$

and the Schrödinger equation reduces to $(iS'' - S'^2 + k^2)e^{iS} = 0$, or

$$\begin{aligned} S' &= \pm\sqrt{k^2(x) + iS''(x)} \\ &= \pm k(x)\sqrt{1 + iS''(x)/k^2} \end{aligned} \tag{2.38}$$

(Note that if k were a constant, $S'' = 0$ and $S' = \pm k$.)

We now attempt to solve the above equation by iteration, using $S' = \pm k$ as the first guess, and as a second guess we use:

$$\begin{aligned} S' &= \pm k\sqrt{1 \pm ik'(x)/k^2} \\ &\approx \pm k\left(1 \pm \frac{i}{2}\frac{k'(x)}{k^2}\right) \\ &\approx \pm k + \frac{i}{2}\frac{k'(x)}{k} \end{aligned} \tag{2.39}$$

where we have assumed that the corrections are small. Then, we have

$$\begin{aligned} \frac{dS}{dx} &= \pm k + \frac{i}{2}\frac{k'}{k} \\ S(x) &\sim \pm\int^x k(x')dx' + \frac{i}{2}\int^x \frac{k'(x')}{k(x')}dx' + c \end{aligned} \tag{2.40}$$

The second integral is a perfect differential $(d\ \ln k)$, so

$$\begin{aligned} S(x) &= \pm\int^{x} k(x')dx' + \frac{i}{2}\ln k + c \\ \psi &= e^{iS} \\ &= C\, e^{\pm i\int^{x} k(x')dx'} e^{-\frac{1}{2}\ln k} \\ &= \frac{C}{\sqrt{k(x)}} e^{\pm i\int^{x} k(x')dx'} \end{aligned} \tag{2.41}$$

Note that in making the expansion, we have assumed that $\frac{k'}{k^2} \ll 1$ or $\frac{\lambda}{2\pi}\frac{dk}{dx} \ll k$, i.e. that the change in k in one wavelength is much smaller than k. Alternatively, one has $\lambda\frac{dV}{dx} \ll \frac{\hbar^2 k^2}{m}$ so that the change in V in one wavelength is much smaller than the local kinetic energy.

Note that in the classically forbidden regions, $k^2 < 0$, one puts $k = iK(x)$ and carries through the above derivation to get

$$\begin{aligned} \psi(x) &= \frac{C}{\sqrt{K(x)}} e^{\pm\int^{x} K(x')dx'} \\ K^2 &= \frac{2m}{\hbar^2}(V - E) > 0 \end{aligned} \tag{2.42}$$

Connection Formulae

In our discussion above, it was emphasised that the JWKB method works when the short wavelength approximation holds. This of course breaks down when we hit the classical turning points where $k^2(x) = 0$ (which happens when $E = V$). To overcome this problem, we will derive below equations relating the forms of the solution to both sides of the turning point.

If the potential can be approximated by an increasing linear potential near the turning point $x = a$ (the region $x > a$ being classically forbidden), we can write in the vicinity of the turning point

$$k^2(x) = \frac{2m}{\hbar^2}\left(-\frac{dV}{dx}\right)_{x=a}(x - a) \tag{2.43}$$

The Schrödinger equation near the turning point becomes

$$\psi'' - \left(\frac{dV}{dx}\right)_{x=a}\frac{2m}{\hbar^2}\,(x - a)\psi = 0 \tag{2.44}$$

If we let

$$\begin{aligned} z &= \alpha(x - a) \\ \alpha^3 &= \frac{2m}{\hbar^2}\frac{dV}{dx} \geq 0 \end{aligned} \tag{2.45}$$

then the above differential equation becomes equivalent to **Airy's equation**

$$f''(z) - z\,f(z) = 0\,. \tag{2.46}$$

The solution of this equation is a non-elementary function called the *Airy function* (in fact, there are two linearly independent solutions, as this is a second order equation), and we are particularly interested in its behaviour at large $|z|$. As is often the case with special functions, there is an integral representation of the Airy function, and we can use this to find the large $|z|$ behaviour in a controlled way.

The first thing to note is that the Fourier transform of the equation

$$i\tilde{f}'(k) + k^2\tilde{f}(k) = 0 \tag{2.47}$$

is *first* order, and may be solved easily

$$\tilde{f}(k) = A\exp\left(ik^3/3\right), \tag{2.48}$$

Using the convention $f(z) = \int_{-\infty}^{\infty} e^{ikz}\tilde{f}(k)\,\frac{dk}{2\pi}$. Overall numerical factors aren't important here: it's a linear equation.

with A some constant. Thus all we have to do to find the solution $f(z)$ is compute the Fourier integral

$$f(z) = \frac{1}{2\pi}\int e^{ikz}\tilde{f}(k)\,dk = \frac{A}{2\pi}\int \exp\left(ik^3/3 + ikz\right)\,dk. \tag{2.49}$$

But wait! A linear second order equation has two independent solutions, and it looks like we have only found one. However, we didn't yet specify the contour of integration in Eq. (2.49), and our freedom to choose this allows us to generate more than one solution.

Problem 2.7

Show that $f(z)$ defined by Eq. (2.49) satisfies Airy's equation as long as the integrand vanishes at the endpoints. *Hint*: integrate by parts.

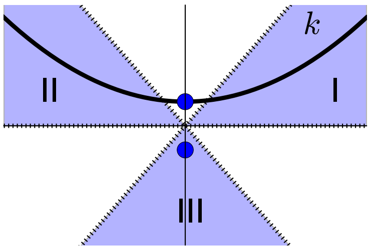

Figure 2.3: A possible contour in the plane of complex k, passing through one of the stationary points of the integrand.

Where does the integrand vanish? We have to go to large $|k|$ in such a way that the dominant term $ik^3/3$ term in the exponent has a negative real part. Writing $k = |k|e^{i\theta}$, we can see that this happens as $|k| \to \infty$ in the three wedges

$$\begin{aligned} \text{I:} &\qquad 0 < \theta < \pi/3 \\ \text{II:} &\qquad 2\pi/3 < \theta < \pi \\ \text{III:} &\qquad 4\pi/3 < \theta < 5\pi/3 \end{aligned} \tag{2.50}$$

Different choices for the starting and ending wedge give different solutions.

Use Cauchy's theorem to convince yourself that only two are independent.

Now comes the key idea. Because the integrand is an exponential, it quickly becomes negligible as we move off into a wedge. The largest contribution should come from the largest value of the real part of the exponent. The stationary points satisfy $k^2 + z = 0$ and lie at

$$k_{\text{sp}} = \begin{cases} \pm i\sqrt{z} & \text{for } z > 0 \\ \pm\sqrt{|z|} & \text{for } z < 0 \end{cases}, \tag{2.51}$$

Why do we look at a stationary point if we only want to maximize the *real* part of the exponent? Think about the Cauchy–Riemann equations.

with the integrand taking the values

$$\exp\left(ik_{\text{sp}}^3/3 + ik_{\text{sp}}z\right) = \begin{cases} \exp\left(\mp\frac{2}{3}z^{3/2}\right) & \text{for } z > 0 \\ \exp\left(\mp i\frac{2}{3}|z|^{3/2}\right) & \text{for } z < 0. \end{cases} \tag{2.52}$$

As we go to large $|z|$, the decay of the integrand as we move away from these stationary points becomes more rapid. Fixing $z > 0$ and expanding the exponent around the saddle point value gives

For an analytic function, all stationary points are saddle points, which is why we use the terms interchangeably here.

$$\exp\left(ik^3/3 + ikz\right) \sim \exp\left(\mp\frac{2}{3}z^{3/2}\right)\exp\left(\mp\sqrt{z}\,(k - k_{\text{sp}})^2\right) \tag{2.53}$$

where the ± signs correspond to the stationary points at $\pm i\sqrt{z}$. For $i\sqrt{z}$, moving parallel to the real axis therefore corresponds to the direction of *steepest descent*, in which the integrand decays fastest. For $-i\sqrt{z}$, the steepest descent direction is parallel to the imaginary axis.

Eq. (2.53) replaces the integrand by a Gaussian of width $\sim z^{-1/4}$, an approximation that obviously improves very quickly as z becomes large. For the contour in Fig. 2.3 which passes through $i\sqrt{z}$, the integral in Eq. (2.49) is then approximately

$$f(z) \sim \frac{A}{2\pi}\frac{\pi^{1/2}}{z^{1/4}} \exp\left(-\frac{2}{3}z^{3/2}\right), \text{ as } z \to \infty. \tag{2.54}$$

The **Airy function** $\mathrm{Ai}(z)$ is defined by this contour, with the (arbitrary) choice $A = 1$. Thus we have

$$\mathrm{Ai}(z) \sim \frac{1}{2\pi^{1/2}z^{1/4}} \exp\left(-\frac{2}{3}z^{3/2}\right), \text{ as } z \to \infty \tag{2.55}$$

The second solution that grows exponentially for $z \to \infty$ is denoted by $\mathrm{Bi}(z)$ and sometimes hilariously called the Bairy function.

The case of $z < 0$ is slightly trickier, as the two stationary points lie on the real axis. In this case we pass through *both* stationary points, and in the Gaussian approximation we can just sum the contribution from each. Near these points the integrand takes the form (c.f. Eq. (2.53))

$$\exp\left(ik^3/3 + ikz\right) \sim \exp\left(\mp i\frac{2}{3}|z|^{3/2}\right)\exp\left(\pm i\sqrt{|z|}\left(k - k_{\mathrm{sp}}\right)^2\right). \tag{2.56}$$

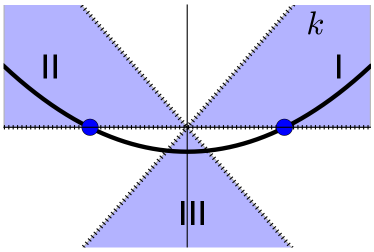

Figure 2.4: For $z < 0$ we pass through *both* stationary points of the integrand.

We see that the steepest descent directions are now at angle $\pm\pi/4$ to the real axis for the saddle point at $\pm\sqrt{|z|}$. Accounting for this rotation of the contour when we do the Gaussian integral gives

$$\mathrm{Ai}(z) \sim \frac{1}{\pi^{1/2}|z|^{1/4}} \sin\left(\frac{2}{3}|z|^{3/2} + \frac{\pi}{4}\right), \text{ as } z \to -\infty. \tag{2.57}$$

The $\pi/4$ phase shift is the ultimate origin of the 'extra' $1/2$ in the Bohr–Sommerfeld quantization condition

$$\oint p(x)dx = h\left(n + \frac{1}{2}\right), \qquad n \text{ integer}, \tag{2.58}$$

where $p(x) = \sqrt{2m\left(E - V(x)\right)}$ is the classical momentum at position x of a particle with energy E moving in a potential $V(x)$.

Problem 2.8

You are familiar with *Stirling's approximation* in the form

$$\ln N! \sim N \ln N - N. \tag{2.59}$$

Sometimes, however, this approximation doesn't cut it. Think of the number of ways of getting 50 heads with 100 coin tosses

$$\binom{100}{50}\left(\frac{1}{2}\right)^{100} = \frac{100!}{(50!)^2}\left(\frac{1}{2}\right)^{100}. \tag{2.60}$$

Eq. (2.59) would tell you that the answer is approximately one. To get something better, we write

$$N! = \int_0^\infty x^N e^{-x}\, dx \tag{2.61}$$

(proof by integration by parts) and use the saddle point method, valid at large N. Show that this yields

$$N! \sim N^N e^{-N}\sqrt{2\pi N}. \tag{2.62}$$

A better estimate for the above probability is then $\frac{1}{5\sqrt{2\pi}} \sim 0.080$.

2.6 *The classical limit*

Now we understand the method of stationary phase, we proceed to discuss the path integral by analogy. The integrand in Eq. (2.19) is

$$\exp\left(\frac{i}{\hbar}S[\mathbf{r}(t)]\right), \tag{2.63}$$

where $S[\mathbf{r}(t)]$ is the action. Planck's constant immediately presents itself as a small parameter on which to base the stationary phase approximation. More precisely, if the ratio of typical variations of the action to Planck's constant is large, we are justified in approximating the path integral as Gaussian in the vicinity of the extremum of the action. But we know that the extremum corresponds to the classical trajectory $\mathbf{r}_{\text{cl}}(t)$. This suggests that, schematically, the propagator can be written approximately as

Such approximations are usually called *semiclassical*. The WKB method is another example.

$$K(\mathbf{r},t;\mathbf{r}',t') \sim (\text{Gaussian integral}) \times \exp\left(\frac{i}{\hbar}S[\mathbf{r}_{\text{cl}}(t)]\right). \tag{2.64}$$

The classical trajectory is the one satisfying $\mathbf{r}_{\text{cl}}(t) = \mathbf{r}$, $\mathbf{r}_{\text{cl}}(t') = \mathbf{r}'$. That is, the endpoints fix the solution, rather than the initial position and velocity.

The result is a beautiful connection between the classical and quantum formalisms. The path integral tells us that the amplitude of a process is the sum of amplitudes for all possible trajectories between two points. But in the classical limit – which corresponds to systems sufficiently large that the variations of the action are much larger that Planck's constant – almost all of these trajectories cancel out because of the wild fluctuations of the phase of the integrand. The dominant contributions are those close to the extremum of the integrand i.e. the classical trajectory.

TANGENT Unfortunately we don't have time to make Eq. (2.64) precise. The result of evaluating the Gaussian path integral is the **van Vleck propagator**[4]. In three dimensions, this is

$$K_{\text{vV}}(\mathbf{r},t;\mathbf{r}',t') = \sum_{\text{classical paths}} \left(\frac{1}{2\pi i\hbar}\right)^{3/2} \det\left(-\frac{\partial^2 S}{\partial\mathbf{r}\,\partial\mathbf{r}'}\right)^{-1/2} \exp\left(\frac{i}{\hbar}S[\mathbf{r}_{\text{cl}}(t)]\right). \tag{2.65}$$

The classical action is a function (not a functional) of $\mathbf{r}$, $\mathbf{r}'$ because $\mathbf{r}_{\text{cl}}(t)$ depends on the endpoints (c.f. Eq. (2.28)). In general there may be more than one classical trajectory connecting two points (if there is periodic motion, say), so we have to sum over all of them, just as when we evaluated the Airy function for $x < 0$.

This doesn't happen for the harmonic oscillator because the period is constant.

[4] See (?). As the date indicates, you don't need the path integral to derive this result!

3
Scattering theory

Scattering experiments play a vital role in modern physics. In a typical scattering experiment, particles approach each other 'from infinity' – which is to say from far outside the range of their interaction with each other – spend a short time in close proximity, and then go their separate ways. As they propagate outwards from the collision region, their interaction ceases but its imprint is left on the scattered waves, ready to be picked up by a detector.

This basic picture encompasses a wide variety of different situations. We list just a few examples

- The scattering of neutrons from a crystal lattice to determine magnetic structure.
- The scattering of α-particles from the nuclei in a layer of gold leaf (**Rutherford scattering**[1]).
- The collision of protons in the LHC.

The usefulness of scattering as an experimental technique therefore hinges on solving the 'inverse problem' of inferring the interactions (i.e. the Hamiltonian) from the scattered waves. Our purpose in this chapter, on the other hand, is to describe the general mathematical structure of scattering.

3.1 Scattering in one dimension

A great many of the concepts of scattering theory can be introduced in one dimension, where certain complexities of our three dimensional world are absent. As an additional simplification, we'll study the scattering of particles from a static potential: the 'target'. The generalization to the scattering of pairs of particles is not difficult – it involves viewing the collision in the centre of mass frame, which as usual reduces to a single particle problem.

The situation we aim to describe is illustrated in Fig. 3.1. A wavepacket approaches the origin from $-\infty$. Near the origin it interacts with a potential $V(x)$. As a result of this interaction, a modified wavepacket is transmitted and another is reflected, and these move to $\pm\infty$.

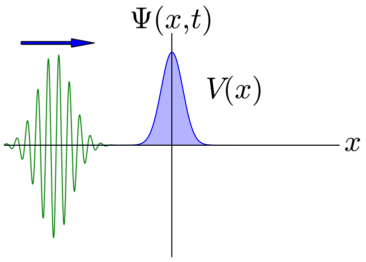

Figure 3.1: Schematic view of scattering in one dimension.

Let's suppose that $V(x)$ either vanishes outside some finite region that includes the origin, or is otherwise negligible (exponentially decaying, say). We'll sometimes refer to this region as the *interaction region*. Long range potentials bring certain complications that need not concern us at the moment. As well as being relevant to a great many scattering experiments, interaction with a localized potential brings the wonderful simplification that outside of

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[1] 'It was quite the most incredible event that has ever happened to me in my life. It was almost as incredible as if you fired a 15-inch shell at a piece of tissue paper and it came back and hit you.'

the range of the potential, the energy eigenstates of the system take the form of plane waves. This allows us to construct the incoming wavepacket from the eigenstates, just as we would construct one from plane waves. If we now imagine the wavepacket becoming more extended in real space, then eventually it becomes indistinguishable from an eigenstate. In a little while, a 'relic' of the wavepacket picture will be required to make sense of some of our expressions, but for the moment let us continue to discuss the eigenstates of the problem.

As we have already mentioned, outside of the interaction region an energy eigenstate must have the form

$$\Psi_k(x) = \begin{cases} a_+ \exp(ikx) + a_- \exp(-ikx) & x \ll 0 \\ b_+ \exp(ikx) + b_- \exp(-ikx) & x \gg 0, \end{cases} \tag{3.1}$$

where the wavevector k is related to the energy of the state by $E_k \equiv \frac{\hbar^2 k^2}{2m}$. Now, the four complex coefficients in Eq. (3.1) are not independent of each other. Rather, they are related by finding the form of the wavefunction within the interaction region, as the following example shows.

Problem 3.1

For a δ-function potential $V(x) = g\delta(x)$, show that the relationship between the coefficients in Eq. (3.1) may be written in terms of the **scattering matrix** $\mathsf{S}(k)$

$$\begin{pmatrix} a_- \\ b_+ \end{pmatrix} = \overbrace{\begin{pmatrix} r_{\text{LL}} & t_{\text{RL}} \\ t_{\text{LR}} & r_{\text{RR}} \end{pmatrix}}^{\mathsf{S}(k)} \begin{pmatrix} a_+ \\ b_- \end{pmatrix}, \tag{3.2}$$

where the **reflection** and **transmission** coefficients have the form

$$r_{\text{LL}} = r_{\text{RR}} = \frac{g}{i\hbar^2 k/m - g}, \qquad t_{\text{RL}} = t_{\text{LR}} = \frac{i\hbar^2 k/m}{i\hbar^2 k/m - g}. \tag{3.3}$$

Hint: think about the boundary conditions obeyed by the wavefunction at the origin.

What property of this problem is responsible for $r_{\text{LL}} = r_{\text{RR}}$, $t_{\text{RL}} = t_{\text{LR}}$?

The scattering matrix expresses the *outgoing* waves (i.e. the wave at $x < 0$ moving to the left and the wave at $x > 0$ moving to the right) in terms of the *incoming* waves. Probably you are familiar with the form

$$\Psi_k(x) = \begin{cases} \exp(ikx) + r_{\text{LL}} \exp(-ikx) & x \ll 0 \\ t_{\text{LR}} \exp(ikx) & x \gg 0 \end{cases}, \tag{3.4}$$

which describes a wave coming in from $-\infty$ only, and corresponds to taking $a_+ = 1$, $b_- = 0$.

Another way to encode the same information is in terms of the **transfer matrix** $\mathsf{T}(k)$, which expresses the amplitudes on one side of the scatterer in terms of those on the other

$$\begin{pmatrix} b_+ \\ b_- \end{pmatrix} = \mathsf{T}(k) \begin{pmatrix} a_+ \\ a_- \end{pmatrix} = \begin{pmatrix} t_{\text{LR}} - r_{\text{RR}} r_{\text{LL}}/t_{\text{RL}} & r_{\text{RR}}/t_{\text{RL}} \\ -r_{\text{LL}}/t_{\text{RL}} & 1/t_{\text{RL}} \end{pmatrix} \begin{pmatrix} a_+ \\ a_- \end{pmatrix} \tag{3.5}$$

The transfer matrix has the nice feature that it can be found for a number of scatterers in series by multiplying together the transfer matrices for each.

The scattering matrix $\mathsf{S}(k)$ exists for any potential $V(x)$, being defined by the relation Eq. (3.2) between the coefficients of the plane wave components of an eigenstate outside of the interaction region. It reduces the number of independent components in Eq. (3.1) from four to two. The goal of scattering theory is to find $\mathsf{S}(k)$ given $V(x)$, or at least to deduce its general properties. Let us discuss some of these properties now.

When $V(x) = 0$ these two independent solutions can of course be taken to be the left and right moving waves.

Flux conservation and unitarity of $\mathsf{S}(k)$

The probability density $P(x,t) = |\Psi(x,t)|^2$ obeys the continuity equation

$$\partial_t P(x,t) + \partial_x j(x,t) = 0, \tag{3.6}$$

where the probability current is

$$j(x,t) = -\frac{i\hbar}{2m}\left[\Psi^*\partial_x\Psi - \Psi\partial_x\Psi^*\right]. \tag{3.7}$$

When we consider an eigenstate (a.k.a. *stationary* state), the probability density does not change in time, and we must have

$$\partial_x j(x) = 0. \tag{3.8}$$

If we integrate over a region $[-L, L]$ containing the interaction region, we get

$$j(-L) = j(L). \tag{3.9}$$

At $x = \pm L$, we can use the form of the wavefunction from Eq. (3.1), giving

$$\frac{\hbar k}{m}\left[|a_+|^2 - |a_-|^2\right] = \frac{\hbar k}{m}\left[|b_+|^2 - |b_-|^2\right] \tag{3.10}$$

(happily the cross terms vanish). Eq. (3.10) has a straightforward physical meaning. $\pm\frac{\hbar k}{m}$ is the velocity of a particle described by a plane wave $e^{\pm ikx}$, and the contribution of a plane wave to the probability current is the product of the velocity and the (spatially constant) probability density.

Problem 3.2

Show that Eq. (3.10) implies that $\mathsf{S}(k)$ is a *unitary* matrix. Check that Eq. (3.2) is unitary. What is the corresponding condition satisfied by $\mathsf{T}(k)$?

Channels and phase shifts

The scattering matrix, like any unitary matrix, can be diagonlized by a unitary transformation U. The eigenvalues are complex numbers of unit magnitude, so we can write

$$\mathsf{U}\mathsf{S}\mathsf{U}^\dagger = \begin{pmatrix} \exp(2i\delta_1) & 0 \\ 0 & \exp(2i\delta_2) \end{pmatrix}, \tag{3.11}$$

which defines the **phase shifts** $\delta_{1,2}$. This means that if we express the amplitudes in Eq. (3.1) as

$$\begin{aligned} \begin{pmatrix} a_+ \\ b_- \end{pmatrix} &= \mathsf{U}^\dagger \begin{pmatrix} c_1^{\text{in}} \\ c_2^{\text{in}} \end{pmatrix} \\ \begin{pmatrix} a_- \\ b_+ \end{pmatrix} &= \mathsf{U}^\dagger \begin{pmatrix} c_1^{\text{out}} \\ c_2^{\text{out}} \end{pmatrix}, \end{aligned} \tag{3.12}$$

then the new amplitudes $c_{1,2}^{\text{in,out}}$ are related by

$$c_{1,2}^{\text{out}} = \exp\left(2i\delta_{1,2}\right) c_{1,2}^{\text{in}}. \tag{3.13}$$

In this way an eigenstate is written as a linear combination of two **scattering channels**, each of which has particular simple scattering properties: there is no 'mixing' between channels.

For $V(x) = 0$, this corresponds to working with $\cos(kx)$ and $\sin(kx)$ instead of $e^{\pm ikx}$.

In one dimension by far the most important example is provided by **parity symmetric** potentials $V(x) = V(-x)$. We know that the energy eigenstates of such potentials can be chosen to have a definite parity. Referring to the general form Eq. (3.1), this means that $a_+ = \pm b_-$, $a_- = \pm b_+$, with a $+$ sign for an even state and a $-$ for an odd one. In this case we can write Eq. (3.12) as

$$\begin{aligned} \begin{pmatrix} a_+ \\ b_- \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} c_{\text{even}}^{\text{in}} \\ c_{\text{odd}}^{\text{in}} \end{pmatrix} \\ \begin{pmatrix} a_- \\ b_+ \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} c_{\text{even}}^{\text{out}} \\ c_{\text{odd}}^{\text{out}} \end{pmatrix}. \end{aligned} \tag{3.14}$$

In this basis Eq. (3.1) takes the form

$$\Psi_k(|x| \gg 0) = c_{\text{even}} \cos\left(k|x| + \delta_{\text{even}}\right) + \operatorname{sgn}(x) c_{\text{odd}} \cos\left(k|x| + \delta_{\text{odd}}\right), \tag{3.15}$$

where for convenience we have defined $c_{\text{even,odd}} = \exp\left(i\delta_{\text{even,odd}}\right) c_{\text{even,odd}}^{\text{in}} / \sqrt{2}$

Problem 3.3

Find δ_{even} and δ_{odd} for the δ-function potential of Problem 3.1, and the form of the corresponding wavefunctions.

Integral equation for scattering amplitudes

All this formalism is well and good, but how do we find $\mathsf{S}(k)$, $\delta_{1,2}(k)$, and so on in general? We are looking for solutions of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\partial_x^2 \Psi(x) + V(x)\Psi(x) = E_k \Psi(x), \tag{3.16}$$

but we know that in general there are two independent solutions at each k, so we need to somehow 'force' the solution to be of the form Eq. (3.4) (say) corresponding to a wave coming from $-\infty$. From the solution we can then read off the scattering amplitudes.

The way to force the solution is to express the wavefunction as

$$\Psi_k(x) = \exp\left(ikx\right) + \Psi_k^{\text{scatt}}(x). \tag{3.17}$$

This defines $\Psi_k^{\text{scatt}}(x)$, the **scattered wave**, as the part of the solution that owes its existence to $V(x)$, and which therefore vanishes as $V(x)$ vanishes. For Eq. (3.4), $\Psi_k^{\text{scatt}}(x)$ has the explicit form

$$\Psi_k^{\text{scatt}}(x) = \begin{cases} r_{\text{LL}} \exp(-ikx) & x \ll 0 \\ (t_{\text{LR}} - 1)\exp(ikx) & x \gg 0 \end{cases}. \tag{3.18}$$

With the definition Eq. (3.17), we can rewrite Eq. (3.16) as

$$\left[E_k + \frac{\hbar^2}{2m}\partial_x^2\right] \Psi_k^{\text{scatt}}(x) = V(x)\Psi_k(x). \tag{3.19}$$

Now let's introduce the *inverse* of the operator on the left hand side. That is, a function satisfying

$$\left[E_k + \frac{\hbar^2}{2m}\partial_x^2\right] G_k(x,x') = \delta(x-x') \tag{3.20}$$

(This is just the Green's function of the operator of the *free* problem, hence the notation). We'll write down $G_k(x,x')$ in a moment, but for now let's use it to rewrite Eq. (3.19) as

$$\Psi_k^{\text{scatt}}(x) = \int dx'\, G_k(x,x')V(x')\Psi_k(x'). \tag{3.21}$$

In terms of $\Psi_k(x)$ this is

$$\Psi_k(x) = \exp(ikx) + \int dx'\, G_k(x,x')V(x')\Psi_k(x'). \tag{3.22}$$

Thus we have passed from a differential equation to an integral equation, known as the **Lippmann–Schwinger equation**. What did we gain by doing this? The point is that once $G_k(x,x')$ is given we have an explicit equation with nothing further to be specified. In particular, there are no boundary conditions that have to be imposed en route to a unique solution, as is the case when we solve a differential equation. This is because the choice of boundary conditions fixes the Green's function uniquely, as we'll see in a moment.

Indeed, the most simple-minded way to go about solving Eq. (3.22) is by iteration

$$\begin{aligned}\Psi_k(x) = \exp(ikx) &+ \int dx'\, G_k(x,x')V(x')\exp\left(ikx'\right) \\ &+ \int dx' dx''\, G_k(x,x')V(x')G_k(x',x'')V(x'')\exp\left(ikx''\right) + \cdots, \end{aligned} \tag{3.23}$$

which generates the **Born series**.

Now let's discuss the Green's function. From Eq. (3.20) we can see that this satisfies the free particle Schrödinger equation with energy E_k when $x \neq x'$. Therefore it has the form

$$G_k(x,x') = \begin{cases} g_+^{<} \exp(ikx) + g_-^{<} \exp(-ikx) & x < x' \\ g_+^{>} \exp(ikx) + g_-^{>} \exp(-ikx) & x > x'. \end{cases} \tag{3.24}$$

To fix the form uniquely we specify:

- $G_k(x,x')$ is continuous at $x = x'$

- At $x = x'$ the derivative jumps

$$\partial_x G_k(x,x')\big|_{x=x'-\epsilon}^{x=x'+\epsilon} = \frac{2m}{\hbar^2}. \tag{3.25}$$

These two conditions follow from the defining Eq. (3.20).

- In order to generate a solution of the form Eq. (3.4), we must have

$$g_+^< = g_-^> = 0, \tag{3.26}$$

which corresponds to only 'outgoing' waves being generated by the scattering potential.

If you are uncomfortable with the solution of a time independent equation being described as coming or going anywhere, don't worry. We'll return to the time dependent view of scattering later.

Imposing these conditions gives

$$G_k^+(x,x') = -i\frac{m}{\hbar^2 k}\exp\left(ik|x-x'|\right). \tag{3.27}$$

We have added a $+$ to indicate this is a *particular* Green's function obeying certain boundary conditions – the reason for this notation will become clear later. Because it enshrines the notion of 'cause' (the scatterer) preceeding 'effect' (the outgoing wave), G_k^+ is called the **retarded** or **causal** Green's function.

We spoke earlier about imposing boundary conditions on the Green's function, but didn't write any explicitly. That's because they look slightly unusual:

$$\lim_{|x-x'|\to\infty}\left[\partial_{|x-x'|} - ik\right] G(x,x') = 0.$$

However, this **radiation condition** has the same content as Eq. (3.26).

Problem 3.4

Solve the Lippmann–Schwinger equation for the case of the δ-function potential and show that the result of Problem 3.1 is reproduced.

TANGENT One dimensional scattering theory is not just pedagogically useful: it also forms a cornerstone of the theory of electrical conduction in nanoscale devices. The idea is that narrow **quantum wires** can act as waveguides for the flow of electrons, quantising the transverse motion and allowing a one dimensional description of the motion along the wire. Scattering is then described by a $2N \times 2N$ scattering matrix, where N is the number of occupied modes, which has the block form

$$S = \begin{pmatrix} r_{\mathrm{LL}} & t_{\mathrm{RL}} \\ t_{\mathrm{LR}} & r_{\mathrm{RR}} \end{pmatrix} \tag{3.28}$$

The N eigenvalues of the transmission matrix $t_{\mathrm{RL}} t_{\mathrm{RL}}^\dagger$ are the **transmission coefficients** T_n ($t_{\mathrm{LR}} t_{\mathrm{LR}}^\dagger$ has the same eigenvalues by unitarity).

By far the most important result here is the **Landauer formula** for the conductance, which gives quantitative form to the idea that *conductance is transmission*

$$G = G_0 \sum_n T_n, \tag{3.29}$$

where $G_0 = 2e^2/h \sim 7.75 \times 10^{-5}\Omega^{-1}$ is the **quantum of conductance**. For much more, see (**?**).

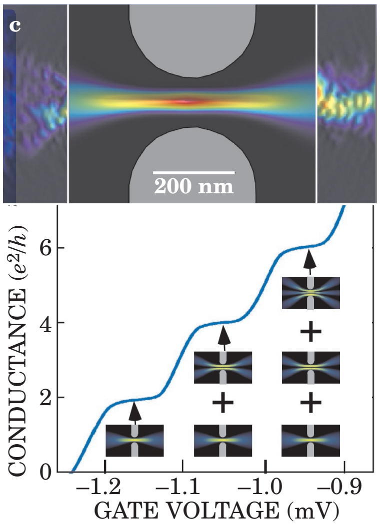

Figure 3.2: (Top) Images (left and right) and simulation (centre) of electron flow in a **quantum point contact**, showing motion confined to a single transverse mode. The experimental images are made using scanning probe microscopy of a two dimensional electron gas in a semiconductor heterostructure. (Bottom) Steps in the conductance as more conduction channels open with changing gate voltage. Images from (**?**).

3.2 *The scattering problem in three dimensions*

We are now ready to begin our assault on three dimensions. We will see that all[2] of the concepts we introduced in studying the one dimensional problem have natural counterparts in 3D.

---

[2] With the exception of the transfer matrix.

The scattering amplitude and cross section

We first seek an analog of Eq. (3.4), in which the wavefunction is written in terms of an incoming plane wave and transmitted and reflected waves. Like Eq. (3.4), its form is fixed by the idea that outside of the interaction region an eigenstate should coincide with a solution of the free particle Schrödinger equation, only deviating from such a solution inside.

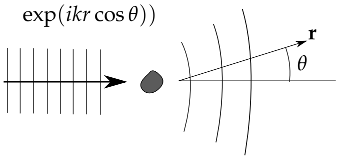

Figure 3.3: Schematic of a scattering experiment. The azimuthal coordinate ϕ corresponds as usual to rotation about the $\theta = 0$ axis.

Let's write down the three dimensional version first, and then spend some time discussing it. Introducing spherical polar coordinates with $\theta = 0$ corresponding to the direction of the incoming wave, we have

$$\boxed{\Psi_k(\mathbf{r}) \xrightarrow[r\to\infty]{} \exp\left(ikz\right) + \frac{f(\theta,\phi)}{r}\exp\left(ikr\right),} \tag{3.30}$$

where $z = r\cos\theta$. The first term represent the incoming plane wave, while the second term is an outgoing scattered wave, which is the reason we have $\exp\left(ikr\right)$ and not $\exp\left(-ikr\right)$.

The main difference from Eq. (3.4) is that Eq. (3.30) is *not* actually a solution of the free particle Schrödinger equation. Rather, it is an *asymptotic* solution, meaning that it comes closer to a solution as $|\mathbf{r}| \to \infty$.

You might argue that Eq. (3.17) is a closer analog of Eq. (3.30) than Eq. (3.4), because of it represents a division into incoming and scattered waves, and we would not disagree. But Eq. (3.17) was defined everywhere, rather than just outside the interaction region. We'll introduce the corresponding expression in the 3D case shortly.

Problem 3.5

Show this. How does the 'correction' required to make Eq. (3.30) a solution decay with r?

Eq. (3.30) amounts to a definition of $f(\theta,\phi)$, which is called the **scattering amplitude**. Note that it has the units of length.

The physical meaning of $f(\theta,\phi)$ can be understood by once again considering the probability current, which in three dimensions has the form

$$\mathbf{j}(\mathbf{r}) = -\frac{i\hbar}{2m}\left[\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right]. \tag{3.31}$$

Calculating the current using Eq. (3.30) gives

$$\mathbf{j}(\mathbf{r}) \xrightarrow[r\to\infty]{} \frac{\hbar k}{m}\left[\hat{\mathbf{z}} + \frac{|f(\theta,\phi)|^2}{r^2}\hat{\mathbf{r}}\right] + \left(\text{cross terms with } \exp\left(\pm ik[r-z]\right) \text{ factors}\right). \tag{3.32}$$

There is also a contribution arising from the angular part of the gradient operator acting on $f(\theta,\phi)$. This contribution decays like $1/r^3$ and will not be important at large distances (it also points perpendicular to $\mathbf{r}$, so doesn't contribute to the outward flux).

The gradient operator in spherical polars is $\nabla = \hat{\mathbf{r}}\partial_r + \frac{\hat{\boldsymbol{\theta}}}{r}\partial_\theta + \frac{\hat{\boldsymbol{\phi}}}{r\sin\theta}\partial_\phi$

But what about the cross terms? The presence of the rapidly oscillating factors $\exp\left(\pm ik[r-z]\right) = \exp\left(\pm ikr[1-\cos\theta]\right)$ means that the average of these terms over some angular range quickly decays to approach zero. Any real detector has some nonzero angular resolution, $\delta\theta$, and since the angular range required to average out the cross terms scales like $1/\left(kr\right)$, they may neglected if the detector is far enough away. Equivalently, provided the spatial extent of the detector $R = r\delta\theta$ is sufficiently large to be able to detect the phase variation of the waves moving in the z direction, i.e. $kR\sin\theta \gtrsim 2\pi$, the detector can discriminate these waves from the scattered waves (which have no phase variation across the detector).

Eq. (3.30) is not normalized. In an infinite system one can normalize states according to the flux they carry. This gives

$$\mathbf{j}(\mathbf{r}) \xrightarrow[r\to\infty]{} j\left[\hat{\mathbf{z}} + \frac{|f(\theta,\phi)|^2}{r^2}\hat{\mathbf{r}}\right]. \tag{3.33}$$

The result is a simple picture of the flow of the probability current due to scattering. The probability per unit time for a *scattered* particle to pass through a solid angle element $d\Omega$ at coordinates (θ,ϕ) is

$$\text{probability / time} = j|f(\theta,\phi)|^2\, d\Omega. \tag{3.34}$$

You might very well ask how a detector would tell the difference between a scattered and an unscattered particle. This is one of the places that the deficiency of our time independent thinking shows up. In the wavepacket viewpoint discussed earlier the incoming wave has both a finite extent parallel and perpendicular to its wavevector. Then the probability of this wave hitting a detector at $\theta \neq 0$ and at a great distance is negligible. Without developing this picture further, Eq. (3.34) will have to remain heuristic.

To define a quantity that depends only on the scatterer, we divide through by the flux. The resulting quantity has the units of area and is called the **differential cross section**

$$\boxed{\frac{d\sigma}{d\Omega}\, d\Omega \equiv \frac{\text{probability / time}}{\text{flux}} = |f(\theta,\phi)|^2\, d\Omega.} \tag{3.35}$$

$\frac{d\sigma}{d\Omega}$ is a function of θ and ϕ, though those arguments are normally omitted because $\frac{d\sigma}{d\Omega}(\theta,\phi)$ looks like a mess. The notation $\frac{d\sigma}{d\Omega}$ is standard, but regrettable: the differential cross section is not the derivative of anything.

You can think of the differential cross section as the area of a wavefront that is 'routed' to the element $d\Omega$. Integrating over all solid angles gives the **total cross section**

$$\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega}\, d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, \frac{d\sigma}{d\Omega} \tag{3.36}$$

The optical theorem

The above picture of the probability current is nice and simple. It is also wrong.

To see that we have a problem, consider integrating the probability current Eq. (3.33) over a sphere centred on the origin. For a stationary state, we should expect to get zero net flux (c.f. Eq. (3.9)). The plane wave contribution, represented by the first term, gives zero, as anything passing in through one hemisphere leaves through the other. So Eq. (3.33) implies

$$\int |f(\theta,\phi)|^2\, d\Omega = \sigma_{\text{tot}} = 0. \tag{3.37}$$

Which doesn't sound good. The problem is that we have been too cavalier with the cross terms in Eq. (3.32). Though it is true that averaging over a small angular range zeroes out these terms when $\theta \neq 0$, $\theta = 0$ has to be treated more carefully. The result will be a relation between σ_{tot} and $f(\theta = 0)$ known as the **optical theorem**.

For a discussion of the history of this theorem, see (**?**), which is where this proof comes from.

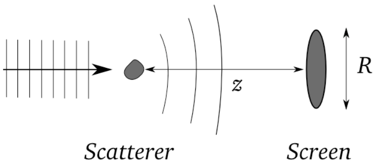

Figure 3.4: Finding the intensity of the wavefunction on a screen.

In Fig. 3.4 we consider again our scattering geometry, only now we erect a circular screen of radius R a distance z away from the scatterer with $z/R \gg 1$, so that the solid angle occupied by the screen as seen from the scatterer is very small.

Using Eq. (3.30), we find the square modulus of the wavefunction to be

$$|\Psi_k(\mathbf{r})|^2 = 1 + \frac{2\,\mathrm{Re}[f(\theta,\phi)e^{ik(r-z)}]}{r} + \frac{|f(\theta,\phi)|^2}{r^2}.$$

When we are far from the scatterer we can evidently neglect the third term relative to the first two. Furthermore

$$r=\sqrt{x^2+y^2+z^2}\sim z+\frac{x^2+y^2}{2z},\qquad z\gg x,y$$

For x, y values on the screen i.e. with $x^2+y^2\leq R^2$, the condition $z/R\gg 1$ allows us to use this approximation, as well as to set $f(\theta,\phi)$ equal to $f(\theta=0)$ (of course, at $\theta=0$ the ϕ variable is redundant). Thus on the screen we can write

$$|\Psi_k(\mathbf{r})|^2\sim 1+\frac{2\,\mathrm{Re}[f(\theta=0)e^{ik(x^2+y^2)/2z}]}{z}$$

Integrating over the screen gives

$$\begin{aligned}\int_{\text{Screen}} dA\,|\Psi_k(\mathbf{r})|^2 &= \int_0^R dr\,2\pi r\left[1+\frac{2\mathrm{Re}[f(\theta=0)e^{ikr^2/2z}]}{z}\right]\\ &= \pi R^2-\frac{4\pi}{k}\,\mathrm{Im}\,f(\theta=0).\end{aligned}\tag{3.38}$$

In the last line we have done the integral in the second term assuming $kR^2/z\gg 1$, which is not inconsistent with the condition $z/R\gg 1$.

Finally we identify the second term, which reduces the value of the integrated probability density below the value πR^2 that we would get if there were no scattering, with the total cross section σ_{tot}. Then we have

$$\sigma_{\text{tot}}=\frac{4\pi}{k}\,\mathrm{Im}\,f(\theta=0),\tag{3.39}$$

which is the optical theorem. This final step may appear confusing: note that we are not calculating a property of the screen (the result comes out to be independent of R) but of the scatterer.

We have considered only the case of *elastic* potential scattering, meaning that the incoming and outgoing energies are identical, and the target is unchanged. In general there will be *inelastic* scattering as well. For example, if the scatterer is an atom it may be ionised in the course of scattering. Then the optical theorem still applies, but with σ_{tot} including all processes, both elastic and inelastic, and $f(\theta=0)$ the purely elastic forward scattering amplitude.

Thus our original expression Eq. (3.33) is not too much in error. The missing contribution that guarantees flux conservation is in the forward direction only. If our detector is off axis, we have nothing to worry about.

The Lippmann–Schwinger equation

Next we turn to the 3D version of the Lippmann–Schwinger equation. In fact, this can be written down without hesitation directly from Eq. (3.22)

$$\Psi_k(\mathbf{r})=\exp(ikz)+\int d\mathbf{r}'\,G_k^+(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\Psi_k(\mathbf{r}').\tag{3.40}$$

It remains only to find the correct form of the retarded Green's function. Recall that this is the function satisfying

$$\left[E_k+\frac{\hbar^2}{2m}\nabla^2\right]G_k^+(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}'),\tag{3.41}$$

and containing only an outward moving wave. Let's write down the answer, and then see why it is correct.

$$G_k^+(\mathbf{r},\mathbf{r}')=-\frac{m}{2\pi\hbar^2}\frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}.\tag{3.42}$$

Do you have trouble remembering the form of the Laplacian in spherical polar coordinates? For the radial part, the following trick is helpful. It's much easier to remember that the radial part of the gradient operator is $\hat{\mathbf{r}}\partial_r$. For $\psi(r)$ and $\varphi(r)$ functions of r only we then have

$$\begin{aligned}\int d\mathbf{r}\,\varphi\left(\nabla^2\psi\right) &= -\int d\mathbf{r}\,(\nabla\varphi)\,(\nabla\psi)\\ &= -\int 4\pi r^2\,\partial_r\varphi\,\partial_r\psi\,dr\\ &= 4\pi\int\varphi\,\partial_r\left(r^2\partial_r\psi\right)\,dr,\end{aligned}$$

assuming boundary terms at infinity vanish in the integrations by parts. Then it's clear that

$$\nabla^2\psi=\frac{1}{r^2}\partial_r\left(r^2\partial_r\psi\right).$$

As in the 1D case, you can verify directly that Eq. (3.42) satisfies the free particle Schrödinger equation when $\mathbf{r} \neq \mathbf{r}'$. To understand the origin of the δ-function, notice that as $\mathbf{r} \to \mathbf{r}'$, the numerator can be neglected and

$$G_k^+ \to -\frac{m}{2\pi\hbar^2}\frac{1}{|\mathbf{r}-\mathbf{r}'|}. \tag{3.43}$$

Now recall that the Green's function for Laplace's equation, satisfying

$$\nabla^2 G_{\mathrm{L}}(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \tag{3.44}$$

is just

$$G_{\mathrm{L}}(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}. \tag{3.45}$$

The E_k term in Eq. (3.41) is not involved in producing the δ-function, and therefore we have verified that Eq. (3.42) does the job.

If you found this a bit slick, a 'constructive' method using the Fourier transform and contour integration is given in the appendix to this chapter.

Now, we would like to be able to check that the solution of the 3D Lippmann–Schwinger equation Eq. (3.40) has the asymptotic behaviour given by Eq. (3.30). To do this, we'll need to investigate the behaviour of the Green's function at large distances. First note that, if $|\mathbf{r}| \gg |\mathbf{r}'|$

$$|\mathbf{r}-\mathbf{r}'| \sim r - \hat{\mathbf{r}}\cdot\mathbf{r}'. \tag{3.46}$$

In the Lippmann–Schwinger equation, the argument $\mathbf{r}'$ is always within the interaction region. This suggests that, as $|\mathbf{r}| \to \infty$, we can replace $G^+(\mathbf{r},\mathbf{r}')$ with

$$G^+(\mathbf{r},\mathbf{r}') \to -\frac{m}{2\pi\hbar^2}\frac{\exp(ikr)}{r}\exp\left(-i\mathbf{k}_{\mathrm{f}}\cdot\mathbf{r}'\right), \tag{3.47}$$

where $\mathbf{k}_{\mathrm{f}} = k\hat{\mathbf{r}}$ is the wavevector of an elastically scattered particle moving in the $\mathbf{r}$ direction. With this replacement, the Lippmann–Schwinger equation becomes

$$\Psi_k(\mathbf{r}) \underset{r\to\infty}{\longrightarrow} \exp(ikz) - \frac{m}{2\pi\hbar^2}\frac{\exp(ikr)}{r}\int d\mathbf{r}' \exp\left(-i\mathbf{k}_{\mathrm{f}}\cdot\mathbf{r}'\right)V(\mathbf{r}')\Psi_k(\mathbf{r}'). \tag{3.48}$$

Comparison with Eq. (3.30) allows us to identify

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int d\mathbf{r}' \exp\left(-i\mathbf{k}_{\mathrm{f}}\cdot\mathbf{r}'\right)V(\mathbf{r}')\Psi_k(\mathbf{r}'). \tag{3.49}$$

By itself, this equation is not very informative, as we still need to know the wavefunction in the interaction region to find $f(\theta,\phi)$, but it's a useful starting point for approximations.

The Born approximation

As we already discussed in Section 3.1, one way to solve the Lippmann–Schwinger equation is by iteration, generating the *Born series* (c.f. Eq. (3.23)). The lowest order approximation amounts to replacing $\Psi_k(\mathbf{r}')$ in Eq. (3.49) with the unscattered plane wave, yielding the **(first) Born approximation** to the scattering amplitude

$$f_{\mathrm{Born}}(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int d\mathbf{r}' \exp\left(-i\mathbf{q}\cdot\mathbf{r}'\right)V(\mathbf{r}'), \tag{3.50}$$

where $\mathbf{q} = \mathbf{k}_\mathrm{f} - \mathbf{k}_\mathrm{i}$ is the **momentum transfer** in the collision. The initial momentum $\mathbf{k}_\mathrm{i} = k\hat{\mathbf{z}}$. If you are wondering where the angles appear on the right hand side: they determine $\mathbf{k}_\mathrm{f}$, which determines $\mathbf{q}$. Eq. (3.50) gives the differential cross section

$$\frac{d\sigma}{d\Omega}_{\text{Born}} = \left| \frac{m}{2\pi\hbar^2} \int d\mathbf{r}' \exp\left(-i\mathbf{q}\cdot\mathbf{r}'\right) V(\mathbf{r}') \right|^2 \tag{3.51}$$

The Born approximation provides a very appealing picture of the relation between the scattering amplitude and the interaction potential: the former is proportional to the Fourier transform of the latter, evaluated at the transferred momentum.

Problem 3.6

Find the scattering amplitude within the lowest Born approximation for the spherical potential

$$V(\mathbf{r}) = \begin{cases} V_0 & |\mathbf{r}| < a_\circ \\ 0 & |\mathbf{r}| > a_\circ \end{cases}. \tag{3.52}$$

The Born approximation relies on $\Psi_k(\mathbf{r})$ being close to a plane wave within the interaction region. By examining the size of the correction in this region, one can obtain the condition

$$V_\mathrm{c} \ll \frac{\hbar^2}{mr_\mathrm{c}^2}, \tag{3.53}$$

For attractive potentials, this means that the potential is much too weak to form a bound state.

at low energies, where V_c and r_c are respectively a characteristic energy and length scale of the potential. Here, low energies means $kr_\mathrm{c} \ll 1$. In the opposite limit, the fast oscillations within the interaction region lead to an additional factor of kr_c, and the condition becomes

$$V_\mathrm{c} \ll kr_\mathrm{c}\frac{\hbar^2}{mr_\mathrm{c}^2}, \tag{3.54}$$

and the Born approximation is *always* satisfied at high enough energies.

The Born approximation can also be derived using Fermi's Golden Rule, applied to the static potential $V(\mathbf{r})$, to compute the rate of scattering between plane wave states $\exp\left(i\mathbf{k}_\mathrm{i}\cdot\mathbf{r}\right)$ and $\exp\left(i\mathbf{k}_\mathrm{f}\cdot\mathbf{r}\right)$ as

$$\Gamma_{\mathrm{i}\to\mathrm{f}} = \frac{2\pi}{\hbar} |\langle \mathbf{k}_\mathrm{f}|V|\mathbf{k}_\mathrm{f}\rangle|^2 \delta(E_{\mathbf{k}_\mathrm{i}} - E_{\mathbf{k}_\mathrm{f}}). \tag{3.55}$$

It is instructive to compare the two derivations.

3.3 *Partial wave analysis*

The picture of scattering in one dimension was greatly simplified for parity symmetric potentials by working with states of definite parity. Instead of having to find a 2×2 unitary scattering matrix we had only to consider phase shifts $\delta_{\text{even,odd}}$ for the two channels. We showed that the wavefunction has the form

$$\Psi_k(|x|\gg 0) = c_{\text{even}}\cos\left(k|x| + \delta_{\text{even}}\right) + \operatorname{sgn}(x)c_{\text{odd}}\cos\left(k|x| + \delta_{\text{odd}}\right). \tag{3.15}$$

An entirely analogous simplification occurs in three dimensions for spherically symmetric potentials $V(\mathbf{r}) = V(r)$ (which are of course quite common!). In this case the relevant symmetry is much larger, corresponding to the continuous group of rotations, rather than the discrete parity transformation. By working in a basis that transforms 'nicely'[3] under rotations, we can obtain scattering channels that decouple from each other. Of course, you are already familiar with such a basis: it is provided by the spherical harmonics $Y_{lm}(\theta, \phi)$.

Time independent scattering states are solutions of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + V(r)\Psi(\mathbf{r}) = E_k\Psi(\mathbf{r}). \tag{3.56}$$

We are going to seek a solution of the form

$$\Psi(\mathbf{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{lm} Y_{lm}(\theta,\phi) R_l(r). \tag{3.57}$$

The terms in the expansion are the **partial waves** that give this technique its name. Substitution in Eq. (3.56) yields an equation for $R_l(r)$

$$\frac{d^2R_l}{dr^2} + \frac{2}{r}\frac{dR_l}{dr} + \left[k^2 - \frac{l(l+1)}{r^2}\right]R_l = \frac{2mV(r)}{\hbar^2}R_l \tag{3.58}$$

The Laplacian can be written

$$\nabla^2 = \frac{1}{r^2}\partial_r\left(r^2\partial_r\right) - \frac{\mathbf{L}^2}{\hbar^2 r^2}$$

where $\mathbf{L} = \mathbf{r}\times\mathbf{p}$ is the orbital angular momentum. It's a useful exercise to check this directly starting from

$$(\mathbf{r}\times\mathbf{p})^2 = x_j p_k x_j p_k - x_j p_k x_k p_j$$

and then using the canonical commutation relations.

The spherical harmonics $Y_{lm}(\theta,\phi)$ are eigenfunctions of $\mathbf{L}^2$ with eigenvalue $\hbar^2 l(l+1)$.

Just as in one dimension, the partial waves must satisfy the free particle Schrödinger equation outside of the interaction region. For the partial waves, the radial part satisfies Eq. (3.58) with zero on the right hand side. Writing $R_l(r) = r_l(kr)$ gives the equation

$$\rho^2\frac{d^2r_l}{d\rho^2} + 2\rho\frac{dr_l}{d\rho} + \left[\rho^2 - l(l+1)\right]r_l = 0. \tag{3.59}$$

The general solution of this equation is a superposition of two solutions $j_l(\rho)$ and $n_l(\rho)$ known as the **spherical Bessel function** and **spherical Neumann function** (of order l) respectively. You can think of these as roughly the 3D versions of the $\sin(kx)$ and $\cos(kx)$ solutions of the free particle Schrödinger equation in 1D. In fact, for $l = 0$, the equation

$$\frac{d^2r_0}{d\rho^2} + \frac{2}{\rho}\frac{dr_0}{d\rho} + r_0 = 0 \tag{3.60}$$

can be simplified by writing $r_0(\rho) = u(\rho)/\rho$ to give

$$u'' + u = 0. \tag{3.61}$$

There is some potential for confusion here. Separating variables to find the eigenvalues of the Laplacian in *cylindrical* coordinates yields plain **Bessel functions** $J_\alpha(\rho)$ (of order α) which satisfy **Bessel's equation**

$$\rho^2 J''_\alpha + \rho J'_\alpha + \left(\rho^2 - \alpha^2\right)J_\alpha = 0.$$

The two are in fact related

$$j_l(\rho) = \sqrt{\frac{\pi}{2\rho}}J_{l+1/2}(\rho)$$

Interestingly, while the Bessel functions are in general not *elementary* functions – meaning that they cannot be built from combinations of exponentials, logs and roots – the spherical Bessel functions are, as Eq. (3.65) makes clear.

Then we have

$$j_0(\rho) = \frac{\sin\rho}{\rho}, \qquad n_0(\rho) = -\frac{\cos\rho}{\rho}. \tag{3.62}$$

Note that $j_0(\rho)$ is finite as $\rho\to 0$, while $n_0(\rho)\to -\rho^{-1}$.

Alternatively, we can work with the **spherical Hankel functions**

$$\begin{aligned} h_l^{(1)}(\rho) &= j_l(\rho) + i n_l(\rho) \\ h_l^{(2)}(\rho) &= \left[h_l^{(1)}(\rho)\right]^* \end{aligned}, \tag{3.63}$$

which play the role of $\exp(\pm ikx)$. For example

$$h_0^{(1)}(\rho) = \frac{\exp(i\rho)}{i\rho}. \tag{3.64}$$

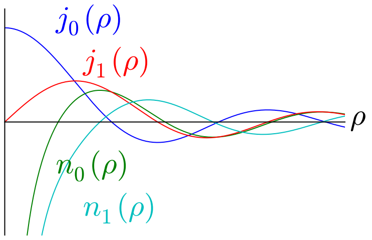

Figure 3.5: The first two spherical Bessel and Neumann functions.

[3] More properly, the basis forms a group *representation*, but more about this in Chapter 6.

PLOUGHING through the properties of these functions can feel like a bit of a mathematical death march. In fact, everything that we will need follows fairly painlessly from **Rayleigh's formulas**

$$\begin{aligned} j_l(\rho) &= (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\sin\rho}{\rho} \\ n_l(\rho) &= -(-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\cos\rho}{\rho} \end{aligned} \tag{3.65}$$

Problem 3.7

Show that these functions satisfy Eq. (3.59).

Let's use these formulas to obtain the behaviour at small and large arguments.

Problem 3.8

Show that the asymptotic behaviour at small arguments is

$$\begin{aligned} j_l(\rho) &\to \frac{\rho^l}{(2l+1)!!} \\ n_l(\rho) &\to -\frac{(2l-1)!!}{\rho^{l+1}} \end{aligned}. \tag{3.66}$$

Hint: Write $\frac{1}{\rho}\frac{d}{d\rho} = 2\frac{d}{du}$ with $u = \rho^2$

A really minimal derivation of this property uses the substitution $r_l(\rho) = u_l(\rho)/\rho$ to write Eq. (3.59) as

$$u_l'' + \left[u - \frac{l(l+1)}{\rho^2}\right] = 0.$$

The series solution then must start with a term ρ^{l+1} or ρ^{-l}.

Problem 3.9

Show that for large arguments

$$\begin{aligned} j_l(\rho) &\to \frac{1}{\rho}\sin\left(\rho - \frac{l\pi}{2}\right) \\ n_l(\rho) &\to -\frac{1}{\rho}\cos\left(\rho - \frac{l\pi}{2}\right) \\ h_l^{(1)}(\rho) &\to -\frac{i}{\rho}\exp\left(i\left[\rho - \frac{l\pi}{2}\right]\right) \end{aligned} . \tag{3.67}$$

Eq. (3.67) substantiate the analogy drawn above between these functions and $\sin(kx)$ and $\cos(kx)$ in one dimension.

NOW, in considering the superposition of $j_l(\rho)$ and $n_l(\rho)$ (or $h_l^{(1)}(\rho)$ and $h_l^{(1)}(\rho)$) that form the partial wave outside of the interaction region, we are going to appeal to the intuition provided by Eq. (3.15). Recall the chain of argument that lead us to this result:

- Conservation of probability flux led to a unitary scattering matrix.
- Finding the scattering channels gave components in which the incoming and outgoing wave are related by the phase shifts, because there is no mixing between channels.

Since we have the scattering channels in the 3D problem, it's hopefully plausible that flux conservation relates the incoming and outgoing waves in these channels by a phase shift only, so that up to an overall factor the partial wave takes the form

It is not a problem that the wavefunction outside the interaction region contains some contribution from the Neumann function, which diverges at the origin. Inside the interaction region the wavefunction has a different form because the potential $V(r)$ is nonzero.

$$h_l^{(1)}(\rho)\exp(i\delta_l)+h_l^{(2)}(\rho)\exp(-i\delta_l)\xrightarrow[r\to\infty]{}\frac{2}{\rho}\sin\left(\rho-\frac{l\pi}{2}+\delta_l\right). \tag{3.68}$$

This defines the phase shifts in the 3D case.

Problem 3.10

Of course that's a bit fluffy. So let's compute the flux through a large sphere of a wave with the general form

$$\Psi(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\theta,\phi)\left[c_{lm}^{\text{out}}h_l^{(1)}(kr)+c_{lm}^{\text{in}}h_l^{(2)}(kr)\right] \tag{3.69}$$

Use the asymptotic form Eq. (3.67) and the orthogonality relation for the spherical harmonics

$$\int d\Omega\, Y_{lm}^{*}(\theta,\phi)Y_{l'm'}(\theta,\phi)=\delta_{ll'}\delta_{mm'}. \tag{3.70}$$

You should find

$$\text{Flux}=\frac{\hbar}{mk}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left[|c_{lm}^{\text{out}}|^2-|c_{lm}^{\text{in}}|^2\right]. \tag{3.71}$$

This calculation is the analogue of that giving Eq. (3.10) in the 1D case.

Expansion of a plane wave

While this is all very nice, real scattering experiments do not involve spherical waves, but a situation closer to that described by our earlier expression

$$\Psi_k(\mathbf{r})\xrightarrow[r\to\infty]{}\exp(ikz)+\frac{f(\theta,\phi)}{r}\exp(ikr). \tag{3.30}$$

We want to connect the two pictures, and ultimately find the relation between the scattering amplitude $f(\theta,\phi)$ and the phase shifts $\{\delta_l\}$.

The first stage in that program is to find an expression for the plane wave in terms of partial waves. Once we have done that, all we need to do is modify the *outgoing* partial waves by appropriate the phase shift.

We write a plane wave in the $+\hat{\mathbf{z}}$ direction as an expansion

$$\exp(ikr\cos\theta)=\sum_{l=0}^{\infty}a_l j_l(kr)P_l(\cos\theta). \tag{3.72}$$

This expansion contains no contribution from the Neumann functions $n_l(kr)$ because these are singular at the origin, and only the $m=0$ spherical harmonics

$$Y_{l0}(\theta,\phi)=\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta) \tag{3.73}$$

by virtue of azimuthal symmetry. The functions $P_l(\cos\theta)$ are l^{th} order polynomials called the **Legendre polynomials**. Now it is straightforward to fix

The Legendre polynomials can be generated from **Rodrigues' formula**

$$P_n(x)=\frac{1}{2^n n!}\frac{d^n}{dx^n}\left(x^2-1\right)^n,$$

from which we see that the coefficient of x^n is $\frac{2n!}{2^n(n!)^2}=\frac{(2n-1)!!}{n!}$. In a moment, we'll use another property: $P_n(1)=1$, which you should also be able to the coefficients, because $P_l(\cos\theta)$ contains only $\cos^p\theta$ for $p \leq l$ and $j_l(kr)$ contains $(kr)^q$ for $q \geq l$ (c.f. Eq. (3.66)). Thus the l^{th} term of the expansion of the left hand side, containing $(kr\cos\theta)^l$, arises only from the l^{th} term of the right hand side,

$$a_l = i^l(2l+1) \tag{3.74}$$

Adding the phase shifts

We write out this plane waves expansion once more, this time in terms of the Hankel functions

$$\exp\left(ikr\cos\theta\right) = \frac{1}{2}\sum_{l=0}^{\infty} i^l\left(2l+1\right)P_l(\cos\theta)\left[h_l^{(1)}(kr) + h_l^{(2)}(kr)\right]. \tag{3.75}$$

How should this expansion be changed to allow for the scattered wave? We already know that the incoming and outgoing waves will be related by the phase shifts δ_l. Now we invoke causality to argue that it must be only the *outgoing* wave that is modfied, and hence

$$\Psi_k(\mathbf{r}) = \frac{1}{2}\sum_{l=0}^{\infty} i^l\left(2l+1\right)P_l(\cos\theta)\left[\exp\left(2i\delta_l\right)h_l^{(1)}(kr) + h_l^{(2)}(kr)\right]. \tag{3.76}$$

The scattered wave can then be found by subtracting off the plane wave contribution. In the asymptotic region where Eq. (3.30) is valid, the yields the desired relation between $f(\theta,\phi)$ and the phase shifts

$$\boxed{f(\theta,\phi) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[\exp\left(2i\delta_l\right)-1\right]P_l(\cos\theta).} \tag{3.77}$$

The hard work is done, but there are a few relations still to work out. The differential cross section is of course $\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2$. We get the total cross section by integrating over solid angles and using the orthogonality relation for the Legendre polynomials.

This is of course just the $m = m' = 0$ case of Eq. (3.70).

$$\int_{-1}^{1} dx\, P_l(x)P_{l'}(x) = \frac{2}{2l+1}\delta_{ll'}, \tag{3.78}$$

to give

$$\boxed{\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l.} \tag{3.79}$$

Because $0 \leq \sin^2\delta_l \leq 1$, the contribution σ_l that each partial wave can make to scattering is limited by

$$\sigma_l \leq \frac{4\pi}{k^2}\left(2l+1\right), \tag{3.80}$$

which is known as the **unitarity bound**, and is saturated for $\delta_l = \left(n+\frac{1}{2}\right)\pi$, for integer n, a situation known as **resonant scattering**.

As a check on the correctness of these formulas, we calculate

$$\operatorname{Im} f(\theta=0) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l = \frac{k\sigma_{\text{tot}}}{4\pi}, \tag{3.81}$$

(We used the property $P_l(1) = 1$) which is the optical theorem. Compared to our earlier proof, this one is limited to the case of spherical symmetry, and doesn't give a clear sense of the underlying physics. On the other hand, it is short.

Problem 3.11

Let's consider the case of the *hard sphere* potential

$$V(\mathbf{r}) = \begin{cases} \infty & r < a_\circ \\ 0 & r > a_\circ \end{cases}, \tag{3.82}$$

which is simple enough to allow explicit solution, at least for the $l = 0$ partial wave.

1. Show that the phase shifts satisfy

$$\frac{j_l(ka_\circ)}{n_l(ka_\circ)} = \tan\delta_l. \tag{3.83}$$

2. Find δ_0 explicitly, and show that at small k

$$\delta_l(k) \to -\frac{(ka_\circ)^{2l+1}}{(2l+1)\left[(2l-1)!!\right]^2}. \tag{3.84}$$

3. Find the low k limit of σ_{tot}.

Problem 3.12

For the spherical potential of Eq. (3.52), show that

$$\delta_0(k) = \arctan\left(\frac{ka_\circ}{k'a_\circ}\tan k'a_\circ\right) - ka_\circ \tag{3.85}$$

where $k' = \sqrt{2m(E - V_0)}/\hbar$. Compare this with the Born approximation result of Problem 3.6.

3.4 *Low energy scattering, bound states and resonances*

The results of Problem 3.11 illustrate an important feature of scattering at low energies: it is dominated by the *s*-wave ($l = 0$) component. To see this more generally, we imagine solving Eq. (3.58) for the radial function $R_l(r)$ from the origin to some point r *outside* of the interaction region, where it can be expressed in terms of $j_l(\rho)$ and $n_l(\rho)$.

Problem 3.13

By matching $R_l(r)$ and $R_l'(r)$ to a linear combination of $j_l(\rho)$ and $n_l(\rho)$, show that the phase shift satisfies

$$\tan\delta_l = \frac{kj_l'(kr) - \gamma j_l(kr)}{kn_l'(kr) - \gamma n_l(kr)} \tag{3.86}$$

where $\gamma = R_l'(r)/R_l(r)$. Deduce that $\delta_l \to k^{2l+1}$ as $k \to 0$.

The low energy behaviour of δ_0 defines a length scale a, called the **scattering length** by

$$\delta_0(k) \xrightarrow[k\to 0]{} -ka. \tag{3.87}$$

Thus, no matter how complicated the scattering potential, the behaviour of the scattering at low energies is characterised by a single number.

To grasp its physical meaning, consider the equation for $R_0(r)$. Making the substitution $R_0(r) = u(r)/r$ once more gives

$$-\frac{\hbar^2}{2m}\partial_r^2 u(r) + V(r)u(r) = E_k u(r). \tag{3.88}$$

This is just the Schrödinger equation for 1D motion. $u(r)$ obeys the boundary condition $u(0) = 0$[4]. Now consider the limit of *zero energy*, when the right hand side of Eq. (3.88) vanishes. Outside of the interaction region the behaviour of $u(r)$ is extremely simple: it is just a straight line

$$u(r) = A(r-a). \tag{3.89}$$

The fact that the intercept with the r axis is identified with the scattering length follows from the form of the $l=0$ partial wave

$$\frac{\sin[kr+\delta_0(k)]}{kr} \xrightarrow[k\to 0]{} 1 - \frac{a}{r}. \tag{3.90}$$

By considering the form of the zero energy wavefunction inside the interaction region, it's not hard to convince yourself that repulsive potentials lead to *positive* scattering lengths, while weak attractive potentials lead to *negative* scattering lengths. However, stronger attraction can lead to a divergence of the scattering length to $-\infty$, followed by a return to positive values.

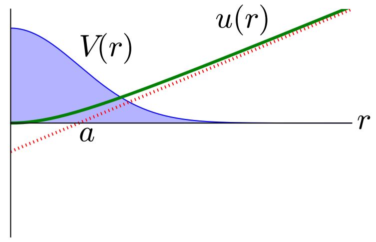

Figure 3.6: Zero energy wavefunction for a repulsive potential, leading to positive scattering length.

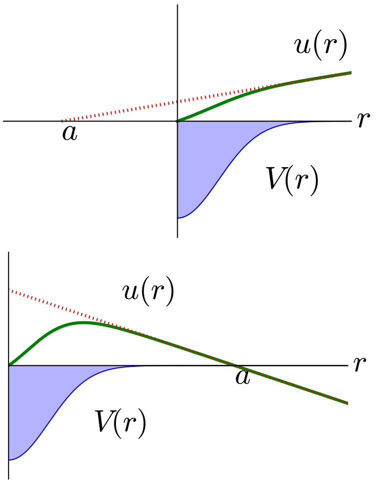

Figure 3.7: (Top) Zero energy wavefunction for an attractive potential, leading to negative scattering length. (Bottom) Stronger attraction leads to a diverging, and then a positive scattering length.

Problem 3.14

Confirm this behaviour of the scattering length for the spherical potential in Problem 3.12.

The divergence of the scattering length coincides with the formation of a bound state. If the (positive) scattering length greatly exceeds the range of the potential, it is possible to relate it to the bound state energy. The bound state wavefunction has the form $u(r) = \exp(-\kappa r)$ outside of the interaction region, and we can identify $\kappa = a^{-1}$. Then

$$E_{\text{bound}} = -\frac{\hbar^2\kappa^2}{2m} \sim -\frac{\hbar^2}{2ma^2} \tag{3.91}$$

TANGENT A somewhat related situation involves **resonant scattering**, in which we 'almost' have a bound state at positive energy (i.e. above the limiting value of $V(\mathbf{r})$ as $|\mathbf{r}| \to \infty$). We can think of this as a bound state $\psi_{\text{res}}(\mathbf{r})$ weakly coupled to the outside world.

Working in one dimension for simplicity, a minimal description of this situation is provided by the **Fano–Anderson model**

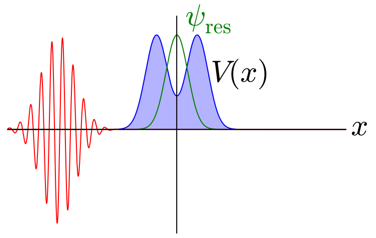

Figure 3.8: Resonant scattering

$$\begin{aligned}-\frac{\hbar^2}{2m}\partial_x^2\Psi(x) + t\delta(x)\psi_{\text{res}} &= E_k\Psi(x)\\ \mathcal{E}_{\text{res}}\psi_{\text{res}} + t\Psi(0) &= E_k\psi_{\text{res}}.\end{aligned} \tag{3.92}$$

---

[4] Why? Think about the kinetic energy.

where δ is a parameter that describes the coupling of the resonant level to the continuum of states in the outside world. The odd solutions are unaffected by the resonant level, as they vanish at the origin. We write the even solutions as

$$\Psi_{\text{even}}(x) = \cos[k|x| + \delta_{\text{even}}(k)] \tag{3.93}$$

The first of Eq. (3.92) tells us that

$$\sin \delta_{\text{even}}(k) = -\frac{mt}{\hbar^2 k}\psi_{\text{res}}. \tag{3.94}$$

After solving the second for ψ_{res} we arrive at

$$\tan \delta_{\text{even}}(k) = \frac{m}{\hbar^2 k}\frac{t^2}{\mathcal{E}_{\text{res}} - E_k}. \tag{3.95}$$

The phase shift increases from 0 to π as we cross the resonance, taking the value $\pi/2$ when $E_k = \mathcal{E}_{\text{res}}$.

Problem 3.15

Show that the reflection probability has the **Breit–Wigner** form

$$|r(k)|^2 = \frac{\gamma^2/4}{(E_k - \mathcal{E}_{\text{res}})^2 + \gamma^2/4} \tag{3.96}$$

for some γ.

3.A *Finding the Green's function*

We promised a more methodical derivation of the Green's function Eq. (3.42). Starting from the defining equation Eq. (3.41)

$$\left[E_k + \frac{\hbar^2}{2m}\nabla^2\right] G_k(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'), \tag{3.41}$$

we find that the Fourier transform

$$G_k(\mathbf{r}, \mathbf{r}') = \int \frac{d\mathbf{q}}{(2\pi)^3}\tilde{G}_k(\mathbf{q}) \exp\left(i\mathbf{q} \cdot [\mathbf{r} - \mathbf{r}']\right) \tag{3.97}$$

satisfies

$$\left[k^2 - \mathbf{q}^2\right] \tilde{G}_k(\mathbf{q}) = \frac{2m}{\hbar^2}. \tag{3.98}$$

The Green's function is then given by the integral

$$\begin{aligned} G_k(\mathbf{r}, \mathbf{r}') &= \frac{2m}{\hbar^2}\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{\exp\left(i\mathbf{q} \cdot [\mathbf{r} - \mathbf{r}']\right)}{k^2 - \mathbf{q}^2} \\ &= \frac{m}{\pi^2\hbar^2|\mathbf{r} - \mathbf{r}'|}\int_0^\infty \frac{\sin q|\mathbf{r} - \mathbf{r}'|}{k^2 - q^2} q\, dq \\ &= \frac{m}{2\pi^2 i\hbar^2|\mathbf{r} - \mathbf{r}'|}\int_{-\infty}^\infty \frac{\exp(iq|\mathbf{r} - \mathbf{r}'|)}{k^2 - q^2} q\, dq, \end{aligned} \tag{3.99}$$

where in the second line we have done the angular integral, and in the third we have extended the integral to whole of the real axis. This is done in order to evaluate using the residue theorem. The integrand has poles at $q = \pm k$, which lie on the integration contour. The residues at these poles are

$$\mp\frac{1}{2}\exp\left(\pm ik|\mathbf{r} - \mathbf{r}'|\right) \text{ at } q = \pm k. \tag{3.100}$$

We close the contour by adding a semicircle 'at infinity' in the upper half plane. **Jordan's lemma** tells us that the integral is unchanged.

Notice that the residue at $q = +k$ corresponds to an *outgoing* wave, while that at $q = -k$ corresponds to an *incoming* wave. As in our treatment of the Airy function in Section 2.5, the physically relevant solution can be selected by choosing the integration contour appropriately. In this case, the retarded Green's function is obtained by including only the pole at $q = +k$.

An alternative to deforming the contour is to add an infinitesimal quantity in the denominator

$$G_k^+(\mathbf{r}, \mathbf{r}') = \frac{m}{2\pi i\hbar^2|\mathbf{r}-\mathbf{r}'|}\int_{-\infty}^{\infty}\frac{\exp(iq|\mathbf{r}-\mathbf{r}'|)}{k^2-q^2+i\epsilon}q\,dq, \tag{3.101}$$

which has the effect of pushing the pole at $q = +k$ up a little bit, and that at $q = -k$ down. Evaluating using the residue theorem gives Eq. (3.42).

Problem 3.16

Verify that Eq. (3.27), the Green's function in 1D, is reproduced correctly by this method.

Propagator and Green's function

Now is a good opportunity to connect the Green's function with the propagator of Chapter 2. Recall that the propagator is defined by

$$\begin{gathered}\left[i\hbar\frac{\partial}{\partial t} - H\right]K(\mathbf{r}, t|\mathbf{r}', t') = i\hbar\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \text{ and}\\ K(\mathbf{r}, t|\mathbf{r}', t') = 0 \text{ for } t < t'.\end{gathered} \tag{2.8}$$

For a time independent Hamiltonian, we can represent the solution as a Fourier integral over angular frequency as

$$K(\mathbf{r}, t|\mathbf{r}', t') = \int_{-\infty}^{\infty}K_\omega(\mathbf{r}|\mathbf{r}')\exp\left(-i\omega\left[t-t'\right]\right)\frac{d\omega}{2\pi}. \tag{3.102}$$

The first part of Eq. (2.8) tells us that $K_\omega(\mathbf{r}|\mathbf{r}')$ satisfies

$$[\hbar\omega - H]\,K_\omega(\mathbf{r}|\mathbf{r}') = i\hbar\delta(\mathbf{r}-\mathbf{r}'). \tag{3.103}$$

Comparison of Eq. (3.103) and Eq. (3.41) suggests that for $H_0 \equiv -\frac{\hbar^2}{2m}\nabla^2$

$$K_\omega(\mathbf{r}|\mathbf{r}') \overset{?}{=} i\hbar G_k(\mathbf{r}, \mathbf{r}') \tag{3.104}$$

with $\frac{\hbar^2k^2}{2m} = \hbar\omega$. But what about the second part of Eq. (2.8)? For $t < t'$ we can, by Jordan's lemma, close the contour of integration in Eq. (3.102) in the upper half plane. If the integrand is analytic in this region, the integral vanishes, as required. From Eq. (3.101), we can see that the '$+i\epsilon$' prescription that we introduced to move the poles in the appropriate way also has the effect of making $G_k^+(\mathbf{r}, \mathbf{r}')$ analytic in the upper half plane of $\omega = \frac{\hbar k^2}{2m}$, so that the Fourier integral over ω has the desired property. Thus we conclude

$$K_\omega(\mathbf{r}|\mathbf{r}') = i\hbar G_k^+(\mathbf{r}, \mathbf{r}'). \tag{3.105}$$

This establishes the connection that we have been using all along between the retarded nature of the propagator (in time) and the fact that $G_k^+(\mathbf{r}, \mathbf{r}')$ contains only outgoing waves.

3.B Formal scattering theory

It is sometimes useful – if only to produce more compact expressions – to write the Lippmann–Schwinger equation in a basis independent, operator form:

$$|\Psi_k\rangle = |\mathbf{k}_\mathrm{i}\rangle + G_k^+ V |\Psi_k\rangle\,, \tag{3.106}$$

where $|\mathbf{k}_\mathrm{i}\rangle$ is a plane wave state describing the incoming particle, and the operator expression for the retarded Green's function is

$$G_k^+ = (E_k - H_0 + i\epsilon)^{-1}\,. \tag{3.107}$$

Here we have used the '$+i\epsilon$' prescription discussed above. The n^{th} order term in the Born series can then be written

$$\langle\mathbf{k}_\mathrm{f}|\,\overbrace{G_k^+ V \cdots G_k^+ V}^{n\text{ times}}\,|\mathbf{k}_\mathrm{i}\rangle\,. \tag{3.108}$$

Using the normalization $\langle\mathbf{r}|\mathbf{k}\rangle = \exp(i\mathbf{k}\cdot\mathbf{r})/(2\pi)^{3/2}$

Translating the formula Eq. (3.49) for the scattering amplitude gives

$$f(\mathbf{k}_\mathrm{f},\mathbf{k}_\mathrm{i}) = -\frac{\sqrt{2\pi}m}{\hbar^2}\langle\mathbf{k}_\mathrm{f}|V|\Psi_k\rangle\,. \tag{3.109}$$

It's convenient to define a **transition operator** T by

$$T|\mathbf{k}_\mathrm{i}\rangle = V|\Psi_k\rangle\,. \tag{3.110}$$

From Eq. (3.106), we see that T obeys the operator equation

$$T = V + VG_k^+ T. \tag{3.111}$$

The scattering amplitude is then given by the matrix elements of the transition operator between initial and final plane wave states

$$f(\mathbf{k}_\mathrm{f},\mathbf{k}_\mathrm{i}) = -\frac{4\pi^2 m}{\hbar^2}\langle\mathbf{k}_\mathrm{f}|T|\mathbf{k}_\mathrm{i}\rangle\,. \tag{3.112}$$

Note that T is not Hermitian by virtue of the '$+i\epsilon$' in the Green's function.

As an illustration of this formalism, consider the following computation

$$\begin{aligned}\langle\Psi_k|V|\Psi_k\rangle &= \langle\Psi_k|T|\mathbf{k}_\mathrm{i}\rangle\\ &= \langle\Psi_k|V|\mathbf{k}_\mathrm{i}\rangle + \langle\Psi_k|VG_k^+T|\mathbf{k}_\mathrm{i}\rangle\\ &= \langle\mathbf{k}_\mathrm{i}|T^\dagger|\mathbf{k}_\mathrm{i}\rangle + \langle\mathbf{k}_\mathrm{i}|T^\dagger G_k^+ T|\mathbf{k}_\mathrm{i}\rangle\end{aligned} \tag{3.113}$$

The left hand side is manifestly real.

Problem 3.17

By taking the imaginary part of the right hand side, show that this yields (yet another) proof of the optical theorem. *Hint*: Use the formula

$$\frac{1}{x+i\epsilon} = \mathcal{P}\frac{1}{x} - i\pi\delta(x) \tag{3.114}$$

where $\mathcal{P}$ denotes the principal value.

3.C *The quantum point contact*

This discussion is based on (**?**).

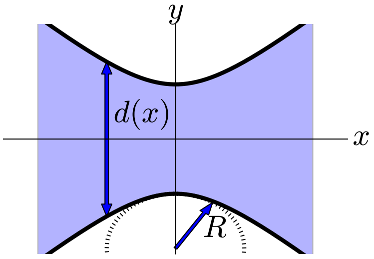

Figure 3.9: Schematic view of a quantum point contact.

The quantum point contact (see Fig. 3.1) is a waveguide with width $d(x)$ varying with position x along the contact. Motion along the contact in the n^{th} transverse mode can be described by the one dimensional Schrödinger equation.

$$\left[-\frac{\hbar^2}{2m}\partial_x^2 + \mathcal{E}_n(x)\right]\Psi(x) = E_k\Psi(x), \tag{3.115}$$

where

$$\mathcal{E}_n(x) = \frac{\hbar^2}{2m}\frac{\pi^2 n^2}{d(x)^2} \tag{3.116}$$

is the transverse quantisation energy at x. Close to the centre of the contact we can write

$$d(x) \sim d_0 + \frac{x^2}{R} \tag{3.117}$$

where R is the radius of curvature of the edge of the waveguide. In this region Eq. (3.115) takes the form

$$\left[-\partial_x^2 - \frac{1}{2}k_n x^2\right]\Psi(x) = \left(k^2 - \frac{\pi^2 n^2}{d_0^2}\right)\Psi(x), \tag{3.118}$$

where

$$k_n = \frac{4\pi^2 n^2}{d_0^3 R} \tag{3.119}$$

Eq. (3.118) is an inverted harmonic oscillator, and is soluble in terms of parabolic cylinder functions. However, there is a way to understand what is going on without getting our hands too dirty. If the energy is large enough, we expect the WKB form of the wavefunction to be valid (see §2.5)

$$\Psi_{\text{WKB}}(x) = \frac{A}{\sqrt{p(x)}}\exp\left(\frac{i}{\hbar}\int^x p(x')dx'\right) + \frac{B}{\sqrt{p(x)}}\exp\left(-\frac{i}{\hbar}\int^x p(x')dx'\right). \tag{3.120}$$

Now recall the trick we used to solve the Landau–Zener problem in Section 1.3. There we used a path in the plane of complex t, the time, on which adiabaticity was not violated to solve a non-adiabatic problem. In exactly the same way, we can use a path in complex x to solve a problem in which the WKB approximation breaks down for real x. In fact, it's more or less the same problem, as the functions $\pm p(x)$ that appear in the exponential are identical to the $E_\pm(t)$ of Eq. (1.66).

The only difference is that the exponential factor analogous to Eq. (1.71) is now the ratio of the reflection to transmission coefficients, because one outgoing wave becomes the other as we pass around the branch point (c.f. Eq. (3.5))

$$\frac{R}{T} = \exp\left(-z_n\pi^2\sqrt{\frac{2R}{d_0}}\right), \qquad z_n = \frac{kd_0}{\pi} - n, \tag{3.121}$$

where in the exponent we have made the simplification $k^2 - \pi^2 n^2/d_0^2 \sim \frac{2\pi n}{d_0}\left(k - \pi n/d_0\right)$ for $k \sim \pi n/d_0$.

Problem 3.18

Verify this.

Using unitarity $T + R = 1$ we can therefore find the reflection coefficient *exactly*

$$R = \frac{1}{1 + \exp\left(z_n \pi^2 \sqrt{\frac{2R}{d_0}}\right)}. \tag{3.122}$$

This shows that even for energies greater than the quantisation energy in the middle of the waveguide there is **overbarrier reflection**, though the effect is small because of the numerical factors in the exponent. This explains the sharp conductance plateaux observed with relatively smooth constrictions (c.f. Fig. 3.1).

4
Second quantization

> Each photon then interferes only with itself. Interference between two different photons never occurs.
>
> Dirac, *Principles of Quantum Mechanics*

Dirac was wrong about this, as we'll see in this chapter.

A system of N particles is described by a wavefunction of N position arguments $\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$. For indistinguishable particles, you will have already met the idea that the wavefunction should be taken to be totally symmetric or totally antisymmetric under exchange of any pair of particles (see **AQP**). We'll review this idea and its consequences in the next section.

The wavefunction language is not a convenient one, however, when we come to discuss the quantum mechanics of a truly macroscopic number of particles. Only in certain special cases can a compact expression for the wavefunction be obtained for an arbitrary number of particles (we'll meet such an example shortly). Even then, evaluating observables typically involves integrals over every particle coordinate: an arduous task. Fortunately, there is a formalism that is well suited to the general case, in which indistinguishability is built in from the outset rather than imposed upon the wavefunction. This formalism is called **second quantization**.

The name is very obscure, but will become a bit clearer later.

4.1 *Quantum indistinguishability: bosons and fermions*

A pair of particles is described by a wavefunction $\Psi(\mathbf{y}, \mathbf{x})$. If the particles are indistinguishable, the associated probability density must be unchanged upon exchange of the positions of any pair[1]

$$|\Psi(\mathbf{y}, \mathbf{x})|^2 = |\Psi(\mathbf{x}, \mathbf{y})|^2. \tag{4.1}$$

More precisely, $\Psi(\mathbf{x}, \mathbf{y})$ and $\Psi(\mathbf{y}, \mathbf{x})$ must correspond to the *same quantum state*, meaning that they can differ only by a (constant) phase

$$\Psi(\mathbf{y}, \mathbf{x}) = e^{i\theta}\Psi(\mathbf{x}, \mathbf{y}).$$

What can we say about θ? Take another two positions $\mathbf{x}'$, and $\mathbf{y}'$, then

$$\Psi(\mathbf{y}', \mathbf{x}') = e^{i\theta}\Psi(\mathbf{x}', \mathbf{y}'),$$

but there's nothing to stop us taking $\mathbf{x} = \mathbf{y}'$, and $\mathbf{y} = \mathbf{x}'$, in which case we can combine these two expressions to give

$$\Psi(\mathbf{x}, \mathbf{y}) = e^{2i\theta}\Psi(\mathbf{x}, \mathbf{y}) \tag{4.2}$$

that is $e^{i\theta} = \pm 1$ and the wavefunction for two particles is either *symmetric* or *antisymmetric*.

[1] This is what we *mean* by indistinguishable.

A more formal approach is to consider the **exchange operator** P_{12} that exchanges the two arguments

$$P_{12}\Psi(\mathbf{x},\mathbf{y}) = \Psi(\mathbf{y},\mathbf{x})$$

which is evidently a linear operator that furthermore squares to give the identity $P_{12}^2 = 1$. The eigenvalues of P_{12} are therefore ± 1, with the corresponding eigenstates being symmetric or antisymmetric respectively.

The exchange operator commutes with the Hamiltonian of a pair of identical particles. As an example, consider the Hamiltonian for a pair of electrons

$$H = -\frac{\hbar^2}{2m_e}\left[\nabla_x^2 + \nabla_y^2\right] + \frac{e^2}{|\mathbf{x}-\mathbf{y}|} \tag{4.3}$$

evidently it doesn't matter whether we apply P_{12} before or after H. Thus $[H, P_{12}] = 0$ and basic ideas of quantum mechanics tell us that

1. Eigenstates of the Hamiltonian have definite exchange symmetry[2].
2. The symmetry of the wavefunction is a constant of the motion.

From two to many

What changes when we consider systems of N identical particles? The wavefunction is now a function of the N coordinates $\Psi(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_N})$, and we can consider an exchange operator P_{ij} that swaps the i^{th} and j^{th} arguments. The same physical reasoning as before singles out eigenstates of the $\{P_{ij}\}$. Note that $[P_{12}, P_{23}] \neq 0$, and thus one might worry whether it is *mathematically* possible to have a simultaneous eigenstate of all the P_{ij}. We see straightaway that a *totally symmetric* state with all eigenvalues equal to $+1$ is allowed. What about a *totally antisymmetric* state with all eigenvalues -1? This too is possible for the following reason. Any given permutation may be written in many different ways as a product of exchanges (see the next problem for an example). For a given permutation, however, these different possibilities either involve only even numbers of exchanges, or only odd numbers, a fact we'll prove below.

Problem 4.1

By showing that $P_{12}P_{23}P_{12} = P_{13} = P_{23}P_{12}P_{23}$ prove that a simultaneous eigenstate of all the P_{ij} must have all eigenvalues $+1$ or all -1, that is, be totally symmetric or totally antisymmetric.

All of this shows that any given species of quantum particle will fall into one of two fundamental classes: symmetric **bosons** and antisymmetric **fermions**, named for Bose and Fermi respectively (the whimsical terminology is Dirac's). The distinction works equally well for composite particles, provide we ignore the internal degrees of freedom and discuss only the center of mass coordinate. All matter in the universe is made up of fermions: electrons, quarks, etc., but you can easily convince yourself that an even number of fermions make a composite boson (e.g. a ^{4}He atom with two electrons, two neutrons and two protons) and an odd number make a composite fermion (^{3}He has one fewer neutron, which in turn is made up of 3 quarks).

Easy for us to say. Here's Dirac again: 'The solution with antisymmetrical eigenfunctions, though, is probably the correct one for gas molecules, since it is known to be the correct one for electrons in an atom, and one would expect molecules to resemble electrons more closely than light-quanta.' (?)

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[2] In a real two-electron system overall antisymmetry is guaranteed by the appropriate choice of spin wavefunction.

If we dealt with *distinguishable* particles, the wavefunction of a pair of particles in states φ_1 and φ_2 would be

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \varphi_1(\mathbf{r}_1)\varphi_2(\mathbf{r}_2). \tag{4.4}$$

Accounting for indistinguishability, we have either

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}[\varphi_1(\mathbf{r}_1)\varphi_2(\mathbf{r}_2) \pm \varphi_2(\mathbf{r}_1)\varphi_1(\mathbf{r}_2)] \tag{4.5}$$

The $1/\sqrt{2}$ yields a normalized wavefunction *if* $\varphi_{1,2}(\mathbf{r})$ are *orthonormal*.

with the upper sign for bosons and the lower for fermions. Note in particular that when $\varphi_1 = \varphi_2$ the fermion wavefunction *vanishes*. This illustrates the **Pauli exclusion principle**, that no two identical fermions can be in the same quantum state. There is no such restriction for bosons.

Problem 4.2

Classically, if you had a function $P_1(\mathbf{r}_1)$ describing the probability density of finding particle 1 at position $\mathbf{r}_1$, and the corresponding quantity for an independent particle 2, you would have no hesitation in concluding that the joint distribution is

$$P_{12}(\mathbf{r}_1,\mathbf{r}_2) = P_1(\mathbf{r}_1)P_2(\mathbf{r}_2). \tag{4.6}$$

This also follows from taking the square modulus of Eq. (4.4). What is the result implied by the wavefunction Eq. (4.5) for a pair of identical bosons or fermions?

Most people find this result rather counterintuitive. It shows that, because probabilities arise from the squares of amplitudes, identical particles in quantum mechanics are never truly independent.

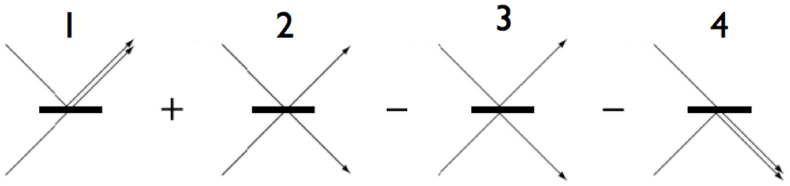

Figure 4.1: Four possible outcomes after the passage of two bosons through a beam splitter.

Problem 4.3

One dramatic illustration of this deviation from our classical intuition is provided by the **Hong–Ou–Mandel** effect in quantum optics (Fig. 4.1). In simplified terms, we imagine wavepackets describing two bosons approaching a 50:50 beam splitter from either side. Because of the unitarity of scattering, the two bosons end up in orthogonal states. For example,

$$\frac{1}{\sqrt{2}}\left(|\text{Left}\rangle \pm |\text{Right}\rangle\right). \tag{4.7}$$

Apply the result of the previous problem to deduce the probabilities of the four possible outcomes.

The Hamiltonian of a system of N identical noninteracting particles is a sum of N identical **single particle** Hamiltonians, that is, with each term acting on a different particle coordinate

$$H = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r_i}) \right] \tag{4.8}$$

where m is the particle mass, and $V(\mathbf{r_i})$ is a potential experienced by the particles. Let's denote the eigenstates of the single particle Hamiltonian by $\{\varphi_\alpha(\mathbf{r})\}$, and the corresponding eigenenergies by $\{E_\alpha\}$, where α is a shorthand for whatever quantum numbers are used to label the states. A set of labels $\{\alpha_i\}$ $i = 1, 2, \ldots N$ tells us the state of each of the particles. Thus we can write an eigenstate of N *distinguishable* particles with energy $E = \sum_{i=1}^{N} E_{\alpha_i}$ as[3]

$$|\Psi_{\alpha_1\alpha_2\cdots\alpha_N}\rangle = \varphi_{\alpha_1}(\mathbf{r_1})\varphi_{\alpha_2}(\mathbf{r_2}) \cdots \varphi_{\alpha_N}(\mathbf{r_N}). \tag{4.9}$$

A general state will be expressed as a superposition of such states, of course. As we've just discussed, however, we should really be dealing with a totally symmetric or totally antisymmetric wavefunction, depending on whether our identical particles are bosons or fermions. To write these down we introduce the operators of *symmetrization* and *antisymmetrization*

$$\mathcal{S} = \frac{1}{N!} \sum_P P, \qquad \mathcal{A} = \frac{1}{N!} \sum_P \operatorname{sgn}(P) P. \tag{4.10}$$

The sums are over all $N!$ permutations of N objects, P denotes the corresponding permutation operator, and $\operatorname{sgn}(P)$ is the **signature** of the permutation, equal to $+1$ for permutations involving an even number of exchanges, and -1 for an odd number. This allows us to write the totally symmetric and totally antisymmetric versions of Eq. (4.9) as

$$\begin{aligned} \left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle &= \sqrt{\frac{N!}{\prod_\alpha N_\alpha!}}\, \mathcal{S}\, \varphi_{\alpha_1}(\mathbf{r_1})\varphi_{\alpha_2}(\mathbf{r_2}) \cdots \varphi_{\alpha_N}(\mathbf{r_N}) \\ \left|\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle &= \sqrt{N!}\, \mathcal{A}\, \varphi_{\alpha_1}(\mathbf{r_1})\varphi_{\alpha_2}(\mathbf{r_2}) \cdots \varphi_{\alpha_N}(\mathbf{r_N}) \end{aligned} \tag{4.11}$$

The normalization factors yield normalized wavefunctions *if* the single particle state $|\varphi_\alpha\rangle$ are orthonormal (as the eigenstates of the single particle Hamiltonian are).

Such states are called **product states**. The normalization factor in the boson case involves the **occupation numbers** $\{N_\alpha\}$ giving the number of particles in state α. In the fermion case each N_α is either 0 or 1 so the prefactor simplifies. Since the order of the α indices is irrelevant in the boson case, and amounts only to a sign in the fermion case, states based on a given set of single particle states are more efficiently labeled by the occupation numbers. In terms of these numbers the total energy is

$$E = \sum_{i=1}^{N} E_{\alpha_i} = \sum_\alpha N_\alpha E_\alpha \tag{4.12}$$

[3] We will frequently switch between the wavefunction ($\varphi(\mathbf{x})$) and bra-ket notation ($|\varphi\rangle$). In the latter notation the product wavefunction in Eq. (4.4) is written $|\varphi_1\rangle\,|\varphi_2\rangle$.

Problem 4.4

Find

1. The totally antisymmetric state of three fermions in states φ_1, φ_2, and φ_3
2. The totally symmetric state of three bosons, with two in state φ_1 and one in state φ_2.

Problem 4.5

Verify that the normalization factors in Eq. (4.11) are correct.

A more formal way of putting things is as follows. We first consider the space spanned by states of the form Eq. (4.9). Then we introduce the operators $\mathcal{S}$ and $\mathcal{A}$, noting that $\mathcal{S}^2 = \mathcal{S}$ and $\mathcal{A}^2 = \mathcal{A}$. In other words, there's no point symmetrizing or antisymmetrizing more than once (we say that the operators are **idempotent**). Any eigenvalue of one of these operators is therefore either one or zero. The states with $\mathcal{S} = 1$ are the symmetric states, and those with $\mathcal{A} = 1$ are antisymmetric. You can easily convince yourself that if a state has one of $\mathcal{S}$ or $\mathcal{A}$ equal to one, the other is zero. This defines symmetric and antisymmetric subspaces, consisting of the admissible boson and fermion wavefunctions.

Note that the fermion wavefunction takes the form of a determinant (usually called a **Slater determinant**[4])

$$\left|\Psi^{A}_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_{\alpha_1}(\mathbf{r_1}) & \varphi_{\alpha_1}(\mathbf{r_2}) & \cdots & \varphi_{\alpha_1}(\mathbf{r_N}) \\ \varphi_{\alpha_2}(\mathbf{r_1}) & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \varphi_{\alpha_N}(\mathbf{r_1}) & \cdots & \cdots & \varphi_{\alpha_N}(\mathbf{r_N}) \end{vmatrix}. \tag{4.13}$$

The vanishing of a determinant when two rows or two columns are identical means that the wavefunction is zero if two particle coordinates coincide ($\mathbf{r}_i = \mathbf{r}_j$), or if two particles occupy the same state ($\alpha_i = \alpha_j$).

TANGENT We pause here to note that the above arguments – which appear in most textbooks in one variant or another – suffer from a deficiency that remained undiscovered until (**?**). The weak point is that nothing requires that the wavefunction of a pair be *single-valued*, as we tacitly assumed in writing Eq. (4.2).

Let's examine the argument a little more closely. Imagine our pair of particles remain always at the same distance from each other, and only relative motion is important. In terms of the unit vector $\mathbf{n} = (\mathbf{x} - \mathbf{y})/|\mathbf{x} - \mathbf{y}|$, an exchange then corresponds to $\mathbf{n} \to -\mathbf{n}$ i.e. tracing a path on the unit sphere that starts and finishes at antipodal points. A double exchange corresponds to a complete circumnavigation. We associate a phase factor $e^{2i\theta}$ with this path. Assuming that this phase is independent of the path, we can now consider contracting this path to nothing, which shows that our original conclusion that $e^{2i\theta} = 1$ is solid.

The situation changes drastically if we consider particles confined to *two* spatial dimensions. Then our double exchange corresponds to going once around a *circle*. Such a path cannot be deformed smoothly to nothing, and as a result $e^{2i\theta}$ can in principle be anything at all. Particles whose statistics lie in this continuum of possibilities between bosons and fermions in two dimensions were dubbed **anyons** by Frank Wilczek (**?**).

Compare this situation with our discussion of Berry's phase in Section 1.4. In that case the phase accumulated *does* depend on the path, because the associated vector potential has a non-zero 'magnetic field'. This has a dynamical effect even for a classical particle. The present discussion is more closely related to the Aharonov–Bohm, which you met briefly in **AQP**, where the particle moves in a region of zero magnetic field.

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[4] Though it appears first in (**?**).

Of course, our world is three dimensional, which seems to make this possibility of limited interest. Even if we happen to confine particles to two dimensions, the fact that they can really move in three means that the original argument applies. This reasoning does not hold, however, for *collective* excitations of a many body system confined to two dimensions. Remarkably, anyonic excitations do in fact occur in the **fractional quantum Hall effect**, a phenomenon observed in two dimensional electron systems in high magnetic fields.

4.2 *Example: particles on a ring*

Let's consider perhaps the simplest many particle system one can think of: non-interacting particles on a ring. If the ring has circumference L, the single particle eigenstates are

$$\varphi_n(x) = \frac{1}{\sqrt{L}}\exp\left(\frac{2\pi i n x}{L}\right), \quad n = 0, \pm 1, \pm 2, \ldots \tag{4.14}$$

with energies $E_n = \frac{h^2 n^2}{2mL^2}$. Let's find the N particle ground state. For bosons every particle is in the state φ_0 with zero energy: $N_0 = N$. Thus (ignoring normalization)

$$\Psi^S(x_1, x_2, \ldots x_N) = 1.$$

That was easy! The fermion case is harder. Since the occupation of each level is at most one, the lowest energy is obtained by filling each level with one particle, starting at the bottom. If we have an odd number of particles, this means filling the levels with $n = -(N-1)/2, -(N-3)/2, \ldots, -1, 0, 1 \ldots (N-1)/2$ (for an even number of particles we have to decide whether to put the last particle at $n = \pm N/2$). Introducing the complex variables $z_i = \exp(2\pi i x_i/L)$, the Slater determinant in Eq. (4.13) becomes

$$\begin{vmatrix} z_1^{-(N-1)/2} & z_2^{-(N-1)/2} & \cdots & z_N^{-(N-1)/2} \\ z_1^{-(N-3)/2} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ z_1^{(N-1)/2} & \cdots & \cdots & z_N^{(N-1)/2} \end{vmatrix}. \tag{4.15}$$

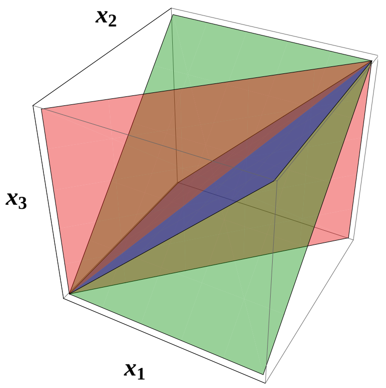

Figure 4.2: Nodal surfaces $x_i = x_j$ for three fermions. Because of the periodic boundary conditions, the three dimensional space of particle coordinates is divided into two regions, corresponding to the even (123, 231, 312) and odd (132, 321, 213) permutations.

Let's evaluate this complicated looking expression in a simple case. With three particles we have

$$\begin{vmatrix} z_1^{-1} & z_2^{-1} & z_3^{-1} \\ 1 & 1 & 1 \\ z_1 & z_2 & z_3 \end{vmatrix} = \frac{z_1}{z_2} - \frac{z_2}{z_1} + \frac{z_3}{z_1} - \frac{z_1}{z_3} + \frac{z_2}{z_3} - \frac{z_3}{z_2} \tag{4.16}$$

$$= \left(\sqrt{\frac{z_3}{z_1}} - \sqrt{\frac{z_1}{z_3}}\right)\left(\sqrt{\frac{z_1}{z_2}} - \sqrt{\frac{z_2}{z_1}}\right)\left(\sqrt{\frac{z_2}{z_3}} - \sqrt{\frac{z_3}{z_2}}\right) \tag{4.17}$$

$$\propto \sin\left(\frac{\pi[x_1 - x_2]}{L}\right)\sin\left(\frac{\pi[x_3 - x_1]}{L}\right)\sin\left(\frac{\pi[x_2 - x_3]}{L}\right). \tag{4.18}$$

The vanishing of the wavefunction when $x_i = x_j$ (see Figure 4.2) is consistent with the Pauli principle. You should check that additionally it is periodic and totally antisymmetric.

Problem 4.6

Show that this generalizes for any (odd) N so that Eq. (4.15) is proportional to

$$\prod_{i<j}^{N} \sin\left(\frac{\pi[x_i - x_j]}{L}\right) \tag{4.19}$$

You will need the **Vandermonde** determinant

$$\begin{vmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & \cdots \\ z_1^2 & z_2^2 & \cdots & \cdots \\ \cdots z_1^{N-1} & z_2^{N-1} & \cdots & z_N^{N-1} \end{vmatrix} = \prod_{i<j}^{N} (z_i - z_j) \tag{4.20}$$

which can be proved in a variety of ways. Proving directly that Eq. (4.19) is an eigenstate of the Hamiltonian is not easy, but can be accomplished using the identity

$$\cot(x-y)\cot(y-z) + \cot(y-z)\cot(z-x) + \cot(z-x)\cot(x-y) = 1. \tag{4.21}$$

Check carefully that Eq. (4.19) is periodic and totally antisymmetric. Note that explicitly finding a totally antisymmetric function of N variables is tantamount to proving the statement of Section 4.1 that a given permutation can be written in terms of only even numbers of exchanges, or only odd numbers, not both.

Let's take the opportunity to introduce some terminology. The wavevector of the last fermion added is called the **Fermi wavevector** and denoted k_F. In this case $k_F = \frac{(N-1)\pi}{L}$. The corresponding momentum $p_F = \hbar k_F$ is the **Fermi momentum**; the corresponding energy $E_F = \frac{\hbar^2 k_F^2}{2m}$ the **Fermi energy**, and so on.

4.3 *Creation and annihilation operators*

We have already gleaned the essential idea of second quantization. Instead of working with totally symmetric or antisymmetric states $\left|\Psi^{S/A}_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle$, we'd rather label states purely by the occupation numbers that describe how particles populate the single particle states. The second quantization formalism is based upon **creation** and **annihilation** operators that add and remove particles from the one particles states, that is, change the occupation numbers N_α[5]. We generally want the number of particles to be conserved, so observables of interest are typically products of equal number of creation and annihilation operators whose overall effect is to redistribute particles among the single particle states. The operators are defined by their effect on the states in Eq. 4.9. A first guess at defining a **creation operator** that puts a particle in state $|\varphi_\alpha\rangle$ would be

$$c_\alpha : |\Psi_{\alpha_1\alpha_2\cdots\alpha_N}\rangle \xrightarrow{?} \sqrt{N+1}\,|\varphi_\alpha\rangle\,|\Psi_{\alpha_1\alpha_2\cdots\alpha_N}\rangle = \sqrt{N+1}\,|\Psi_{\alpha\alpha_1\alpha_2\cdots\alpha_N}\rangle \tag{4.22}$$

(the origin of the $\sqrt{N+1}$ will become clear shortly). This operator acts on a state with N particles and produces one with $N+1$ particles. Since

Formally, the space of distinguishable N particle states is $\mathcal{H}_N = \overbrace{\mathcal{H}_1 \otimes \cdots \mathcal{H}_1}^{\text{n times}}$. The creation operator acts in the space $\mathbb{C} \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots$, or rather the symmetric subspace of this space, which is called (bosonic) **Fock space**.

[5] It is often convenient, but by no means necessary, to chose the single particle states $\{\varphi_\alpha\}$ to be eigenstates of the single particle Hamiltonian, as we did earlier.

any state can be written as a linear combination of the states $\{|\Psi_{\alpha_1\alpha_2\cdots\alpha_N}\rangle\}$, the action of c_α can be extended to any state by linearity. Eq. 4.22 has an obvious shortcoming, however, in that it does not preserve the symmetry of the wavefunction. This is easily remedied by applying the symmetrization operator that we introduced in Eq. 4.10 after adding a particle (we discuss the boson case first), so a better definition is

$$c_\alpha : \left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle \to \sqrt{N+1}\mathcal{S}\,|\varphi_\alpha\rangle \left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle, \quad \text{for bosons.} \tag{4.23}$$

Problem 4.7

Bearing in mind the normalization factors in Eq. 4.11, show that this implies

$$c_\alpha : \left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle \to \sqrt{N_\alpha+1}\left|\Psi^S_{\alpha\alpha_1\alpha_2\cdots\alpha_N}\right\rangle. \tag{4.24}$$

If we label totally symmetric states by their occupation numbers, so that $\left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle = |N_0, N_1 \ldots\rangle$, this equation may be written

$$c_\alpha\,|N_0, N_1, \ldots N_\alpha, \ldots\rangle \to \sqrt{N_\alpha+1}\,|N_0, N_1, \ldots N_\alpha+1, \ldots\rangle\,. \tag{4.25}$$

By considering matrix elements $\langle N_0, N_1, \ldots\,|\,c_\alpha\,|\,N_0', N_1', \ldots\rangle$ we can conclude

$$c_\alpha^\dagger\,|N_0, N_1, \ldots N_\alpha, \ldots\rangle \to \sqrt{N_\alpha}\,|N_0, N_1, \ldots N_\alpha-1, \ldots\rangle\,. \tag{4.26}$$

In other words, the conjugate of the creation operator is a **destruction operator**, that removes one particle from a given state. From Eq. 4.25 and Eq. 4.26 come the fundamental relationships

$$\begin{aligned}\left[c_\alpha^\dagger, c_\beta\right] &= \delta_{\alpha\beta}\\ \left[c_\alpha, c_\beta\right] = \left[c_\alpha^\dagger, c_\beta^\dagger\right] &= 0.\end{aligned} \tag{4.27}$$

For reasons that will become clear shortly we normally write things in terms of the annihilation operator $a_\alpha \equiv c_\alpha^\dagger$, in which case the above takes the form

$$\begin{aligned}\left[a_\alpha, a_\beta^\dagger\right] &= \delta_{\alpha\beta}\\ \left[a_\alpha, a_\beta\right] = \left[a_\alpha^\dagger, a_\beta^\dagger\right] &= 0\end{aligned} \tag{4.28}$$

The same relations describe the ladder operators of a set of independent harmonic oscillators, revealing a deep connection between these two systems. The combination $\mathsf{N}_\alpha \equiv a_\alpha^\dagger a_\alpha$ is called the **number operator** for state α for obvious reasons

$$\mathsf{N}_\alpha\,|N_0, N_1, \ldots N_\alpha, \ldots\rangle = N_\alpha\,|N_0, N_1, \ldots N_\alpha, \ldots\rangle\,. \tag{4.29}$$

From Eq. 4.28 it follows that

$$\begin{aligned}\left[a_\alpha, \mathsf{N}_\alpha\right] &= a_\alpha\\ \left[a_\alpha^\dagger, \mathsf{N}_\alpha\right] &= -a_\alpha^\dagger.\end{aligned} \tag{4.30}$$

You can think of the first of these as 'count then destroy minus destroy then count', for example.

It follows that a normalized state $|\Psi^S_{\alpha_1\alpha_2\ldots\alpha_N}\rangle$ of the many boson system may be written as

$$|N_0, N_1, \ldots\rangle = \frac{\left(a_0^\dagger\right)^{N_0}}{\sqrt{N_0!}} \frac{\left(a_1^\dagger\right)^{N_1}}{\sqrt{N_1!}} \cdots |0, 0, \ldots\rangle \tag{4.31}$$

The state with no particles $|0, 0, \ldots\rangle$ is known as the **vacuum state**. We will often denote it by $|\mathrm{VAC}\rangle$ for brevity. In terms of a wavefunction, you can think of it as equal to 1, so that Eq. 4.23 works out. Alternatively, you can take the relations in Eq. 4.28 as fundamental, in which case $|\mathrm{VAC}\rangle$ has the defining property

$$a_\alpha |\mathrm{VAC}\rangle = 0, \quad \text{for all } \alpha$$

$|\mathrm{VAC}\rangle$ is not to be confused with $|0\rangle$, which will denote the ground state of our many body system with a fixed number of particles.

Now we move on the slightly trickier matter of fermions. Eq. 4.23 suggests that the creation operator should be defined by

$$c_\alpha : \left|\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle \to \sqrt{N+1}\mathcal{A}\,|\varphi_\alpha\rangle \left|\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle, \quad \text{for fermions.} \tag{4.32}$$

For the fermion annihilation operators $a_\alpha = c_\alpha^\dagger$ the result corresponding to Eq. 4.28 is

$$\begin{gathered} \left\{a_\alpha, a_\beta^\dagger\right\} = \delta_{\alpha\beta} \\ \left\{a_\alpha, a_\beta\right\} = \left\{a_\alpha^\dagger, a_\beta^\dagger\right\} = 0 \end{gathered} \tag{4.33}$$

where $\{A, B\} = AB + BA$ denotes the **anticommutator**.

Problem 4.8

Prove this.

Of course, you *could* calculate the commutator, but it proves to be complicated (and uninteresting). The number operators, together with Eq. 4.30 (with commutators!), work as in the boson case. Eq. 4.33 implies that $\left(a_\alpha^\dagger\right)^2 = 0$, so we can't add two particles to the same single particle state, consistent with the Pauli principle. Similarly, since $N_\alpha = 0$ or 1, $\left(a_\alpha\right)^2 = 0$, meaning that we can't remove two particles from the same state.

The state $\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}$ has the representation

$$|N_0, N_1, \ldots\rangle = \left(a_0^\dagger\right)^{N_0} \left(a_1^\dagger\right)^{N_1} \cdots |0, 0, \ldots\rangle, \tag{4.34}$$

which is the same as Eq. 4.31, since $N_\alpha = 0$ or 1 only are allowed.

Note that this equation defines the overall sign of the state $|N_0, N_1, \ldots\rangle$. Two states $\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}$ and $\Psi^A_{\alpha'_1\alpha'_2\cdots\alpha'_N}$ with the same occupation numbers, that is, with $\{\alpha'_n\}$ a permutation of $\{\alpha_n\}$, may differ by a sign depending upon the signature of the permutation.

Suppose we want to move to a different basis of single particle states $\{|\tilde{\varphi}_\alpha\rangle\}$, corresponding to a unitary transformation

$$|\tilde{\varphi}_\alpha\rangle = \sum_\beta \langle \varphi_\beta \,|\, \tilde{\varphi}_\alpha \rangle \, |\varphi_\beta\rangle \,. \tag{4.35}$$

From Eq.s 4.25 and 4.32, the one particle states with the wavefunctions $\{\varphi_\alpha(\mathbf{r})\}$ are just $\{a_\alpha^\dagger |\mathrm{VAC}\rangle\}$. So we see that the above basis transformation gives a new set of creation operators

$$\tilde{a}_\alpha^\dagger \equiv \sum_\beta \langle \varphi_\beta \,|\, \tilde{\varphi}_\alpha \rangle \, a_\beta^\dagger. \tag{4.36}$$

Often we will work in the basis of position eigenstates $\{|\mathbf{r}\rangle\}$. In this case the matrix elements of the unitary transformation are $\langle \varphi_\beta \,|\, \mathbf{r} \rangle = \varphi_\beta^*(\mathbf{r})$, just the complex conjugate of the wavefunction. Denoting the corresponding creation operator (sometimes called **field operator**) as $\psi^\dagger(\mathbf{r})$, Eq. 4.36 becomes

$$\psi^\dagger(\mathbf{r}) \equiv \sum_\beta \varphi^*_\beta(\mathbf{r}) a^\dagger_\beta. \tag{4.37}$$

Now we can see why we chose to work with the annihilation operator rather than the creation operator. The conjugate of Eq. 4.37 is

$$\psi(\mathbf{r}) \equiv \sum_\beta \varphi_\beta(\mathbf{r}) a_\beta, \tag{4.38}$$

and involves the wavefunctions $\varphi_\beta(\mathbf{r})$, rather than their conjugates. The relations satisfied by these operators are easily found from the corresponding relations in Eq. (4.28) and Eq. (4.33), together with the completeness relation

$$\sum_\alpha \varphi^*_\alpha(\mathbf{r}) \varphi_\alpha(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{4.39}$$

We find

$$\begin{aligned} \psi(\mathbf{r})\psi^\dagger(\mathbf{r}') \mp \psi^\dagger(\mathbf{r}')\psi(\mathbf{r}) &= \delta(\mathbf{r}-\mathbf{r}') \\ \psi(\mathbf{r})\psi(\mathbf{r}') \mp \psi(\mathbf{r}')\psi(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}') \mp \psi^\dagger(\mathbf{r}')\psi^\dagger(\mathbf{r}) &= 0 \end{aligned} \tag{4.40}$$

with the upper sign for bosons, and the lower for fermions. Just as the position representation is very one convenient one for quantum states, the position basis creation and annihilation operators provide a convenient basis for many of the many body operators we will encounter.

A compact way of writing creation and annihilation operators without choosing a basis at the outset is to associate an $a_{|\alpha\rangle}$ and $a^\dagger_{|\alpha\rangle}$ with any single particle state $|\alpha\rangle$ and declare the (anti-)commutation relations

$$a_{|\alpha\rangle} a^\dagger_{|\beta\rangle} \mp a^\dagger_{|\beta\rangle} a_{|\alpha\rangle} = \langle\alpha|\beta\rangle .$$

For an orthonormal basis the RHS is $\delta_{\alpha\beta}$.

As an example, let our original basis be the eigenbasis of the free particle Hamiltonian $H = \frac{\mathbf{p}^2}{2m}$ with periodic boundary conditions

$$|\mathbf{k}\rangle = \frac{\exp(i\mathbf{k}\cdot\mathbf{r})}{\sqrt{V}}, \quad \mathbf{k} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right), \quad n_{x,y,z} \text{ integer}, \tag{4.41}$$

with $V = L_x L_y L_z$. The matrix elements of the transformation between this original basis and the position basis $\{|\mathbf{r}\rangle\}$ are $\langle \mathbf{k} \,|\, \mathbf{r}\rangle = \exp(-i\mathbf{k}\cdot\mathbf{r})/\sqrt{V}$, so we have

$$\psi^\dagger(\mathbf{r}) \equiv \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \exp(-i\mathbf{k}\cdot\mathbf{r}) a^\dagger_{\mathbf{k}}, \tag{4.42}$$

and similarly

$$\psi(\mathbf{r}) \equiv \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{r}) a_{\mathbf{k}}. \tag{4.43}$$

TAKING A breath at this point, we can see that the cumbersome basis set $\left\{\left|\Psi^{S/A}_{\alpha 1 \alpha_2 \cdots \alpha_N}\right\rangle\right\}$ has been hidden away behind a much more compact algebra of operators that generates it. Once we figure out how to write physical observables in terms of these operators, we can – if we wish – purge our formalism completely of wavefunctions with N arguments!

Problem 4.9

(**Bogoliubov transformation**) Consider the Hamiltonian

$$H = \epsilon\left(a^\dagger a + b^\dagger b\right) + \Delta\left(a^\dagger b^\dagger + ba\right)$$

This Hamiltonian is slightly unusual, as it doesn't conserve the number of particles.

1. Let's first consider the case of bosons. Then all operators commute except
$$[a, a^\dagger] = [b, b^\dagger] = 1.$$
Define new operators
$$\begin{aligned}\alpha &= a\cosh\kappa - b^\dagger \sinh\kappa \\ \beta &= b\cosh\kappa - a^\dagger \sinh\kappa\end{aligned}$$
for some κ to be determined. Show that α, $\alpha^\dagger$, and β, $\beta^\dagger$ satisfy the same commutation relations.
2. Show that κ can be chosen so that, when written in terms of α and β, there are no 'anomalous' terms in H (i.e. no terms $\alpha\beta$ or $\alpha^\dagger\beta^\dagger$). In this way find the eigenvalues of the Hamiltonian.
3. Now repeat the problem for fermions. The first thing you will need to figure out is what kind of transformation preserves the anticommutation relations.
4. It's natural to expect that, since the algebraic relations are preserved by this transformation, it may be written as a unitary transformation on the operators
$$\begin{aligned}\alpha &= UaU^\dagger \\ \beta &= UbU^\dagger, \qquad U^\dagger = U^{-1}\end{aligned}$$
Show that $U = \exp\left[\kappa\left(a^\dagger b^\dagger - ba\right)\right]$ does the job for both fermions and bosons.

4.4 *Representation of operators*

We now turn to the matter of representing operators of the many particle system in terms of creation and annihilation operators.

One particle operators

A **one particle** operator consists of a sum of terms, one for each particle, with each term acting solely on that particle's coordinate[6]. In the terminology that we introduced in Section , a one-particle operator is a sum of single particle operators, one for each particle. By assumption each term is the same, consistent with the indistinguishability of the particles. We've already met one important example, namely the Hamiltonian for identical noninteracting particles in Eq. 4.8. In general, the action of an operator A on the single particle states may written in terms of the matrix elements

[6] More formally, each term acts on one factor in the product $\mathcal{H}_1 \otimes \cdots \mathcal{H}_1$ of single particle Hilbert spaces.

$\langle \varphi_\alpha | A | \varphi_\beta \rangle$

$$A |\varphi_\beta\rangle = \sum_\alpha |\varphi_\alpha\rangle \langle \varphi_\alpha | A | \varphi_\beta \rangle . \tag{4.44}$$

In words, the action of A is to take the particle from state $|\varphi_\beta\rangle$ to a superposition of states with amplitudes given by the matrix elements $A_{\alpha\beta} \equiv \langle \varphi_\alpha | A | \varphi_\beta \rangle$. Now it's not hard to see that this action can be replicated on the one particle states $a^\dagger_\alpha |\mathrm{VAC}\rangle$ with

$$\hat{A} \equiv \sum_{\alpha,\beta} A_{\alpha\beta} a^\dagger_\alpha a_\beta \tag{4.45}$$

(for the moment we'll use hats for the second quantized operator, but later we'll drop this distinction). To see this, first note that Eq. (4.30) can be generalized to

$$\begin{aligned} \left[a_\alpha, a^\dagger_\beta a_\gamma\right] &= \delta_{\alpha\beta} a_\gamma \\ \left[a^\dagger_\alpha, a^\dagger_\beta a_\gamma\right] &= -\delta_{\alpha\gamma} a^\dagger_\beta . \end{aligned} \tag{4.46}$$

Using the second of these relations, together with the fact that $\hat{A}\,|\mathrm{VAC}\rangle = 0$

$$\begin{aligned} \hat{A}\, a^\dagger_\beta |\mathrm{VAC}\rangle &= \left(\left[\hat{A}, a^\dagger_\beta\right] + a^\dagger_\beta \hat{A}\right) |\mathrm{VAC}\rangle \\ &= \sum_\alpha A_{\alpha\beta} a^\dagger_\alpha |\mathrm{VAC}\rangle , \end{aligned} \tag{4.47}$$

which is precisely Eq. (4.44).

Problem 4.10

Show that on 2 particle states $\hat{A}$ acts in the following way

$$\begin{aligned} \hat{A} \left|\Psi^{S/A}_{\alpha\beta}\right\rangle = \mathcal{N}_{\alpha\beta} \sum_\gamma \Big(& A_{\gamma\alpha} \mathcal{N}^{-1}_{\gamma\beta} \left|\Psi^{S/A}_{\gamma\beta}\right\rangle \\ & + A_{\gamma\beta} \mathcal{N}^{-1}_{\gamma\alpha} \left|\Psi^{S/A}_{\alpha\gamma}\right\rangle \Big) \end{aligned} \tag{4.48}$$

where

$$\mathcal{N}^{-1}_{\alpha\beta} = \begin{cases} 1 & \alpha \neq \beta \\ \sqrt{2} & \alpha = \beta \end{cases} \tag{4.49}$$

Notice that $\hat{A}$ *looks* formally like the expectation value of A in a single particle state $\sum_\alpha a_\alpha |\varphi_\alpha\rangle$. The difference, of course, is that the a_α in $\hat{A}$ are operators, so that the order is important, while those in the preceding expression are amplitudes. The replacement of amplitudes, or wavefunctions, by operators is the origin of the rather clumsy name 'second quantization', which is traditionally introduced with the caveat that what we are doing is not in any way 'more quantum' than before.

To repeat the above prescription for emphasis: *A one particle operator $\hat{A}$ has a second quantized representation formally identical to the expectation value of its single particle counterpart A.*

This probably all looks a bit abstract, so let's turn to a one particle operator that we have already met, namely the noninteracting Hamiltonian in Eq. (4.8). According to the above prescription, this should have the second quantized form

$$\hat{H} \equiv \sum_{\alpha,\beta} \langle \varphi_\alpha | H | \varphi_\beta \rangle a^\dagger_\alpha a_\beta , \tag{4.50}$$

where H is the single particle Hamiltonian $H = -\frac{\hbar^2}{2m}\nabla_i^2 + V(\mathbf{r_i})$. This takes on a very simple form if the basis $\{|\varphi_\alpha\rangle\}$ is just the eigenbasis of this Hamiltonian, in which case $\langle \varphi_\alpha \mid H \mid \varphi_\beta \rangle = E_\alpha \delta_{\alpha\beta}$ and

$$\hat{H} \equiv \sum_\alpha E_\alpha a_\alpha^\dagger a_\alpha = \sum_\alpha E_\alpha \mathsf{N}_\alpha. \tag{4.51}$$

Evidently this is correct: the eigenstates of this operator are just the N particle basis states $\left|\Psi^{S/A}_{\alpha 1 \alpha_2 \cdots \alpha_N}\right\rangle$, and eigenvalues coincide with Eq. (4.12).

Alternatively, we can look at things in the position basis. By recalling how the expectation value of the Hamiltonian looks in this basis, we come up with

$$\begin{aligned}\hat{H} &= \int d\mathbf{r}\left[-\frac{\hbar^2}{2m}\psi^\dagger(\mathbf{r})\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\right] \\ &= \int d\mathbf{r}\left[\frac{\hbar^2}{2m}\nabla\psi^\dagger(\mathbf{r})\cdot\nabla\psi(\mathbf{r}) + V(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\right],\end{aligned} \tag{4.52}$$

where in the second line we have integrated by parts, assuming that boundary terms at infinity vanish. The equality of (4.52) and (4.51) may be seen by using Eq. (4.38).

The Heisenberg equation of motion corresponding to Eq. (4.52) is

$$\begin{aligned} i\hbar\partial_t\psi(\mathbf{r},t) &= -\left[\hat{H},\psi(\mathbf{r},t)\right] \\ &= -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r})\psi(\mathbf{r},t),\end{aligned} \tag{4.53}$$

which is the time-dependent Schrödinger equation but for the *field operator*!

As a second example, consider the particle density. This is not something that one encounters very often in few particle quantum mechanics, but is obviously an observable of interest in an extended system of many particles. The single particle operator for the density at $\mathbf{x}$ is

$$\rho(\mathbf{x}) \equiv \delta(\mathbf{x}-\mathbf{r}). \tag{4.54}$$

This may look like a rather strange definition, but its expectation value on a single particle state $\varphi(\mathbf{r})$ is just $\rho(\mathbf{x}) = |\varphi(\mathbf{x})|^2$, which is just the probability to find the particle at $\mathbf{x}$. Following our prescription, the second quantized form of the operator is then

$$\hat{\rho}(\mathbf{x}) \equiv \psi^\dagger(\mathbf{x})\psi(\mathbf{x}). \tag{4.55}$$

As a check, integrating over position should give the total number of particles

$$\hat{N} = \int d\mathbf{x}\,\psi^\dagger(\mathbf{x})\psi(\mathbf{x}) = \sum_\alpha a_\alpha^\dagger a_a = \sum_\alpha \mathsf{N}_\alpha, \tag{4.56}$$

as it does! Another useful thing to know is the expectation value of the density on a basis state $|N_0, N_1 \ldots\rangle$

$$\langle N_0, N_1 \ldots \mid \hat{\rho}(\mathbf{r}) \mid N_0, N_1 \ldots\rangle = \sum_\alpha N_\alpha \left|\varphi_\alpha(\mathbf{r})\right|^2 \tag{4.57}$$

which is most easily proved by substituting the representation (4.38). This seems like a very reasonable generalization of the single particle result: the density is given by sum of the probability densities in each of the constituent single particle state, weighted by the occupancy of the state. Note that the symmetry of the states played no role here.

As a final example of a one particle operator, the particle current has the second quantized form

$$\hat{\mathbf{j}}(\mathbf{r}) = -i\frac{\hbar}{2m}\left[\psi^\dagger(\mathbf{r})\left(\nabla\psi(\mathbf{r})\right) - \left(\nabla\psi^\dagger(\mathbf{r})\right)\psi(\mathbf{r})\right]. \tag{4.58}$$

Often we consider the Fourier components of the density or current

$$\begin{aligned}\hat{\rho}_{\mathbf{q}} &\equiv \int d\mathbf{r}\,\hat{\rho}(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}} = \sum_{\mathbf{k}} a^\dagger_{\mathbf{k}-\mathbf{q}/2}a_{\mathbf{k}+\mathbf{q}/2} \\ \hat{\mathbf{j}}_{\mathbf{q}} &\equiv \int d\mathbf{r}\,\hat{\mathbf{j}}(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}} = \sum_{\mathbf{k}} \frac{\mathbf{k}}{m} a^\dagger_{\mathbf{k}-\mathbf{q}/2}a_{\mathbf{k}+\mathbf{q}/2}.\end{aligned} \tag{4.59}$$

The $\mathbf{q} = 0$ modes are just the total particle number and $\frac{1}{m}$ times the total momentum, respectively.

Problem 4.11

The operator for the density of spin of a system of spin-1/2 fermions is

$$\mathbf{S}(\mathbf{r}) = \frac{1}{2}\sum_{s,s'}\psi^\dagger_s(\mathbf{r})\sigma_{ss'}\psi_{s'}(\mathbf{r}),$$

where $\sigma = (\sigma_x, \sigma_y, \sigma_x)$ are the Pauli matrices and $\psi^\dagger(\mathbf{r})$, $\psi(\mathbf{r})$ satisfy

$$\{\psi_s(\mathbf{r}), \psi^\dagger_{s'}(\mathbf{r}')\} = \delta_{ss'}\delta(\mathbf{r}-\mathbf{r}').$$

1. Find the commutation relations $[S_i(\mathbf{r}), S_j(\mathbf{r}')]$.
2. For the Hamiltonian

   $$H = \frac{\hbar^2}{2m}\sum_s \int d^3\mathbf{r}\,\nabla\psi^\dagger_s\nabla\psi_s$$

   find the form of the Heisenberg equation of motion

   $$\partial_t\mathbf{S}(\mathbf{r},t) = i[H, \mathbf{S}(\mathbf{r},t)]/\hbar.$$

   Interpret your result.

Single particle density matrix

We can also define a quantity, whose usefulness will become apparent as we go on, called the **single particle density matrix**

$$g(\mathbf{r},\mathbf{r}') \equiv \left\langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}')\right\rangle \tag{4.60}$$

Notice that $g(\mathbf{r},\mathbf{r}) = \langle\hat{\rho}(\mathbf{r})\rangle$. It may not be immediately obvious what this has to do with the density matrices of Chapter 5. However, in terms of the many body wavefunction $\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ we have

$$g(\mathbf{r},\mathbf{r}') = N\int d\mathbf{r}_2\cdots d\mathbf{r}_N\,\Psi^*(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)\Psi(\mathbf{r}', \mathbf{r}_2, \ldots, \mathbf{r}_N). \tag{4.61}$$

In other words, $g(\mathbf{r},\mathbf{r}')$ arises from the N particle pure state density matrix $\rho_N = |\Psi\rangle\langle\Psi|$ by 'tracing out' $N-1$ particle coordinates.

A slight generalization of the above calculation for the density gives for the state $|N_0, N_1 \ldots\rangle$

$$g(\mathbf{r},\mathbf{r}') = \sum_\alpha N_\alpha \varphi^*_\alpha(\mathbf{r})\varphi_\alpha(\mathbf{r}'). \tag{4.62}$$

Let's evaluate this for the ground state of noninteracting Fermi gas. Recall that in this case $N_\mathbf{k} = 1$ for $|\mathbf{k}| < k_F$, and 0 otherwise. Thus we have

$$\begin{aligned} g(\mathbf{r},\mathbf{r}') = \frac{1}{V}\sum_{|\mathbf{k}|<k_F} e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} &= \int_{|\mathbf{k}|<k_F} \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} \\ &= \frac{k_F^3}{2\pi^2}\left[\frac{\sin\left(k_F|\mathbf{r}'-\mathbf{r}|\right)}{(k_F|\mathbf{r}'-\mathbf{r}|)^3} - \frac{\cos\left(k_F|\mathbf{r}'-\mathbf{r}|\right)}{(k_F|\mathbf{r}'-\mathbf{r}|)^2}\right]. \end{aligned} \tag{4.63}$$

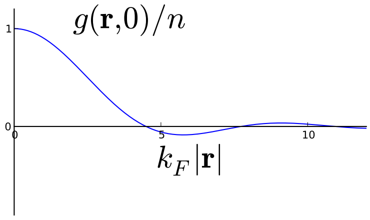

Figure 4.3: Single particle density matrix for the Fermi gas.

Note that $g(\mathbf{r},\mathbf{r}) = \frac{k_F^3}{6\pi^2} = n$, as it should (see your condensed matter course for the relation between density and Fermi wavevector). Also, $g(\mathbf{r},\mathbf{r}') \to 0$ as $|\mathbf{r}-\mathbf{r}'| \to \infty$.

Correlation functions

We are now going to drop the hats for second quantized operators: the distinction is no longer important.

The function $g(\mathbf{r},\mathbf{r}')$ appears as an ingredient in many calculations. As an example, let's consider the **density-density correlation function**. This is defined as

$$C_\rho(\mathbf{r},\mathbf{r}') \equiv \langle : \rho(\mathbf{r})\,\rho(\mathbf{r}') : \rangle. \tag{4.64}$$

Sandwiching operators between colons denotes the operation of **normal ordering**, meaning that we write the constituent creation and annihilation operators so that all annihilation operators stand to the right of all creation operators. In the case of fermions we include the signature of the permutation (the sign that tells us whether the permutation corresponding to our rearrangement is even or odd). Thus

$$a_\alpha a^\dagger_\beta = \delta_{\alpha\beta} \pm a^\dagger_\beta a_\alpha, \text{ while } : a_\alpha a^\dagger_\beta := \pm a^\dagger_\beta a_\alpha,$$

with the upper sign for bosons, and the lower for fermions.

In the present case you can easily convince yourself that

$$\langle \rho(\mathbf{r})\,\rho(\mathbf{r}')\rangle = \langle : \rho(\mathbf{r})\,\rho(\mathbf{r}') : \rangle + \delta(\mathbf{r}-\mathbf{r}')\,\langle \rho(\mathbf{r})\rangle. \tag{4.65}$$

Before ploughing on, let's first motivate the above definition. Imagine dividing space into a fine lattice of cubic sites, such that the probability of finding two particles inside one cube can be neglected. This means that the cube should have linear dimension much smaller than the interparticle spacing. We denote by N_i the number of particles in cube i, centered at $\mathbf{r}_i$. Of course

$$N_i = \int_{\text{cube } i} d\mathbf{r}\,\rho(\mathbf{r}). \tag{4.66}$$

Since N_i is only 0 or 1 by assumption, the probability of cube i being occupied is

$$P(\text{cube } i \text{ occupied}) = \langle N_i \rangle,$$

that is, the mean occupancy. Likewise the probability of having cubes i and j occupied is

$$P(i \text{ and } j \text{ occupied}) = \langle N_i N_j \rangle = \int_{\text{cube } i} d\mathbf{r} \int_{\text{cube } j} d\mathbf{r}'\, \langle \rho(\mathbf{r})\,\rho(\mathbf{r}')\rangle.$$

This tells us that $\langle \rho(\mathbf{r})\, \rho(\mathbf{r}') \rangle$ is equal to the joint probability density of finding a pair of particles at $\mathbf{r}$ and $\mathbf{r}'$, but this interpretation only works for $\mathbf{r} \neq \mathbf{r}'$, since for $i = j$

$$\left\langle N_i N_j \right\rangle = \left\langle N_i^2 \right\rangle = \langle N_i \rangle ,$$

which shows that $\langle \rho(\mathbf{r})\, \rho(\mathbf{r}') \rangle$ always has an additional contribution $\delta(\mathbf{r} - \mathbf{r}')\, \langle \rho(\mathbf{r}) \rangle$, determined by the mean density. Eq. (4.65) shows that normal ordering automatically removes this piece. Why? Imagine removing particles at $\mathbf{r}$ and $\mathbf{r}'$ by applying the product of annihilation operator $\psi(\mathbf{r})\psi(\mathbf{r}')$ to the original state, call it $|\Psi\rangle$. This has the effect of picking out that part of the wavefunction where two particles are localized at these positions. The probability (density) of finding two particles at these locations is then the squared modulus of the resulting state, that is

$$\| \psi(\mathbf{r})\psi(\mathbf{r}')\, |\Psi\rangle \, \|^2 = \left\langle \psi^\dagger(\mathbf{r}')\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\psi(\mathbf{r}') \right\rangle , \tag{4.67}$$

which is just the normal ordered form $\langle : \rho(\mathbf{r})\, \rho(\mathbf{r}') : \rangle$!

With the physical meaning of $C_\rho(\mathbf{r}, \mathbf{r}')$ established, let's proceed to the calculation. As in the derivation of Eq. (4.57), we substitute the representation (4.38) to give

$$\left\langle \rho(\mathbf{r})\, \rho(\mathbf{r}') \right\rangle = \sum_{\alpha,\beta,\gamma,\delta} \varphi^*_\alpha(\mathbf{r})\varphi_\beta(\mathbf{r})\varphi^*_\gamma(\mathbf{r}')\varphi_\delta(\mathbf{r}') \left\langle a^\dagger_\alpha a_\beta a^\dagger_\gamma a_\delta \right\rangle . \tag{4.68}$$

If we are considering the expectation in a state of the form $|N_0, N_1, \ldots\rangle$, we can see that an annihilation operator for a given single particle state must be accompanied by a creation operator for the same state. There are therefore two possibilities

$$\begin{aligned} &\alpha = \beta,\ \gamma = \delta,\ \text{or} \\ &\alpha = \delta,\ \beta = \gamma, \end{aligned}$$

which give rise to two groups of terms. The first contains the average $\left\langle a^\dagger_\alpha a_\alpha a^\dagger_\gamma a_\gamma \right\rangle = N_\alpha N_\gamma$, while the second involves

$$\left\langle a^\dagger_\alpha a_\gamma a^\dagger_\gamma a_\alpha \right\rangle = N_\alpha (1 \pm N_\gamma).$$

Here we have used

$$\begin{aligned} a^\dagger_\alpha a_\alpha &= \mathsf{N}_\alpha \\ a_\gamma a^\dagger_\gamma &= 1 \pm a^\dagger_\gamma a_\gamma = 1 \pm \mathsf{N}_\gamma . \end{aligned} \tag{4.69}$$

Overall we have[7]

$$\begin{aligned} \left\langle \rho(\mathbf{r})\, \rho(\mathbf{r}') \right\rangle = &\sum_{\alpha,\gamma} \varphi^*_\alpha(\mathbf{r})\varphi_\alpha(\mathbf{r})\varphi^*_\gamma(\mathbf{r}')\varphi_\gamma(\mathbf{r}') N_\alpha N_\gamma \\ &+ \sum_{\alpha,\gamma} \varphi^*_\alpha(\mathbf{r})\varphi_\gamma(\mathbf{r})\varphi^*_\gamma(\mathbf{r}')\varphi_\alpha(\mathbf{r}') N_\alpha (1 \pm N_\gamma). \end{aligned} \tag{4.70}$$

This illustrates a general result – known as **Wick's theorem** – that expectation values in a state $|N_0, N_1, \ldots\rangle$ can be computed by pairing the indices of creation and annihilation operators in all possible ways and using Eq. (4.69).

Using the completeness relation Eq. (4.39) the above result can be written

$$\left\langle \rho(\mathbf{r})\, \rho(\mathbf{r}') \right\rangle = \delta(\mathbf{r} - \mathbf{r}')\, \langle \rho(\mathbf{r}) \rangle + \langle \rho(\mathbf{r}) \rangle \, \langle \rho(\mathbf{r}') \rangle \pm g(\mathbf{r}, \mathbf{r}') g(\mathbf{r}', \mathbf{r}). \tag{4.71}$$

[7] You might notice that this expression does not handle the case $\alpha = \beta = \gamma = \delta$ correctly in the case of bosons. In the limit of a large system this does not matter (consider the case of properly normalized plane waves if you are not sure).

or

$$C_\rho(\mathbf{r},\mathbf{r}') = \langle\rho(\mathbf{r})\rangle\langle\rho(\mathbf{r}')\rangle \pm g(\mathbf{r},\mathbf{r}')g(\mathbf{r}',\mathbf{r}). \tag{4.72}$$

For the fermion case, we see that the correlation function vanishes as the separation $|\mathbf{r}-\mathbf{r}'| \to 0$, because $g(\mathbf{r},\mathbf{r}) = \langle\rho(\mathbf{r})\rangle$ (Figure 4.4). This is, of course, another manifestation of the exclusion principle: it is not possible for two fermions to sit on top of each other. The scale of the 'hole' in the correlation function (**anti-bunching**) is of course set by the mean interparticle separation, which is to say the Fermi wavelength.

For bosons the situation is very different. If $g(\mathbf{r},\mathbf{r}') \to 0$ as $|\mathbf{r}-\mathbf{r}'| \to \infty$, the value of the correlation function as $|\mathbf{r}-\mathbf{r}'| \to 0$ is *twice* the value at $|\mathbf{r}-\mathbf{r}'| \to \infty$. This characteristic behavior is often termed **bunching**: a pair of bosons is more likely to be found at two nearby points than at two distant points.

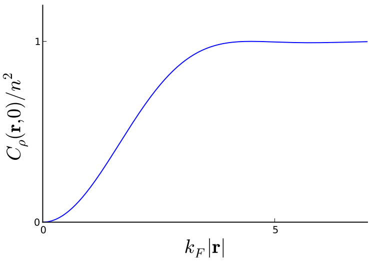

Figure 4.4: Density correlation function for the Fermi gas.

Note when we have a Bose condensate $g(\mathbf{r},\mathbf{r}')$ tends to a finite value as $|\mathbf{r}-\mathbf{r}'| \to \infty$.

Problem 4.12

Re-derive Eq. (4.71) by starting from the many-body wavefunction of the ground state (that is the totally symmetric or antisymmetric function $\Psi^{S/A}_{\alpha_1\alpha_2\cdots\alpha_N}(\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_N)$). Remember that in the first quantized representation, the density operator is $\rho(\mathbf{x}) = \sum_i^N \delta(\mathbf{x}-\mathbf{r}_i)$.

Two particle operators and interactions

A **two particle** operator consists of a sum of terms acting pairwise on the particles. The most important example of such an operator is that describing the potential energy of interaction between pairs of particles

$$H_{\text{int}} = \sum_{i<j}^{N} U(\mathbf{r}_i - \mathbf{r}_j). \tag{4.73}$$

Here $U(\mathbf{r}-\mathbf{r}')$ is the potential energy of a pair of particles at positions $\mathbf{r}$ and $\mathbf{r}'$, and the sum ensures that we count each *pair* of particles once. Recalling the form of the density operator in the first quantized representation: $\rho(\mathbf{x}) = \sum_i^N \delta(\mathbf{x}-\mathbf{r}_i)$, we see that

$$H_{\text{int}} \overset{?}{=} \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\,\rho(\mathbf{r})U(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}') \tag{4.74}$$

almost replicates Eq. (4.73). This expression is familiar from electrostatics, where it represents the electric potential energy of a continuous charge distribution, with $U(\mathbf{r}-\mathbf{r}')$ the Coulomb potential. The factor of $\frac{1}{2}$ ensures that we only sum over each pair once. The problem with Eq. (4.74), however, is that it includes the terms with $i = j$ that are excluded from Eq. (4.73), that is, it allows a particle to interact with itself! From Problem 4.12 you will recall that it is precisely these terms that are responsible for generating the δ-function contribution to Eq. (4.71). Here, as before, the remedy is to normal order the operators

$$H_{\text{int}} = \frac{1}{2}\int d\mathbf{r}\,d\mathbf{r}'\ :\rho(\mathbf{r})U(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}'): = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\,\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}). \tag{4.75}$$

After doing so, it is clear that at least two particles, rather than one, are required for the interaction energy to be non-vanishing. The removal of these 'self-interaction' terms was of particular importance historically. The divergent 'self-energy' of the electron, due to the singular nature of the Coulomb interaction, was an entrenched difficulty of the classical theory. Jordan and Klein (**?**), who pioneered the modern form of second quantization for bosons[8], saw the existence of the above simple prescription in quantum mechanics as a particular benefit. We have taken the more usual modern approach (in nonrelativistic physics) of assuming interactions between pairs only at the outset.

Using Eq. (4.72) we can immediately write down the expectation value of H_{int} in a state $|N_0, N_1, \ldots\rangle$

$$\langle H_{\text{int}}\rangle = \frac{1}{2}\int d\mathbf{r}\,d\mathbf{r}'\,\langle\rho(\mathbf{r})\rangle U(\mathbf{r}-\mathbf{r}')\langle\rho(\mathbf{r}')\rangle \pm \frac{1}{2}\int d\mathbf{r}\,d\mathbf{r}'\,U(\mathbf{r}-\mathbf{r}')g(\mathbf{r},\mathbf{r}')g(\mathbf{r}',\mathbf{r}) \tag{4.76}$$

The two terms are known as the **Hartree** and **Fock** (or **exchange**) contributions, respectively. This expression lies at the core of the variational **Hartree–Fock method** for many body systems, which approximates the ground state by a product state.

WE PAUSE to present the final form of the second quantized Hamiltonian, including an external potential and pairwise interactions

$$\begin{aligned} H = \int d\mathbf{r}\left[\frac{\hbar^2}{2m}\nabla\psi^\dagger(\mathbf{r})\cdot\nabla\psi(\mathbf{r}) + V(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\right] \\ + \frac{1}{2}\int d\mathbf{r}\,d\mathbf{r}'\,\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}). \end{aligned} \tag{4.77}$$

Understanding the properties of this Hamiltonian, and its extensions that include different spin states and particle species, is the central problem of many body physics.

4.5 *Interference of Bose–Einstein condensates*

Consider a gas of N noninteracting bosons occupying the lowest energy level of some potential well: a **Bose condensate**. If the ground state wavefunction is $\varphi_0(\mathbf{r})$, the N-body wavefunction for such a state is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \prod_i^N \varphi_0(\mathbf{r}_i), \tag{4.78}$$

which we can write in second quantized notation as

$$|\Psi\rangle = \frac{1}{\sqrt{N!}}\left(a_0^\dagger\right)^N |\text{VAC}\rangle\,, \tag{4.79}$$

where $a_0^\dagger$ creates a particle in the state $\varphi_0(\mathbf{r})$. Imagine that we took another well, also filled with N bosons, and placed it alongside the first. If we switch off the potentials at some instant, the particles will fly out, with wavefunctions orginating in the two wells overlapping. Precisely this experiment was reported in (**?**). What do we expect to see?

Let us denote by $\varphi_L(\mathbf{r})$ and $\varphi_R(\mathbf{r})$ the ground states of two spatially separated potential wells. First, consider a state where each boson is in a superposition of $\varphi_L(\mathbf{r})$ and $\varphi_R(\mathbf{r})$. Such a situation could arise by starting from a

[8] The formalism was subsequently extended to fermions by Jordan and Wigner (**?**).

single well and adiabatically splitting in two. We can write such a state as

$$|\bar{N}_L, \bar{N}_R\rangle_\theta \equiv \frac{1}{\sqrt{N!}}\left[\sqrt{\frac{\bar{N}_L}{N}}e^{-i\theta/2}a_L^\dagger + \sqrt{\frac{\bar{N}_R}{N}}e^{i\theta/2}a_R^\dagger\right]^N |\text{VAC}\rangle\,, \qquad (4.80)$$

where $\bar{N}_{L,R}$ are the expectation values of particle number in each state $N = \bar{N}_L + \bar{N}_R$. We allow the system to evolve for some time t, so that the two 'clouds' begin to overlap (typically achieved by allowing free expansion i.e. turning off the confining potentials). Ignoring interactions between the particles, the many-particle state is just Eq. (4.80) with the wavefunctions $\varphi_{L,R}$ evolving freely. We compute the subsequent expectation value of the density using the second quantized representation

$$\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r}), \qquad \psi(\mathbf{r}) = \varphi_L(\mathbf{r})a_L + \varphi_R(\mathbf{r})a_R + \cdots$$

where the dots denote the other states in some complete orthogonal set that includes $\varphi_L(\mathbf{r})$ and $\varphi_R(\mathbf{r})$: we can ignore them because they are empty. A simple calculation gives

$$\langle\rho(\mathbf{r},t)\rangle_\theta = \bar{N}_L|\varphi_L(\mathbf{r},t)|^2 + \bar{N}_R|\varphi_R(\mathbf{r},t)|^2 + \overbrace{2\sqrt{\bar{N}_L\bar{N}_R}\operatorname{Re} e^{i\theta}\, \varphi_L^*(\mathbf{r},t)\varphi_R(\mathbf{r},t)}^{\equiv\rho_{\text{int}(\mathbf{r},t)}}\,. \qquad (4.81)$$

If the clouds begin to overlap, the last term in Eq. (4.81) comes into play. Its origin is in quantum interference between the two coherent subsystems, showing that the *relative phase* has a real physical effect.

As an illustration, consider the evolution of two Gaussian wavepackets with width R_0 at $t = 0$, separated by a distance $d \gg R_0$

$$\varphi_{L,R}(\mathbf{r},t) = \frac{1}{\left(\pi R_t^2\right)^{3/4}}\exp\left[-\frac{(\mathbf{r}\pm\mathbf{d}/2)^2\left(1 - i\hbar t/mR_0^2)\right)}{2R_t^2}\right], \qquad (4.82)$$

with

$$R_t^2 = R_0^2 + \left(\frac{\hbar t}{mR_0}\right)^2.$$

Eq. (4.82) illustrates a very important point about the expansion of a gas. After a long period of expansion, the final density distribution is a reflection of the initial *momentum* distribution. This is simply because faster moving atoms fly further, so after time t an atom with velocity $\mathbf{v}$ will be at position $\mathbf{r} = \mathbf{v}t$ from the center of the trap, provided that this distance is large compared to R_0, the initial radius of the gas. The $t \to \infty$ limit of Eq. (4.82) gives

$$|\varphi_{L,R}(\mathbf{r}, t\to\infty)|^2 \propto \exp\left[-\left(\frac{mR_0\left[\mathbf{r}\pm\mathbf{d}/2\right]}{\hbar t}\right)^2\right], \qquad (4.83)$$

reflecting a Gaussian initial momentum distribution of width $\hbar/R_0$. Imaging the density distribution after expansion is one of the most commonly used experimental techniques in ultracold physics, and yields information about the momentum distribution $n(\mathbf{p}) \equiv a_\mathbf{p}^\dagger a_\mathbf{p}$ before expansion.

The final term of Eq. (4.81) is then

$$\rho_{\text{int}}(\mathbf{r},t) = A(\mathbf{r},t)\cos\left[\theta + \frac{\hbar\mathbf{r}\cdot\mathbf{d}}{mR_0^2R_t^2}t\right]$$
$$A(\mathbf{r},t) = \frac{2\sqrt{\bar{N}_L\bar{N}_R}}{\pi^{3/2}R_t^3}\exp\left(-\frac{\mathbf{r}^2+\mathbf{d}^2/4}{R_t^2}\right) \qquad (4.84)$$

The interference term therefore consists of regularly spaced fringes, with a separation at long times of $2\pi\hbar t/md$.

Now we imagine doing the same thing with two condensates of fixed particle number, which bear no phase relation to one another. The system is described by the product state

The F is for Fock, as product states are sometimes known as **Fock states**.

$$|N_L, N_R\rangle_F \equiv \frac{1}{\sqrt{N_L! N_R!}} (a_L^\dagger)^{N_L} (a_R^\dagger)^{N_R} |\text{VAC}\rangle .$$

Computing the density in the same way yields

$$\langle \rho(\mathbf{r}, t) \rangle_F = N_L |\varphi_L(\mathbf{r}, t)|^2 + N_R |\varphi_R(\mathbf{r}, t)|^2, \tag{4.85}$$

which differs from the previous result by the absence of the interference term.

This is not the end of the story, however. When we look at an absorption image of the gas, we are not looking at an *expectation value* of $\rho(\mathbf{r})$ but rather the measured value of some observable(s) $\rho(\mathbf{r})$. The expectation value just tells us the result we would expect to get if we repeated the same experiment many times and averaged the result. We get more information by thinking about the correlation function of the density at two different points.

Problem 4.13

Show that

$$\begin{aligned} \left\langle : \rho(\mathbf{r}) \rho(\mathbf{r}') : \right\rangle_F = \langle \rho(\mathbf{r}) \rangle_F \langle \rho(\mathbf{r}') \rangle_F &+ N_L N_R \varphi_L^*(\mathbf{r}) \varphi_R^*(\mathbf{r}') \varphi_L(\mathbf{r}') \varphi_R(\mathbf{r}) \\ &+ N_L N_R \varphi_R^*(\mathbf{r}) \varphi_L^*(\mathbf{r}') \varphi_R(\mathbf{r}') \varphi_L(\mathbf{r}). \end{aligned} \tag{4.86}$$

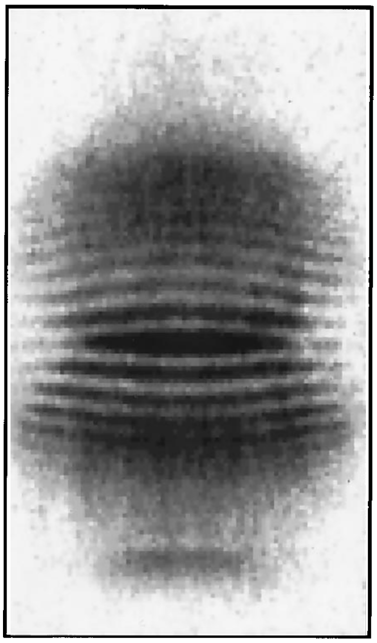

Figure 4.5: Interference fringes observed between two Bose condensates (**?**).

We see that the second line contains interference fringes, with the same spacing as before. The correlation function gives the relative probability of finding an atom at $\mathbf{r}'$ if there is one at $\mathbf{r}$. We conclude that in each measurement of the density, fringes are present but with a phase that varies between measurements, even if the samples are identically prepared.

The rather surprising implication is that predictions for measured quantities for a system in a Fock state are the same as in a relative phase state, but with a subsequent averaging over the phase.

Problem 4.14

Prove this by showing that the density matrix

$$\rho = \int_0^{2\pi} \frac{d\theta}{2\pi} \, |\bar{N}_L, \bar{N}_R\rangle_\theta \, \langle \bar{N}_R, \bar{N}_L|_\theta$$

coincides with that of a mixture of Fock states with binomial distribution of atoms into states φ_L, φ_r. At large N this distribution becomes sharply peaked at occupations $\bar{N}_L$, $\bar{N}_R$.

The interference of two independent condensates was observed in 1997 in (**?**). The related question of whether two independent light sources give rise to interference was discussed much earlier in (**?**)[9].

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[9] This article opens by recalling Dirac's comment that appears at the start of this chapter. Since Dirac invented second quantization (though the term itself is Jordan's) to describe many photon states we give him a pass.

4.6 *The Hanbury Brown and Twiss effect*

As another example, let's consider the problem of **noise correlations** in time-of-flight images of an expanded gas. As we saw above, the density distribution after expansion reflects the initial momentum distribution. This observation applies not just to the *average* of the momentum distribution $n(\mathbf{p}) \equiv a^\dagger_{\mathbf{p}} a_{\mathbf{p}}$, but also to its correlation functions. Thus even images from a single experiment that seem to show only small fluctuations in density superimposed on a smooth background can reveal information when the correlation function is computed.

In (**?**), atoms were initially prepared in an optical lattice in a **Mott state**, meaning that each site in the lattice had a fixed number of atoms. The wavefunction of such a state may then be written

$$\prod_i a^\dagger_i \left|\mathrm{VAC}\right\rangle , \tag{4.87}$$

where $a^\dagger_i$ creates a particle localized at site $\mathbf{r}_i$ in the lattice, with (let's say) Gaussian wavefunction

$$\varphi_i(\mathbf{r}) = \frac{1}{(\pi R^2)^{3/4}} \exp\left[-\frac{(\mathbf{r}-\mathbf{r}_i)^2}{2R^2}\right]$$

This experiment is a realization of the **Hanbury Brown and Twiss effect**, which is the work of two people (not three): Robert Hanbury Brown and Richard Q. Twiss. For the history and early applications of this effect, see (**??**).

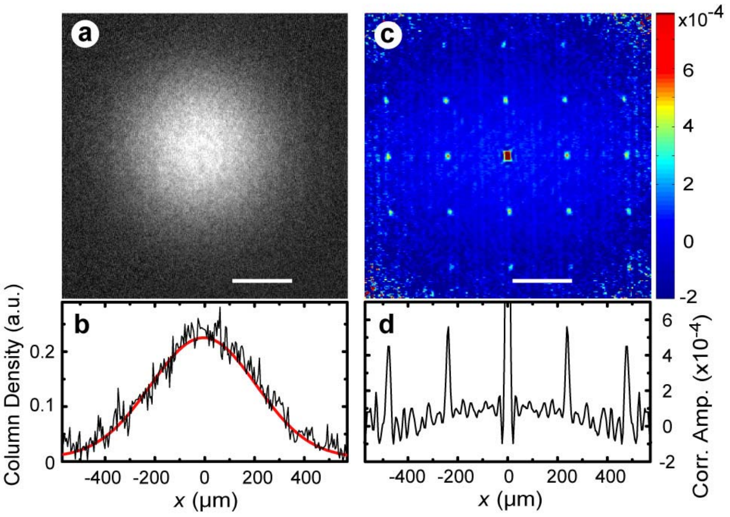

Figure 4.6: (a) raw image (b) density of an atomic cloud following expansion from a Mott state. (c) and (d) noise correlation signal extracted from the same image. From (**?**).

Problem 4.15

Show that the correlation function of momentum state occupancies is

$$\langle : n(\mathbf{p}) n(\mathbf{p}') : \rangle = \sum_{i,j} \tilde{\varphi}^*_i(\mathbf{p}) \tilde{\varphi}_i(\mathbf{p}) \tilde{\varphi}^*_j(\mathbf{p}') \tilde{\varphi}_j(\mathbf{p}') \pm \tilde{\varphi}^*_i(\mathbf{p}) \tilde{\varphi}_j(\mathbf{p}) \tilde{\varphi}^*_j(\mathbf{p}') \tilde{\varphi}_i(\mathbf{p}'). \tag{4.88}$$

where $\tilde{\varphi}_i(\mathbf{p})$ is the Fourier transform of the spatial wavefunction. Evaluate the Fourier transform and explain the structure of the noise correlations in Fig. 4.6.

5
Density matrices

> There are known knowns; there are things we know that we know. There are known unknowns; that is to say there are things that, we now know we don't know. But there are also unknown unknowns – there are things we do not know we don't know.
>
> Donald Rumsfeld

The formalism of quantum mechanics that you have encountered up to now is designed to deal with uncertainty. However, soon after the development of the modern form of the theory, it was realised that a tool was needed to describe a *statistical distribution* of quantum states. As we'll see, such distributions arise in many situations, notably in quantum statistical mechanics.

The appropriate concept, introduced independently in 1927 by von Neumann, Landau, and Bloch, is the **density matrix** (or operator). Before we define it, let's see exactly why such a thing is necessary.

5.1 Two kinds of probability

Recall the **Stern–Gerlach** experiment of 1922, in which a beam of silver atoms was split in two by a inhomogeneous magnetic field, on account of the spin $1/2$ of the outermost electron. Supposing that the atoms are independent, how should we describe the beam?

Recall that the most general state of a spin $1/2$ is

$$|\mathbf{n}\rangle = \begin{pmatrix} \cos\left(\theta/2\right) e^{-i\phi/2} \\ \sin\left(\theta/2\right) e^{i\phi/2}. \end{pmatrix} \tag{5.1}$$

This state has the property that it is an eigenstate of $\mathbf{n}\cdot\mathbf{S}$ with eigenvalue $+\hbar/2$, where

$$\mathbf{n} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}. \tag{5.2}$$

It's clear that a single state of this form cannot describe the outermost electron of each silver atom in the beam. If this were the case, orienting the magnetic field parallel to $\mathbf{n}$ would give a single, deflected beam, showing that there was a preferred axis present.

We therefore need to describe the beam by an *ensemble* of quantum states, characterised by a probability distribution $P(\mathbf{n})$. The expectation value of any observable $\mathcal{O}$ can then be written as the integral over the unit sphere

$$\overline{\langle\mathcal{O}\rangle} = \int d\Omega_{\mathbf{n}} P(\mathbf{n}) \left\langle\mathbf{n}|\mathcal{O}|\mathbf{n}\right\rangle. \tag{5.3}$$

The bar on the left hand side indicates we have taken an additional ensemble average, as well as the quantum average denoted by the angular brackets. We can rewrite this expression by introducing the operator

$$\rho_P \equiv \int d\Omega_{\mathbf{n}} P(\mathbf{n}) \left|\mathbf{n}\right\rangle \left\langle\mathbf{n}\right| . \tag{5.4}$$

Then we have

$$\overline{\langle \mathcal{O} \rangle} = \operatorname{tr}\left[\rho_P \mathcal{O}\right], \tag{5.5}$$

where tr denotes the trace. The operator ρ_P is called the **density matrix**. One immediate benefit of phrasing things in terms of ρ_P is that it makes it clear that $P(\mathbf{n})$ contains a great deal of redundancy. ρ_P is a 2×2 Hermitian matrix

$$\rho_P^\dagger = \rho_P, \tag{5.6a}$$

and therefore depends on only 4 real parameters, rather than a continuous function. In fact, there is are two more conditions. By taking $\mathcal{O} = 1$ in Eq. (5.5)

$$\operatorname{tr} \rho_P = 1. \tag{5.6b}$$

Thus there are only *three* real parameters. Finally, it is clear from the definition Eq. (5.4) and the positivity of the probability distribution that

$$\langle \Psi | \rho_P | \Psi \rangle \geq 0 \tag{5.6c}$$

for all $|\Psi\rangle$. We say that ρ_P is **positive semi definite**.

At this point let's dispense with $P(\mathbf{n})$ altogether, and *define* a density matrix to be any operator satisfying the three conditions Eqs. (5.6). The expectation value of any observable is given by Eq. (5.5)

Problem 5.1

Show that the most general form of a spin 1/2 density matrix is

$$\rho = \frac{1}{2}\mathbb{1} + \frac{r}{2}\mathbf{n} \cdot \boldsymbol{\sigma} \tag{5.7}$$

for $0 \leq r \leq 1$. Thus, the space of spin 1/2 density matrices is identified with the unit ball (**Bloch sphere**).

The density matrix reflects our ignorance of the quantum state of the system. A system described by a general density matrix is said to be in a **mixed state**.

Since ρ is Hermitian, it has a representation in terms of its eigenvalues and (orthogonal) eigenstates

$$\rho = \sum_\alpha P_\alpha \left|\varphi_\alpha\right\rangle \left\langle\varphi_\alpha\right| . \tag{5.8}$$

The conditions Eq. (5.6b) and Eq. (5.6c) imply

$$\sum_\alpha P_\alpha = 1 \text{ and } P_\alpha \geq 0. \tag{5.9}$$

Thus, although the definition provided by Eqs. (5.6) looked abstract, we see that it is equivalent to specifying a probability distribution $\{P_\alpha\}$ on an orthogonal basis of states $\{|\varphi_\alpha\rangle\}$, which could be discrete or continuous. The expectation value Eq. (5.5) takes the form

$$\overline{\langle \mathcal{O} \rangle} = \sum_\alpha P_\alpha \left\langle \varphi_\alpha | \mathcal{O} | \varphi_\alpha \right\rangle \tag{5.10}$$

Problem 5.2

What is the density matrix appropriate for spins in the Stern–Gerlach experiment?

A **pure state** corresponds to having one of the $P_\alpha = 1$, in which case $\rho = |\varphi_\alpha\rangle \langle\varphi_\alpha|$, a projector on the corresponding state.

We'll return to the Stern–Gerlach experiment shortly, after we have discussed the density matrix in the position representation.

TANGENT Although we won't pursue it further, the representation of the density matrix given by Eq. (5.4) is often used in quantum optics and is called the **P representation**. For modes of the light field $|\mathbf{n}\rangle$ is replaced by a coherent state $|\alpha\rangle$ (see **AQP**), and integration over the plane of complex α replaces integration over the unit sphere. In this context, the P representation is known as the **Sudarshan–Glauber representation** (for which Glauber was awarded the Nobel prize in 2005 – you may very well wonder what happened to Sudarshan).

Very roughly, the idea of this representation is to describe the quantum state in terms of a distribution function of a classical quantity, such as an amplitude α or spin direction $\mathbf{n}$. However, this viewpoint is subject to various complications. One drawback of the P representation is that it is not positive. That is, a non-negative ρ_P can correspond to a P that is not everywhere positive. An alternative representation is the **Husimi** or **Q representation**

$$Q(\alpha) = \frac{1}{\pi} \langle\alpha|\rho|\alpha\rangle \,, \tag{5.11}$$

which *is* manifestly positive. For more on the applications of these ideas in quantum optics, see (**?**). The bible of coherent states is (**?**).

The position representation

The density matrix is simple enough for the two dimensional space of spin 1/2, but in general we need to work with infinite dimensional spaces. Barring any mathematical mishaps, the defining conditions Eqs. (5.6) carry over to the general case. We can then form the position representation of the density matrix by taking matrix elements in the usual way

$$\rho(\mathbf{r}, \mathbf{r}') = \langle\mathbf{r}|\rho|\mathbf{r}'\rangle \,. \tag{5.12}$$

In terms of the matrix elements of an observable $\mathcal{O}(\mathbf{r}, \mathbf{r}') = \langle\mathbf{r}|\mathcal{O}|\mathbf{r}'\rangle$, the expectation value may be written

$$\overline{\langle\mathcal{O}\rangle} = \operatorname{tr}[\rho\mathcal{O}] = \int d\mathbf{r}\, d\mathbf{r}'\, \rho(\mathbf{r}, \mathbf{r}')\mathcal{O}(\mathbf{r}', \mathbf{r}) \tag{5.13}$$

Problem 5.3

Show that the expectation value of the momentum is

$$\overline{\langle\mathbf{p}\rangle} = i\hbar \int d\mathbf{r}\, \nabla_{\mathbf{r}} \rho(\mathbf{r}, \mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}} . \tag{5.14}$$

In terms of the eigenvalues and eigenstates of the density matrix we have

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_\alpha P_\alpha \varphi_\alpha(\mathbf{r})\varphi_\alpha^*(\mathbf{r}') \tag{5.15}$$

where $\varphi_\alpha(\mathbf{r}) = \langle \mathbf{r} | \varphi_\alpha \rangle$. The diagonal element of the density matrix

$$\rho(\mathbf{r}, \mathbf{r}) = \sum_\alpha P_\alpha |\varphi_\alpha(\mathbf{r})|^2, \tag{5.16}$$

gives the probability of finding the particle at position $\mathbf{r}$. This is a general feature of the diagonal matrix elements in any *orthogonal* basis.

5.2 *Time evolution of the density matrix*

The equation of motion of the density matrix is easy to obtain from the time dependent Schrödinger equation describing the evolution of an arbitrary state

$$i\hbar \frac{d}{dt} |\Psi\rangle = H |\Psi\rangle \,. \tag{5.17}$$

Applied to the spectral representation Eq. (5.8), this immediately gives the **von Neumann equation**

Note the sign difference between the von Neumann equation and Heisenberg's equation of motion $\frac{d\mathcal{O}}{dt} = \frac{i}{\hbar}[H, \mathcal{O}]$. In the present case we stay within the Schrödinger picture i.e. the states are evolving, rather than the obervables.

$$\boxed{\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] \,.} \tag{5.18}$$

The formal solution of this equation is

$$\rho(t) = U(t, t')\rho(t')U^\dagger(t, t'), \tag{5.19}$$

where $U(t, t')$ is the unitary operator of time evolution. This evolution preserves the eigenvalues $\{P_\alpha\}$ of the density matrix.

Problem 5.4

Describe the evolution of the spin $1/2$ density matrix of Problem 5.1 when $H = \mathbf{H} \cdot \mathbf{S}$.

With the equation of motion in hand we can return to the Stern–Gerlach experiment. The wavefunction of our spin $1/2$ particles consists of a spin component and a spatial part (the internal structure of the atoms can be ignored, in the spirit of the adiabatic approximation), so our density matrix has the general form

$$\begin{pmatrix} \rho_{\uparrow\uparrow}(\mathbf{r}, \mathbf{r}') & \rho_{\uparrow\downarrow}(\mathbf{r}, \mathbf{r}') \\ \rho_{\downarrow\uparrow}(\mathbf{r}, \mathbf{r}') & \rho_{\downarrow\downarrow}(\mathbf{r}, \mathbf{r}'). \end{pmatrix} \tag{5.20}$$

We suppose that the magnetic field varies only in a direction transverse to the beam direction, so the longitudinal motion of the particles factors out of the problem. The Hamiltonian can then be taken to be

$$H = -\frac{\hbar^2}{2m}\partial_x^2 - \mu B' x \sigma_z, \tag{5.21}$$

where B' is the magnetic field gradient and μ is the magnetic moment. Let $\Psi_0(x, t)$ be the wavefunction of a particle in the **absence** of a field gradient. In this case the density matrix would evolve as

$$\rho(x, x'; t) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \Psi_0(x, t)\Psi_0^*(x', t). \tag{5.22}$$

The Hamiltonian Eq. (5.21) is diagonal in the spin, so we just need to find how the wavepackets of an up spin and down spin particle evolve in the presence of the field gradient. Because the gradient is constant, this turns out to be very simple

$$\Psi_{\uparrow,\downarrow}(x,t) = \exp\left(i\theta_{\uparrow,\downarrow}(x,t)/\hbar\right)\Psi_0(x \mp \mu B' t^2/2m, t), \tag{5.23}$$

where the phase $\theta_{\uparrow,\downarrow}(x,t)$ is

$$\theta_{\uparrow,\downarrow}(x,t) = \pm\mu B' x t - \frac{(\mu B')^2 t^3}{6m} \tag{5.24}$$

Problem 5.5

Prove this.

Notice that – apart from the phase factor – the effect of the gradient is to shift the wavepacket to the point $\pm\mu B' t^2/2m$, which corresponds to the classical trajectory of a particle in a linear potential.

The evolution of the density matrix is then

$$\rho(x,x';t) = \frac{1}{2}\begin{pmatrix} \Psi_\uparrow(x,t)\Psi^*_\uparrow(x',t) & 0 \\ 0 & \Psi_\downarrow(x,t)\Psi^*_\downarrow(x',t) \end{pmatrix}. \tag{5.25}$$

The diagonal elements take on a particularly simple form

$$\begin{aligned} \rho_{\uparrow\uparrow}(x,x;t) &= \frac{1}{2}|\Psi_0(x-\mu B' t^2/2m,t)|^2 \\ \rho_{\downarrow\downarrow}(x,x;t) &= \frac{1}{2}|\Psi_0(x+\mu B' t^2/2m,t)|^2. \end{aligned} \tag{5.26}$$

Remembering that the diagonal elements of the density matrix give the probability to be in a particular location with a particular spin component, we see that this describes the splitting of the beam into two.

Comparing Eq. (5.22) and Eq. (5.25), we see that in the first case the spin and position degrees of freedom of the particles are independent of each other – the density matrix factorizes – while in the second case they are **entangled**[1].

TANGENT The von Neumann equation is the quantum counterpart of **Liouville's equation** of classical mechanics

$$\frac{\partial\rho}{\partial t} = -\left\{\rho, H\right\}_{\mathrm{P}}, \tag{5.27}$$

where $\rho(\mathbf{q},\mathbf{p},t)$ is the phase space density and $\{\cdot,\cdot\}$ denotes the **Poisson bracket**

$$\{f,g\}_{\mathrm{P}} = \frac{\partial f}{\partial \mathbf{q}}\cdot\frac{\partial g}{\partial \mathbf{p}} - \frac{\partial f}{\partial \mathbf{p}}\cdot\frac{\partial g}{\partial \mathbf{q}}. \tag{5.28}$$

Eq. (5.27) can be written as a continuity equation

$$\frac{\partial\rho}{\partial t} + \partial_i\left(v_i\rho\right) = 0, \tag{5.29}$$

and describes a flow in phase space due to the **Hamiltonian vector field**

$$v_i = \begin{cases} \frac{\partial H}{\partial p_i} & i = 1,\ldots,N \\ -\frac{\partial H}{\partial q_{i-N}} & i = N+1,\ldots,2N, \end{cases} \tag{5.30}$$

where the first N coordinates are the positions and the second N are the momenta. Note that in writing Eq. (5.29) we used the fact that the flow is incompressible ($\partial_i v_i = 0$), which is the content of **Liouville's theorem**.

Note the appearance of a partial derivative on the left hand side of Liouville's equation compared to a total derivative in von Neumann's equation. This is just because ρ in a classical mechanics is a function on phase space. We mention this because Liouville's equation is sometimes written as $\frac{d\rho}{dt} = 0$, which includes the variation due to the time dependence of $(\mathbf{q}(t),\mathbf{p}(t))$, evolving according to Hamilton's equations.

[1] This term was introduced by Schrödinger, who called it '*the* characteristic trait of quantum mechanics'.

The resemblance between Eq. (5.27) and Eq. (5.18) is an example of the more general correspondence

$$\{A, B\} \longleftrightarrow -\frac{i}{\hbar}\left[A, B\right], \tag{5.31}$$

between Poisson brackets in classical mechanics and commutators of operators in quantum theory.

Of course, this relationship is purely formal, as functions on phase space and operators in Hilbert space are very different things. A closer link may be established by considering the **Wigner function**

$$\varrho(\mathbf{q}, \mathbf{p}) = \int d\mathbf{r}\, \rho(\mathbf{q} + \mathbf{r}/2, \mathbf{q} - \mathbf{r}/2) \exp\left(-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}\right) \tag{5.32}$$

obtained by Fourier transforming with respect to the *difference* of the arguments of the density matrix. $\varrho(\mathbf{q}, \mathbf{p})$ is the quantum mechanical analog of the classical phase space density, though in general it is not positive. The von Neumann equation implies the equation of motion for $\varrho(\mathbf{q}, \mathbf{p})$

$$\frac{\partial \varrho}{\partial t} = -\left\{\varrho, H\right\}_{\mathrm{M}}, \tag{5.33}$$

where $\{\cdot, \cdot\}_{\mathrm{M}}$ denotes the **Moyal bracket**

$$\{f, g\}_{\mathrm{M}} = \frac{2}{\hbar} f(\mathbf{q}, \mathbf{p}) \sin\left(\frac{\hbar}{2}\left[\overleftarrow{\partial_{\mathbf{q}}}\cdot\overrightarrow{\partial_{\mathbf{p}}} - \overleftarrow{\partial_{\mathbf{p}}}\cdot\overrightarrow{\partial_{\mathbf{q}}}\right]\right) g(\mathbf{q}, \mathbf{p}). \tag{5.34}$$

If we retain only the leading order term in $\hbar$, corresponding to the classical limit, we recover Liouville's equation.

Problem 5.6

Use Eq. (5.33) to explain why the linear potential in Eq. (5.21) has such a simple effect on the evolution of the density matrix.

5.3 The density matrix in statistical mechanics

Perhaps the most important mixed state that we encounter is that describing thermal equilibrium. Just as our ignorance of the microstate of a system is described in classical statistical mechanics by a probability distribution $\rho(\mathbf{q}, \mathbf{p})$ in phase space, so our ignorance of the quantum microstate of a system corresponds to a density matrix.

There are a number of variants, according to the ensemble we work with.

- In the **microcanonical ensemble**, corresponding to fixed energy E and number of particles, the density matrix takes the form

  $$\rho_{\mathrm{m}} = \frac{1}{N(E, \delta E)} \sum_{\alpha \in \mathcal{A}(E, \delta E)} |\varphi_\alpha\rangle\langle\varphi_\alpha|, \tag{5.35}$$

  where the set $\mathcal{A}(E, \delta E)$ includes all energy eigenstates in the range $(E - \delta E, E + \delta E)$, and $N(E, \delta E)$ is the number of such states, which is needed to correctly normalize the density matrix. δE is a microscopically large but macroscopically small energy interval, meaning that it contains a large number of states but $\delta E/E \ll 1$.

- In the **canonical ensemble**, with fixed temperature T and number of particles, we have

  $$\rho_{\mathrm{c}} = \frac{1}{Z}\exp\left(-\beta H\right), \tag{5.36}$$

where $\beta = 1/(k_B T)$, and k_B is Boltzmann's constant. The normalization factor that guarantees the trace of the density matrix is unity is called the **partition function**

$$Z = \mathrm{tr}\left[\exp\left(-\beta H\right)\right]. \tag{5.37}$$

Finally, in the **grand canonical ensemble**, with fixed temperature and chemical potential μ, we have

$$\rho_{\mathrm{gc}} = \frac{1}{\mathcal{Z}} \exp\left(-\beta\left[H - \mu N\right]\right). \tag{5.38}$$

The grand canonical partition function is defined just as in Eq. (5.37). The difference from the canonical case is that the Hilbert space is now taken to be the **Fock space** of many particle states, and includes states with differing numbers of particles. More on this in Chapter 4.

Note that all of these density matrices, being functions of the Hamiltonian (and number of particles in the grand canonical case), are constant in time.

The partition function and density matrix appear in a great many thermodynamic relationships, of which we list expressions for the average energy, Helmholtz free energy F, and entropy S

$$\begin{aligned} E &= \overline{\langle H \rangle} = -\frac{\partial}{\partial \beta} \ln Z \\ F &= -k_B T \ln Z \\ S &= -k_B \,\mathrm{tr}\left(\rho \ln \rho\right) = -k_B \sum_\alpha P_\alpha \ln P_\alpha. \end{aligned} \tag{5.39}$$

The above expression for the entropy is called the **von Neumann entropy** (the corresponding expression in classical statistical mechanics is called the **Gibbs entropy**).

The same expression appears in information theory, where it quantifies the information content of a message and is known as **Shannon entropy**, after Claude Shannon. It was von Neumann who suggested the name to Shannon, saying: 'You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, no one really knows what entropy really is, so in a debate you will always have the advantage.'.

Problem 5.7

Show that the von Neumann entropy follows from the first two expressions in Eq. (5.39) and the definition $F = E - TS$ of the Helmholtz free energy.

Note that the von Neumann entropy does not coincide with the thermodynamic entropy of an isolated system out of equilibrium, because it does not change in time.

Problem 5.8

Prove this.

However, the von Neumann entropy is useful for other things. In particular, it measures the departure from a pure state, where it vanishes.

The canonical density matrix

As you will be aware, most calculations in statistical mechanics are more easily done at fixed temperature than fixed energy, making the canonical ensemble preferred over the microcanonical ensemble.

In quantum statistical mechanics, there is another reason to favour the canonical ensemble. ρ_c closely resembles the time evolution operator

$$U(t) = \exp\left(-iHt/\hbar\right), \tag{5.40}$$

except that we 'evolve' for an imaginary time $t = -i\hbar\beta$. The wonderful thing about this observation is that all of the techniques that are available to compute the time evolution of a quantum state can immediately be applied to calculate the density matrix.

The evolution is of course not unitary, but this is more of a blessing than a curse as the usual result is to improve convergence in numerical work: the density matrix is real, indeed positive, rather than complex and oscillating.

From our calculation of the free particle propagator Eq. (2.13) , we can immediately write down

$$\langle \mathbf{r}| \exp\left(-\beta H\right) |\mathbf{r}'\rangle = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} \exp\left[-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2\hbar^2\beta}\right]. \tag{5.41}$$

Calculating the normalization for a particle in a box of volume V gives the partition function

$$Z = \frac{V}{\lambda_\mathrm{dB}^3} \tag{5.42}$$

where λ_dB is the **thermal de Broglie wavelength**

$$\boxed{\lambda_\mathrm{dB} \equiv \sqrt{\frac{2\pi\beta\hbar^2}{m}}.} \tag{5.43}$$

Thus we obtain the density matrix

$$\rho_\mathrm{free}(\mathbf{r},\mathbf{r}') = \frac{1}{V} \exp\left(-\frac{\pi|\mathbf{r}-\mathbf{r}'|^2}{\lambda_\mathrm{dB}^2}\right). \tag{5.44}$$

which nicely captures the intuition that at finite temperature a particle has a typical wavelength λ_dB.

Quantum degeneracy corrections to the ideal gas law

To see the density matrix in action, let's compute the partition function of a gas of indistinguishable non interacting particles. To take into account indistinguishability, we must work with totally symmetric or antisymmetric wavefunctions depending on whether we are dealing with bosons or fermions (see Chapter 4 of these notes). This means that we take matrix elements of the density matrix between the states

$$|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle_{S/A} = \frac{1}{\sqrt{N!}} \sum_P \eta_{S/A}(P) \, |\mathbf{r}_{P1},\ldots,\mathbf{r}_{PN}\rangle. \tag{5.45}$$

The sum is over all $N!$ permutations P of N objects. We have introduced $\eta_{S/A}$ in order to write the following expressions in a unified way for bosons (S) and fermions (A). Thus $\eta_S(P) = 1$ and $\eta_A(P) = \mathrm{sgn}(P)$, the **signature** of the permutation[2].

In this way we find the expression for the N particle partition function

$$Z_N = \frac{1}{N!\lambda_\mathrm{dB}^{3N}} \sum_P \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \, \eta_{S/A}(P) \exp\left(-\frac{\pi}{\lambda_\mathrm{dB}^2} \sum_{j=1}^N |\mathbf{r}_j - \mathbf{r}_{Pj}|^2\right). \tag{5.46}$$

[2] The signature of a permutation is equal to $+1$ for permutations involving an even number of exchanges, and -1 for an odd number.

This is a rather fearsome looking expression, but it has a simple meaning: when taking the trace of $\exp(-\beta H)$ we have to account for the fact that the diagonal elements of the density matrix are those where the two sets of particle position labels differ by a permutation.

Of course, evaluating it is another matter! We can, however, make progress in the limit of high temperatures, where the de Broglie wavelength is short. Then the non trivial permutations in Eq. (5.46) hardly contribute, because some of the Gaussian factors that appear will be small.

Retaining only the identity permutation, we get

$$Z_N \sim \frac{1}{N!}\left(\frac{V}{\lambda_{\mathrm{dB}}^3}\right)^N. \tag{5.47}$$

Eq. (5.39) and $p = -\frac{\partial F}{\partial V}\big|_T$ for the pressure then give the ideal gas law $pV = Nk_{\mathrm{B}}T$.

We can do a bit better than this without too much effort, by taking into account those permutations that involve only a single transposition, as these will evidently be the next largest.

Problem 5.9

Show that this yields the correction to the ideal gas law

$$pV = Nk_{\mathrm{B}}T\left[1 \mp \frac{\lambda_{\mathrm{dB}}^3 n}{2^{5/2}} + \cdots\right], \tag{5.48}$$

with the minus sign for boson and the plus sign for fermions. $n = \frac{N}{V}$ is the density.

Coming from high temperatures, where $n\lambda_{\mathrm{dB}}^3 \ll 1$, this is the first indication of a difference in the thermodynamic behaviour of ideal Bose and Fermi gases. Of course, you know that when $n\lambda_{\mathrm{dB}}^3 \sim 1$ this difference is very pronounced, with the possibility of **Bose–Einstein condensation** in the case of bosons.

It's interesting to ask how condensation appears in this framework. Any permutation can decomposed into set of **cycles**. For example, the permutation $(1,2,3,4) \to (4,2,1,3)$ can be written as the cycle $1 \to 4 \to 3 \to 1$ and the trivial cycle $2 \to 2$. In deriving Eq. (5.48) we just took into account 1-cycles and 2-cycles.

(**?**) conjectured that condensation is associated with the appearance of a finite density of *infinite cycles* in the thermodynamic limit, an idea that was later established rigorously.

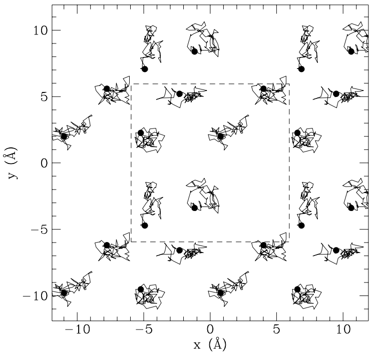

Figure 5.1: Path integral Monte Carlo trajectories of six Helium atoms (periodic boundary conditions). From (**?**).

TANGENT Of course, for noninteracting particles, the above calculation is most easily handled within the grand canonical framework. The canonical picture really comes into its own as a numerical tool called the **path integral Monte Carlo method**. The idea is to represent the partition function of an *interacting* system just as in Eq. (5.46), but with the corresponding propagator taking the place of the free propagator. Because we are working in imaginary time, the integrand for bosons is a positive quantity that can be interpreted as a probability distribution on the space of paths and sampled accordingly. This method has been successfully applied to the study of superfluid Helium, Feynman's original concern in the work mentioned above.

Unfortunately, the minus sign in the case of fermions stymies the straightforward application of this method, a situation generally known as the **fermion sign problem**.

5.4 Density operator for subsystems and quantum entanglement

We introduced density matrices to describe a situation where the quantum state of a system is not definite, but drawn from a probability distribution. We didn't address the question of how such a situation arises in the first place. Of course, the density matrix could just represent the incompleteness of our knowledge of the quantum state. Here, we discuss another natural way in which the density matrix appears when we consider a subsystem of a larger quantum system, itself described by a pure state. We will encounter again the notion of *entanglement*, which we met briefly in Section 5.2. In this section we are going to explore this a little more deeply, using a pair of spins as our main example.

Two spins 1/2 are described by a four dimensional Hilbert space, spanned by the following basis of states

This mathematical term for making a larger space out of two smaller spaces in this way is *tensor product*. It's not hard to see that the dimension of the resulting space is the product of the dimensions of the constituent spaces.

$$\begin{aligned} |A\rangle &= |\uparrow\rangle_1 |\uparrow\rangle_2, \qquad |B\rangle = |\uparrow\rangle_1 |\downarrow\rangle_2 \\ |C\rangle &= |\downarrow\rangle_1 |\uparrow\rangle_2, \qquad |D\rangle = |\downarrow\rangle_1 |\downarrow\rangle_2 . \end{aligned} \tag{5.49}$$

Here $|\uparrow\rangle$ and $|\downarrow\rangle$ are eigenstates of σ_z with eigenvalue ± 1, and the labels 1 and 2 are just to emphasize that we are dealing with the first or second spin (although the position also tells us which).

A pure state of the two spin system is described by the density matrix

$$\rho_{2\text{ spin}} = |\phi\rangle \langle\phi| \tag{5.50}$$

where $|\phi\rangle$ is some linear combination of the states in Eq. (5.49).

$$|\phi\rangle = \alpha |A\rangle + \beta |B\rangle + \gamma |C\rangle + \delta |D\rangle \tag{5.51}$$

Note that $\rho_{2\text{ spin}}$ is a 4×4 matrix. Its explicit form in the above basis is

$$\rho_{2\text{ spin}} = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* & \alpha\gamma^* & \alpha\delta^* \\ \beta\alpha^* & |\beta|^2 & \beta\gamma^* & \beta\delta^* \\ \gamma\alpha^* & \gamma\beta^* & |\gamma|^2 & \gamma\delta^* \\ \delta\alpha^* & \delta\beta^* & \delta\gamma^* & |\delta|^2 . \end{pmatrix} \tag{5.52}$$

As we know, any expectation value can be computed by multiplying the corresponding operator by the density matrix and taking the trace

$$\overline{\langle \mathcal{O} \rangle} = \operatorname{tr}\left[\rho_{2\text{ spin}} \mathcal{O}\right] = \langle \phi | \mathcal{O} | \phi \rangle , \tag{5.53}$$

which in this case is just the pure state expectation value. Now, suppose that the operator $\mathcal{O}$ lives in the Hilbert space of the first spin, e.g. $\mathcal{O}_1 = \sigma_{i,1}$. The expectation value is then

$$\begin{aligned} \overline{\langle \mathcal{O}_1 \rangle} &= \left(|\alpha|^2 + |\beta|^2\right) \langle \uparrow | \mathcal{O} | \uparrow \rangle + \left(|\gamma|^2 + |\delta|^2\right) \langle \downarrow | \mathcal{O} | \downarrow \rangle \\ &(\alpha^*\gamma + \beta^*\delta) \langle \uparrow | \mathcal{O} | \downarrow \rangle + (\alpha\gamma^* + \beta\delta^*) \langle \downarrow | \mathcal{O} | \uparrow \rangle \\ &\equiv \operatorname{tr}[\rho_{1\text{reduced}} \mathcal{O}] \end{aligned} \tag{5.54}$$

where in the last line we have defined the *reduced* density matrix

$$\rho_{1\text{ red}} = \begin{pmatrix} |\alpha|^2 + |\beta|^2 & \alpha\gamma^* + \beta\delta^* \\ \alpha^*\gamma + \beta^*\delta & |\gamma|^2 + |\delta|^2, \end{pmatrix} \tag{5.55}$$

in the $|\uparrow,\downarrow\rangle_1$ basis of spin 1.

In general $\rho_{1\text{ red}}$ describes a *mixed* state of spin 1. More generally, we can write

$$\rho_{1\text{ red}} = \text{tr}_2[\rho_{2\text{ spin}}] \tag{5.56}$$

where $\text{tr}_2\,[\cdots]$ denotes the trace over the space of spin 2. To get a feel for what this means, compare Eq. (5.52) and Eq. (5.55).

The reduced density matrix contains all the information we need about the system if we only ask questions (= make measurements) on spin 1.

Problem 5.10

What about the converse problem? That is, for any density matrix of a single spin, is it possible to view it as the reduced density matrix of a pure state of two spins? If so, is the pure state unique? This process is called *purification* of a density matrix.

The reduced density matrix can be treated like any other density matrix. Its lack of purity is a reflection of the *entanglement* between the two systems that prevents us describing the subsystem by a pure quantum state. We saw that the von Neumann entropy of a density matrix can be used to measure the departure from a pure state. Therefore the quantity

$$S_{\text{ent}} \equiv -\,\text{tr}\left[\rho_{\text{red}} \log \rho_{\text{red}}\right], \tag{5.57}$$

measures the degree of entanglement between two subsystems, and is known as the *entanglement entropy*.

5.5 *Quantum Damping*

The interaction of a quantum system with a reservoir can lead to relaxation or decoherence of the quantum state. Following the general discussion of the previous system, we shall be interested in the dynamics of the reduced density operator for the sub-system. We shall determine how *weak* coupling to the reservoir leads to relaxation and decoherence of the subsystem.

General theory of damping by the environment

We shall write the Hamiltonian as

$$H = H_0 + V(t) \tag{5.58}$$

where H_0 is the Hamiltonian for the decoupled subsystem and reservoir, and $V(t)$ is the (weak) coupling between these two quantum systems. It is convenient to work in the interaction picture, in which all operators are assigned the time-dependence due to H_0, such that the wavefunctions evolve according to $V(t)$. Consequently, the equation of motion for the entire density operator, in the interaction picture, is

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[V(t), \rho] \tag{5.59}$$

This equation can be formally integrated to give

$$\rho(t) = \rho(t_i) - \frac{i}{\hbar}\int_{t_i}^{t}[V(t'),\rho(t')]dt' \tag{5.60}$$

where t_i is an initial time when the coupling $V(t)$ is first turned on. Substituting this result back into the equation of motion leads to

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[V(t),\rho(t_i)] - \frac{1}{\hbar^2}\int_{t_i}^{t}[V(t),[V(t'),\rho(t')]]dt' \tag{5.61}$$

At the initial time t_i, the system and reservoir are decoupled, so we can write

$$\rho(t_i) = \rho_S(t_i)\otimes\rho_R(t_i) \tag{5.62}$$

Assuming that the reservoir is in equilibrium at t_i, if the system and reservoir were to remain decoupled ($V = 0$) the subsequent density operator would be

$$\rho_0(t) = \rho_S(t)\otimes\rho_R(t_i) \tag{5.63}$$

which allows for the possibility that ρ_S was not at equilibrium at $t = t_i$. Since we are interested in weak coupling, we look for a solution to the equations in which

$$\rho(t) = \rho_S(t)\otimes\rho_R(t_i) + \delta\rho(t) \tag{5.64}$$

where $\delta\rho(t)$ is proportional to one or more powers of V, and must satisfy $\mathrm{Tr}\delta\rho = 0$. Substituting (5.64) into the equation of motion (5.61) and retaining terms of order V^2, we find

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[V(t),\rho_S(t_i)\otimes\rho_R(t_i)] - \frac{1}{\hbar^2}\int_{t_i}^{t}\left[V(t),[V(t'),\rho_S(t')\otimes\rho_R(t_i)]\right]dt' \tag{5.65}$$

meaning that the reduced density operator obeys

$$\frac{d\rho_S}{dt} = -\frac{i}{\hbar}\mathrm{Tr}_R[V(t),\rho_S(t_i)\otimes\rho_R(t_i)] - \frac{1}{\hbar^2}\mathrm{Tr}_R\int_{t_i}^{t}\left[V(t),[V(t'),\rho_S(t')\otimes\rho_R(t_i)]\right]dt' \tag{5.66}$$

This equation shows that the time evolution of the reduced density operator depends on its values at earlier times. In practice, for reservoirs in which there is a large number of degrees of freedom, such that the excitations form a continuum of energy levels, this history dependence is unimportant and $\dot\rho_S(t)$ depends only on $\rho_S(t)$ at the same time. We shall see an example of this now.

Two level atom coupled to a thermal reservoir

We shall illustrate the general situation by considering the coupling of a two-level atom to the electromagnetic field. The Hamiltonian for the decoupled system and reservoir is

$$H_0 = \frac{\hbar\omega}{2}\sigma_z + \sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}} \tag{5.67}$$

where the first term describes a two-level atom with energy splitting $\hbar\omega$ (operators acting on the two-level system are the Pauli matrices), and the second term describes the reservoir of photon modes which have wavevector $\mathbf{k}$ and energy $\hbar\omega_{\mathbf{k}} = c|\mathbf{k}|$. Quantising the electromagnetic field amounts to representing each of these modes as a harmonic oscillator, with ladder operators $a^{(\dagger)}$ such that $a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$ is the number of photons in the mode $\mathbf{k}$.

In the interaction picture, and making the rotating wave approximation the interaction is

$$V(t) = \hbar\sum_{\mathbf{k}} g_{\mathbf{k}} \left[a_{\mathbf{k}}^{\dagger}\sigma_- e^{-i(\omega-\omega_{\mathbf{k}})t} + a_{\mathbf{k}}\sigma_+ e^{+i(\omega-\omega_{\mathbf{k}})t}\right] \tag{5.68}$$

These two terms describe processes in which the atom is de-excited (σ_-) and emits a photon ($a_{\mathbf{k}}^{\dagger}$), and in which the atom is excited (σ_+) and absorbs a photon ($a_{\mathbf{k}}$).

The rotating wave approximation amounts to neglecting terms such as $e^{i(\omega+\omega_{\mathbf{k}})t}$. For large $\omega+\omega_{\mathbf{k}}$ these terms oscillate very quickly in time, so their effect averages to zero. This approximation is valid when the frequency of the atomic transition, ω, is large compared to the rate at which energy is exchanged between the system and the reservoir, which is of order Γ defined below.

Using this interaction in the equation of motion for the density operator of the subsystem (5.66) leads to

$$\begin{aligned}\frac{d\rho_S}{dt} \quad = \quad & -i\sum_{\mathbf{k}} g_{\mathbf{k}}\langle a_{\mathbf{k}}^{\dagger}\rangle\left[\sigma_-,\rho_S(t_i)\right]e^{-i(\omega-\omega_{\mathbf{k}})t} - \int_{t_i}^{t}\sum_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}}g_{\mathbf{k}'}\, \{ \\ & \left[\sigma_-\sigma_-\rho_S(t') - 2\sigma_-\rho_S(t')\sigma_- + \rho_S(t')\sigma_-\sigma_-\right] \times e^{-i(\omega-\omega_{\mathbf{k}})t-i(\omega-\omega_{\mathbf{k}'})t'}\langle a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}'}^{\dagger}\rangle \\ & \left[\sigma_-\sigma_+\rho_S(t') - \sigma_+\rho_S(t')\sigma_-\right] \times e^{-i(\omega-\omega_{\mathbf{k}})t+i(\omega-\omega_{\mathbf{k}'})t'}\langle a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}'}\rangle \\ & \left[\sigma_+\sigma_-\rho_S(t') - \sigma_-\rho_S(t')\sigma_+\right] \times e^{i(\omega-\omega_{\mathbf{k}})t-i(\omega-\omega_{\mathbf{k}'})t'}\langle a_{\mathbf{k}}a_{\mathbf{k}'}^{\dagger}\rangle \\ & +\text{h.c.}\}\end{aligned} \tag{5.69}$$

where the angled brackets indicate the average over the density operator of the reservoir.

This lengthy expression can be dramatically simplified by choosing the reservoir to be in thermal equilibrium. Each mode is a simple harmonic oscillator at thermal equilibrium at temperature T. From the results of §5.3 (and noting that we have made a shift in the zero point energy), we find

$$\rho_R = \prod_{\mathbf{k}} \frac{1}{Z_{\mathbf{k}}} \exp\left(-\frac{\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}}{k_{\mathrm{B}}T}\right) \tag{5.70}$$

where $Z_{\mathbf{k}} = \sum_{n=0}^{\infty}\exp\left(-\frac{\hbar\omega_{\mathbf{k}}n}{k_{\mathrm{B}}T}\right) = \left[1-\exp\left(-\frac{\hbar\omega_{\mathbf{k}}}{k_{\mathrm{B}}T}\right)\right]^{-1}$.

Problem 5.11

Show that the thermal density operator (5.70) implies that

$$\begin{aligned}\langle a_{\mathbf{k}}\rangle &= \langle a_{\mathbf{k}}^{\dagger}\rangle = 0 && (5.71)\\ \langle a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}'}\rangle &= \bar{n}_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'} && (5.72)\\ \langle a_{\mathbf{k}}a_{\mathbf{k}'}^{\dagger}\rangle &= (\bar{n}_{\mathbf{k}}+1)\,\delta_{\mathbf{k},\mathbf{k}'} && (5.73)\\ \langle a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}'}^{\dagger}\rangle &= \langle a_{\mathbf{k}}a_{\mathbf{k}'}\rangle = 0 && (5.74)\end{aligned}$$

where

$$\bar{n}_{\mathbf{k}} \equiv \frac{1}{e^{\frac{\hbar\omega_{\mathbf{k}}}{k_{\mathrm{B}}T}}-1} \tag{5.75}$$

is the average photon number in mode $\mathbf{k}$.

Making the simplifications afforded by this, we obtain

$$\begin{aligned}\frac{d\rho_S}{dt} \quad = \quad & -\int_{t_i}^{t}dt'\sum_{\mathbf{k}} g_{\mathbf{k}}^2\left\{\left[\sigma_-\sigma_+\rho_S(t') - \sigma_+\rho_S(t')\sigma_-\right] \times \bar{n}_{\mathbf{k}}e^{-i(\omega-\omega_{\mathbf{k}})(t-t')}\right. && (5.76)\\ & \left. + \left[\sigma_+\sigma_-\rho_S(t') - \sigma_-\rho_S(t')\sigma_+\right] \times (\bar{n}_{\mathbf{k}}+1)e^{i(\omega-\omega_{\mathbf{k}})(t-t')} + \text{h.c.}\right\} && (5.77)\end{aligned}$$

Replacing now the sum over modes by an integral (and allowing for the two polarisation states at each wavevector)

$$\sum_{\mathbf{k}} \to 2\frac{V}{(2\pi)^3}\int d^3\mathbf{k} = 2\frac{V}{(2\pi)^3}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \int_0^{\infty} k^2 dk$$

where V is the volume over which the EM modes are normalised, one finds

$$\begin{aligned} \frac{d\rho_S(t)}{dt} &= -\bar{n}_\omega\frac{\Gamma}{2}\left[\sigma_-\sigma_+\rho_S(t) - \sigma_+\rho_S(t)\sigma_-\right] - (\bar{n}_\omega+1)\frac{\Gamma}{2}\left[\sigma_+\sigma_-\rho_S(t) - \sigma_-\rho_S(t)\sigma_+\right] \\ &\quad + \text{Hermitian conjugate of preceding terms} \end{aligned} \quad (5.78)$$

where $\bar{n}_\omega = \left[e^{\beta\hbar\omega} - 1\right]^{-1}$ is the photon occupation number at frequency ω, and Γ is a rate constant that is related to the coupling of the atom to the electromagnetic field.[3] For a dipole-allowed transition,

$$g_{\mathbf{k}}^2 = \frac{kd^2}{2\hbar c\epsilon_0 V}\cos^2\theta$$

where d is the dipole matrix element between the two atomic levels, and the rate constant is

$$\Gamma = \frac{\omega^3 d^2}{3\pi\epsilon_0\hbar c^3}\,.$$

Equation (5.78) is the final form that we wanted to obtain. Note that, as previously advertised, the dynamics of the density operator depends only on the density operator at the current time. (This arose from the appearance of a delta-function in time, under the integration over the continuum of modes with wavevectors k.)

Denoting the two levels of the atom as "up" (u) and "down" (d) for the high energy and low energy levels respectively, the equations of motion for the elements of the reduced density operator, $\rho_{ij} \equiv \langle i|\hat{\rho}_S|j\rangle$ can be obtained:

$$\dot{\rho}_{uu} = -(\bar{n}_\omega+1)\Gamma\rho_{uu} + \bar{n}_\omega\Gamma\rho_{dd} \quad (5.79)$$

$$\dot{\rho}_{ud} = \dot{\rho}_{du}^* = -\left(\bar{n}_\omega + \frac{1}{2}\right)\Gamma\rho_{ud} \quad (5.80)$$

$$\dot{\rho}_{dd} = -\bar{n}_\omega\Gamma\rho_{dd} + (\bar{n}_\omega+1)\Gamma\rho_{uu} \quad (5.81)$$

Problem 5.12

Verify that Eqn (5.78) leads to equations (5.79-5.81).

Equations (5.79-5.81) for the density operator have a simple physical interpretation: they show that the density operator decays to thermal equilibrium, at a temperature set by the temperature of the reservoir.

Problem 5.13

Use Eqns (5.79-5.81) to show that the long-time behaviour of the density operator is to evolve to the density operator for thermal equilibrium of

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[3] See Scully and Zubairy *Quantum Optics* §6.3 for a derivation of the rate constant Γ.

the atom

$$\begin{aligned} \rho_{uu} &= 1-\rho_{dd}=\frac{1}{1+\exp(\beta\hbar\omega)} && (5.82)\\ \rho_{ud} &= 0 && (5.83) \end{aligned}$$

Furthermore, even if the reservoir is at zero temperature (no photons), the coupling to the reservoir leads to a time-evolution of the system's density operator:

$$\begin{aligned} \dot{\rho}_{uu} &= -\Gamma\rho_{uu} && (5.84)\\ \dot{\rho}_{ud} &= -\frac{\Gamma}{2}\rho_{ud} && (5.85)\\ \dot{\rho}_{dd} &= \Gamma\rho_{uu} && (5.86) \end{aligned}$$

The evolution of the diagonal components of the density operator represent the relaxation of the system into the low-energy atomic state (the "d" state), through the emission of energy as a photon. Simultaneously, we see that there is a decay of the off-diagonal element $\rho_{ud}=\rho^*_{du}$: this decay represents the "decoherence" of any superposition state of the "u" and "d" states, through its coupling to the environment. Thus we have an explicit calculation of the relaxation and decoherence of a quantum system due to its coupling to a reservoir.

6

Introduction to Lie groups

> Good heavens! For more than forty years I have been speaking prose without knowing it.
>
> M. Jourdain, *Le Bourgeois Gentilhomme*

Often without acknowledging it explicitly, we use symmetry repeatedly in our analysis of physical problems. At a very basic level, we assume that the laws of physics are the same at all locations in space and all moments in time. In other words, that physics is invariant under **translations** in space and time.

Other problems are simplified by the use of **rotational** symmetry. For instance, the partial wave expansion of Chapter 3 was only really useful when there was no scattering between the different partial waves, on account of the assumed spherical symmetry of the potential.

As a final example, it's sometimes useful to analyse motion in a reference frame moving relative to our own, exploiting the **principle of relativity**, which comes in **Galilean**, **special** and **general** flavours.

What these three examples have in common is that they are each characterized by a continuum of possible **symmetry transformations**. That is, we can translate arbitrary distances, rotate through arbitrary angles about arbitrary axes, and pass to a frame moving with arbitrary velocity (up to the speed of light, in the case of Einstein's theory). This situation should be contrasted with **discrete symmetry**, where there are only a finite number, or a discrete infinity of such operations. Parity symmetry (just one non-trivial symmetry operation) is an example of the former, whereas the discrete translational invariance of a periodic structure such as a crystal illustrates the latter case.

It would be quite reasonable if the above list of continuous symmetries – which are more or less obvious in the world around us[1] – was exhaustive. Symmetry would still be very useful concept, and well worth studying. Remarkably, however, there are new symmetries in the subatomic world that don't have any analog beyond the scale of the nucleus. Perhaps most importantly, **Quantum Chromodynamics**, the theory of quarks and gluons, involves a symmetry between the three colours of quark called $SU(3)$.

The mathematical structure corresponding to continuous symmetries, of which $SU(3)$ is an example, is called a **Lie group**, and is the subject of this chapter.

[1] This isn't really true for the principle of relativity: it took Galileo to make the point that an experiment below deck on a steadily moving ship could not detect its motion.

6.1 Symmetries in quantum physics

Symmetries are groups

The result of performing one symmetry transformation and then another is itself a symmetry transformation. This basic feature tells us that symmetry transformations form a **group**.

In 1B Maths, you've already met the definition of a group, which is a set of **elements** $\{g_1, g_2, \ldots\}$ and an operation called the **group law**, which takes two elements and gives us a third. We'll normally refer to this operation as a product and write it accordingly i.e. $g_1 g_2$, bearing in mind that in general $g_1 g_2 \neq g_2 g_1$. When $g_1 g_2 = g_2 g_1$ for all pairs of elements the group is called **abelian**. In the case of symmetry transformations, the group law is obvious: perform one symmetry transformation and then the next.

By definition, the group product satisfies the conditions of

- **Associativity** $g_1(g_2 g_3) = (g_1 g_2) g_3$. Probably the only operation you will have met so far where this property fails is the vector product $(\mathbf{a} \times \mathbf{b}) \times \mathbf{c} \neq \mathbf{a} \times (\mathbf{b} \times \mathbf{c})$.
- **Identity** A group must contain the 'do nothing' element, often denoted e, such that $eg = ge = g$ for all g in the group.
- **Inverse** For every g in the group, there's an element, denoted g^{-1}, such that $gg^{-1} = g^{-1}g = e$.

This definition includes a great many things with which you are familiar. For example, the integers form a group with the group law corresponding to addition. In fact, it is so general that it's actually quite hard to think of mathematical objects that physicists make regular use of that are not groups. For this reason, mathematicians narrow things down by specifying further properties. One of the great triumphs of 20th Century mathematics was the classification of **finite simple groups**, which roughly corresponds to those finite groups that can't be broken down into simpler constituents.

Symmetries and unitary transformations

In quantum physics a symmetry transformation leads to a transformation of every quantum state $|\Psi\rangle$ to a unique state $|\Psi'\rangle$. To qualify as a symmetry, the transformation must preserve probabilities

In discussing symmetry in physics, one can always take an **active** or a **passive** view. In the active view, the system is really altered by the symmetry transformation (e.g. rotated). In the passive view, the system is unchanged, but we imagine changing the way our measurements are made (rotating our coordinate axes, for example). In both cases, we have a symmetry if the relations between the new measurements are the same as the relations between the old measurements.

$$\left|\langle\Phi'|\Psi'\rangle\right|^2 = \left|\langle\Phi|\Psi\rangle\right|^2, \tag{6.1}$$

for all pairs $|\Psi\rangle$ and $|\Phi\rangle$. What kind of transformation has this property? Unitary transformations certainly fit the bill. These are linear transformations with the property

$$U^\dagger U = \mathbb{1}. \tag{6.2}$$

All of the symmetries that we will study are described by unitary transformations.

TANGENT If the transformation is linear, then to satisfy Eq. (6.1) it must be unitary. But who said it had to be linear? An important theorem proved by Eugene Wigner, one of the pioneers of the application of the group theory to quantum physics, states that if Eq. (6.1) is satisfied the transformation must have the form

$$|\Psi'\rangle = \exp\left(i\theta(\Psi)\right) U \left|\Psi\right\rangle. \tag{6.3}$$

Here U is either unitary or **antiunitary**, a property we'll define in a moment, and $\theta(\Psi)$ is a phase function that depends on the state $|\Psi\rangle$. We won't discuss the proof of this theorem: see (**?**).

The single most important example of an antiunitary operation is provided by complex conjugation $K : \Psi(\mathbf{r}) \to \Psi^*(\mathbf{r})$. This operation is **antilinear**

$$K(\alpha\Psi(\mathbf{r}) + \beta\Phi(\mathbf{r})) = \alpha^*\Psi^*(\mathbf{r}) + \beta^*\Phi^*(\mathbf{r}) = \alpha^* K\Psi(\mathbf{r}) + \beta^* K\Phi(\mathbf{r}) \tag{6.4}$$

The Hermitian conjugate of $K^\dagger = K$, and we have

$$K^\dagger K = \mathbb{1}. \tag{6.5}$$

This is the same condition that defines a unitary linear operator unitary, but since K is antilinear, we call it antiunitary.

Antilinear operators are unpleasant to work with in the 'bra-ket' notation. Consider the obvious identity

$$\int d\mathbf{r}\, (K\Phi(\mathbf{r}))^* K\Psi(\mathbf{r}) = \int d\mathbf{r}\, \Psi^*(\mathbf{r})\Phi(\mathbf{r}). \tag{6.6}$$

It's tempting to write this in Dirac notation as

$$\langle\Phi|K^\dagger K|\Psi\rangle = (\langle\Phi|\Psi\rangle)^*, \tag{6.7}$$

but of course, this is inconsistent with Eq. (6.5). The problem is that we are used to gamely allowing operators to act to the left or to the right. However, the right hand side of Eq. (6.7) is antilinear in $|\Psi\rangle$ while the left hand side is linear, if $K^\dagger$ is taken to act to the right. It's best to always let operators act on kets, and then take the corresponding bra.

It would be nice to not have to bother with antiunitary operations at all, but unfortunately there is one important example: **time reversal symmetry**. A less snappy, but more accurate name is *symmetry under reversal of motion*, which was the term introduced by Wigner in 1932. This symmetry is fairly evident in Newton's law

$$\ddot{\mathbf{r}} = -\nabla V(\mathbf{r}), \tag{6.8}$$

where $\mathbf{r}(-t)$ is a solution if $\mathbf{r}(t)$ is, on account of the double time derivative (that's why single time derivatives, describing friction or magnetic forces, break time reversal symmetry). In the Schrödinger equation

$$i\hbar\partial_t\Psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r},t). \tag{6.9}$$

The corresponding transformation is $\Psi(\mathbf{r},t) \to \Psi^*(\mathbf{r},-t)$, i.e. just the operation K we introduced above.

Time reversal symmetry is particular interesting for systems with half integer spin (such as an odd number of electrons), where it gives rise to a two fold degeneracy called **Kramers degeneracy**.

6.2 *Rotations as a Lie group*

We are going to take whirlwind tour of some of the properties of **Lie groups**, taking the rotations in three dimensions as our principal example. The net effect will be a lot of new names for things you are already familiar with, but the idea is to develop an appreciation that the ideas have a greater generality.

What is a rotation? It is a transformation that does not distort shape i.e. a *rigid* motion, which also has a point fixed (so that translations are not allowed). It's not hard to see that a rotation is therefore a linear transformation

$$\mathbf{x} \to \mathsf{R}\mathbf{x}, \tag{6.10}$$

subject to

$$\mathsf{R}^T\mathsf{R} = \mathbb{1}. \tag{6.11}$$

That is, rotations are described by **orthogonal** matrices. The orthogonality condition is really 6 conditions ($\mathsf{R}^T\mathsf{R}$ is symmetric), and so reduces the number of free parameters in a 3×3 matrix from 9 to 3. This is consistent with common sense: specifying a rotation involves a choice of axis (2 parameters) and rotation angle.

The product of two orthogonal matrices is an orthogonal matrix: they form a group. This group is denoted $\mathbf{O(3)}$: the group of 3×3 orthogonal matrices. Matrices satsifying Eq. (6.11) have $(\det \mathsf{R})^2 = 1$, so this includes matrices satisfying $\det \mathsf{R} = -1$, which are called **improper rotations**. They are a combination of a rotation and a parity transformation $(x, y, z) \to (-x, -y, -z)$. We now restrict ourselves to proper rotations with $\det \mathsf{R} = 1$, these form a subgroup of $O(3)$ called $\mathbf{SO(3)}$, where the S is for **special**, a not-very-descriptive name designating unit determinant.

The order in which rotations are performed is important, as you can verify by subjecting this handout to quarter turns about various axes. Thus the rotation group is **nonabelian**.

Lie algebras

You are familiar with the angular velocity vector, in terms of which the velocity of a particle may be written

$$\dot{\mathbf{r}} = \boldsymbol{\omega} \times \mathbf{r}. \tag{6.12}$$

This may be written as a matrix equation

$$\dot{\mathbf{r}} = \Omega\mathbf{r}, \tag{6.13}$$

where

$$\Omega = \begin{pmatrix} 0 & -\omega_z & \omega_y \\ \omega_z & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{pmatrix} \quad \text{or} \quad \Omega_{jk} = -\omega_i \varepsilon_{ijk}. \tag{6.14}$$

Note that Ω parametrizes the most general real antisymmetric matrix. If we regard Eq. (6.12) as a differential equation, the solution is (assuming Ω constant)

$$\mathbf{r}(t) = \exp\left(\Omega t\right)\mathbf{r}(0). \tag{6.15}$$

Problem 6.1

Verify that $\exp\left(\Omega t\right)$ is a rotation matrix i.e. it is orthogonal.

Introducing the matrices

$$A_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{6.16}$$

we can write $\Omega = \boldsymbol{\omega} \cdot \mathsf{A}$. The rotation matrices can then be written

$$\mathsf{R} = \exp\left(\boldsymbol{\theta} \cdot \mathsf{A}\right) \tag{6.17}$$

where $\boldsymbol{\theta} \equiv \boldsymbol{\omega} t$ is a vector whose direction gives the axis of rotation, and whose magnitude is the rotation angle.

It is important that we have restricted ourselves to $SO(3)$, the group of proper rotations. The improper rotations cannot be written in this way, as they are not connected to the identity. We say that $O(3)$ has two **connected components**, and $SO(3)$ is the **identity component** of $O(3)$.

Problem 6.2

Show that if $\boldsymbol{\theta} = \theta\hat{\mathbf{n}}$

$$\mathsf{R}\mathbf{r} = \mathbf{r}\cos\theta + \hat{\mathbf{n}} \times \mathbf{r}\sin\theta + \hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \mathbf{r})(1 - \cos\theta). \tag{6.18}$$

The representation of Lie group elements by exponentials is very natural for the following reason. An element X of a general (matrix) Lie group that is close to the identity has the form

$$\mathsf{X} = \mathbb{1} + \epsilon\mathsf{x} + \cdots$$

for ϵ some small quantity. This seems restricted to group elements within an ϵ of the identity, but now we can exploit the group property by raising these elements to a high power. By the definition, the result is still in the group. Furthermore,

$$\lim_{N\to\infty}\left(\mathbb{1} + \frac{\mathsf{x}}{N}\right)^N = \exp(\mathsf{x}) \tag{6.19}$$

Thus, exponentiation of the matrices x describing infinitesimal transformations gives us *finite* transformations.

The defining features of the Lie group imply some conditions on x. For instance, in the case of rotations we have

$$\mathsf{R} = \mathbb{1} + \epsilon\mathsf{r},$$

and

$$\mathsf{R}^T\mathsf{R} = (\mathbb{1} + \epsilon\mathsf{r}^T + \cdots)(\mathbb{1} + \epsilon\mathsf{r} + \cdots) = \mathbb{1} + \epsilon(\mathsf{r} + \mathsf{r}^T) + \cdots = \mathbb{1}$$

Thus $\mathsf{r} = -\mathsf{r}^T$. You have already verified that the finite transformations $\mathsf{R} = \exp(\mathsf{r})$ satisfies the group property.

The matrices x form a vector space called a **Lie algebra**. In order to generate group elements upon exponentiation, they must 'inherit' some defining conditions from the Lie group. These conditions are always expressed as linear equations – antisymmetry in the case of the rotations. By choosing a complete basis of matrices satisfying these conditions a general element can be written as a linear superposition, as we did when we wrote $\mathsf{r} = \boldsymbol{\theta} \cdot \mathsf{A}$ above.

The A_i matrices are known as the **generators** of the rotations. They do not commute with each other

$$\left[\mathsf{A}_i, \mathsf{A}_j\right] = \varepsilon_{ijk}\mathsf{A}_k, \tag{6.20}$$

which gives rise to the nonabelian nature of the rotations, because

$$\mathsf{R}(\boldsymbol{\theta}_1)\mathsf{R}(\boldsymbol{\theta}_2) \neq \mathsf{R}(\boldsymbol{\theta}_1 + \boldsymbol{\theta}_2). \tag{6.21}$$

A natural question is therefore: what $\boldsymbol{\theta}$ does result from this composition of rotations? We can get some idea of what is going on by expanding the exponentials. Retaining only terms to second order gives

$$\begin{aligned} \left[1 + \boldsymbol{\theta}_1 \cdot \mathsf{A} + \frac{1}{2}(\boldsymbol{\theta}_1 \cdot \mathsf{A})^2 + \cdots\right]\left[1 + \boldsymbol{\theta}_2 \cdot \mathsf{A} + \frac{1}{2}(\boldsymbol{\theta}_2 \cdot \mathsf{A})^2 + \cdots\right] &= \\ 1 + (\boldsymbol{\theta}_1 + \boldsymbol{\theta}_2) \cdot \mathsf{A} + \frac{1}{2}((\boldsymbol{\theta}_1 + \boldsymbol{\theta}_2) \cdot \mathsf{A})^2 + \frac{1}{2}[\boldsymbol{\theta}_1 \cdot \mathsf{A}, \boldsymbol{\theta}_2 \cdot \mathsf{A}] \cdots &= \\ 1 + \left(\boldsymbol{\theta}_1 + \boldsymbol{\theta}_2 + \frac{1}{2}\boldsymbol{\theta}_1 \times \boldsymbol{\theta}_2\right) \cdot \mathsf{A} + \frac{1}{2}((\boldsymbol{\theta}_1 + \boldsymbol{\theta}_2) \cdot \mathsf{A})^2 + \cdots. \end{aligned} \tag{6.22}$$

This shows that to second order in the angles, the composition of two rotations is $\mathsf{R}(\boldsymbol{\theta}_1 + \boldsymbol{\theta}_2 + \frac{1}{2}\boldsymbol{\theta}_1 \times \boldsymbol{\theta}_2)$. Note that to obtain this result, all we needed was the *commutation relations* Eq. (6.20). It turns out that this is true generally: if we want to reorder the product of the two series in Eq. (6.22) as a single exponential series in some linear combination of the generators, we just need the commutations relations. This result is known as the **Baker–Campbell-Hausdorff** formula. Just for fun we give the next term to illustrate the point

$$\begin{aligned}\log\left[\mathsf{R}(\boldsymbol{\theta}_1)\mathsf{R}(\boldsymbol{\theta}_2)\right] &= \boldsymbol{\theta}_1\cdot\mathsf{A} + \boldsymbol{\theta}_2\cdot\mathsf{A} + \frac{1}{2}\left[\boldsymbol{\theta}_1\cdot\mathsf{A}, \boldsymbol{\theta}_2\cdot\mathsf{A}\right] \\ &+ \frac{1}{12}\left[\boldsymbol{\theta}_1\cdot\mathsf{A}, \left[\boldsymbol{\theta}_1\cdot\mathsf{A}, \boldsymbol{\theta}_2\cdot\mathsf{A}\right]\right] - \frac{1}{12}\left[\boldsymbol{\theta}_2\cdot\mathsf{A}, \left[\boldsymbol{\theta}_1\cdot\mathsf{A}, \boldsymbol{\theta}_2\cdot\mathsf{A}\right]\right] + \cdots \\ &= \left(\boldsymbol{\theta}_1 + \boldsymbol{\theta}_2 + \frac{1}{2}\boldsymbol{\theta}_1\times\boldsymbol{\theta}_2 + \frac{1}{3}\left[(\boldsymbol{\theta}_1\cdot\boldsymbol{\theta}_2)(\boldsymbol{\theta}_1+\boldsymbol{\theta}_2) - \boldsymbol{\theta}_1^2\boldsymbol{\theta}_2 - \boldsymbol{\theta}_2^2\boldsymbol{\theta}_1\right] + \cdots\right)\cdot\mathsf{A}\end{aligned} \tag{6.23}$$

For harmonic oscillator variables a and $a^\dagger$ Problem 6.3 gives

$$e^{za - z^* a^\dagger} e^{z' a - z'^* a^\dagger} = e^{\left[z+z'\right]a - \left[z^* + z'^*\right]a^\dagger} \times e^{-\operatorname{Im}\left[zz'^* - z^* z'\right]}.$$

Note that the same group law arises from multiplication of the matrices

$$\begin{pmatrix} 1 & z & \frac{1}{2}|z|^2 + it \\ 0 & 1 & z^* \\ 0 & 0 & 1 \end{pmatrix}$$

This is the **Heisenberg group**.

Problem 6.3

Suppose that $[A, B] = C$ commutes with both A and B. Show that

$$\exp(A)\exp(B) = \exp(A+B)\exp\left(\frac{1}{2}[A,B]\right). \tag{6.24}$$

This shows that the commutation relations encode the same information as the group composition law: they define a **Lie algebra**. The relationship between the elements of the Lie algebra and the corresponding Lie group is provided by the **exponential map**. The defining properties of the group elements (orthogonal matrices, in the case of the rotations) correspond to defining properties of the elements of the algebra (antisymmetric matrices).

An **algebra** is a structure which is both a vector space – so one can add elements and multiply them by numbers – and has a bilinear product. A Lie algebra is then an algebra where the product, normally denoted $[\cdot,\cdot]$ is antisymmetric and satisfies the **Jacobi identity**

$$[x,[y,z]] + [z,[x,y]] + [y,[z,x]] = 0$$

The commutator has both of these properties, though one can study the properties of Lie algebras without explicitly identifying $[\cdot,\cdot]$ with a commutator.

Problem 6.4

Show that the commutator of two antisymmetric matrices is antisymmetric.

By convention, the name of the Lie algebra is the name of the corresponding group in lower case: $\mathbf{so}(\mathbf{3})$ in this case.

Representations

We will consider symmetries that act as unitary transformations on the Hilbert space of quantum states. We say that these transformations form a **unitary representation** of the symmetry transformations. For the rotations, this means that we associate with any rotation R a unitary transformation $U(\mathsf{R})$ with the property

$$U(\mathsf{R}_1)U(\mathsf{R}_2) = U(\mathsf{R}_1\mathsf{R}_2). \tag{6.25}$$

Of course, taking $U(\mathsf{R}) = \mathbb{1}$ would do the trick, but that is hardly what we are after. Rather, we seek **faithful** representations, which means that distinct rotations are represented by distinct transformations.

That is, the composition of unitary transformations reflects the group composition law. If states transform as

$$\mathsf{R} : |\Psi\rangle \to |\Psi'\rangle = U(\mathsf{R})\,|\Psi\rangle\,, \tag{6.26}$$

then the wavefunction $\Psi(\mathbf{r}) = \langle \mathbf{r}|\Psi\rangle$ transforms as

$$\mathsf{R} : \Psi(\mathbf{r}) \to \Psi'(\mathbf{r}) = \langle \mathsf{R}^{-1}\mathbf{r}|\Psi\rangle = \Psi(\mathsf{R}^{-1}\mathbf{r}) \tag{6.27}$$

(in the last step we used unitarity). What can we deduce about the form of $U(\mathsf{R})$? We first define

$$L_k = -i\hbar\varepsilon_{klm}x_l\frac{\partial}{\partial x_m}, \tag{6.28}$$

and then observe that

$$L_k\mathbf{x} = -i\hbar\mathsf{A}_k\mathbf{x}. \tag{6.29}$$

$\Psi(\mathsf{R}^{-1}\mathbf{r})$ is a rotation of the wavefunction by R for the same reason that $f(x-y)$ is the function $f(x)$ shifted by y.

You may notice that the commutator of the L_k (Eq. (6.31)) differs by a sign from that implied by Eq. (6.29). This stems from the slightly awkward fact that the effect on the wavefunction of the rotation $\mathsf{R}_1\mathsf{R}_2$ is $\Psi(R_2^{-1}R_1^{-1}\mathbf{r})$.

Problem 6.5

Show that

$$U(\mathsf{R}) = \exp\left(-i\boldsymbol{\theta}\cdot\mathbf{L}/\hbar\right) \tag{6.30}$$

L is of course the operator of orbital angular momentum. We have shown that this is a representation of the generators of rotations (or it generates the representation of rotations, whichever you prefer). As you know, the components of **L** satisfy

$$[L_k, L_l] = i\hbar\varepsilon_{klm}L_m \tag{6.31}$$

Is this a unitary representation? Yes, because it is clear that Eq. (6.27) preserves the inner product between states. Alternatively,

Problem 6.6

Show that the exponential of any anti-Hermitian operator is unitary.

Corresponding to Eq. (6.26), operators transform as

$$\mathsf{R} : \mathcal{O} \to \mathcal{O}' = U^\dagger(\mathsf{R})\mathcal{O}U(\mathsf{R}). \tag{6.32}$$

Quantities that are preserved under rotations therefore commute with the generators. If the Hamiltonian is such a quantity, **L** does not change in time by the Heisenberg equations of motion: it is conserved.

The fact that $\left[\mathbf{L}^2, \mathbf{L}\right] = 0$ means that the representation is **reducible**: it does not mix subspaces corresponding to different eigenvalues of $\mathbf{L}^2$. As you already know, the possible eigenvalues of $\mathbf{L}^2$ are $\hbar^2 l(l+1)$ for $l = 0, 1, \ldots$ and each subspace has dimension $2l+1$. Conventionally, one takes a basis within each subspace consisting of the eigenstates of L_z with eigenvalues $m = l, l-1, \ldots, -l$. The corresponding wavefunctions have angular parts given by the spherical harmonics $Y_{lm}(\theta, \phi)$.

The matrices representing the rotations are therefore **block diagonal**, with the different blocks corresponding to different $\mathbf{L}^2$ values.

Within the subspace corresponding to each l value, the rotations are represented by $(2l+1)\times(2l+1)$ matrices. These representations are **irreducible** – they cannot be reduced further. If you picture $U(\mathsf{R})$ as a big matrix acting in the space spanned by states of different l and m, it will be **block diagonal**, with each square block on the diagonal corresponding to a given l value. If **L** (or more generally total angular momentum) is conserved these irreducible representations correspond to **symmetry multiplets**: degenerate subspaces spanned by states of the same energy.

The three dimensional $l = 1$ representation is the **fundamental** representation – the smallest faithful representation. It corresponds to the original representation in terms of 3×3 orthogonal matrices.

One way to make new representations out of old is to take the **tensor product** of representations.

First we have to understand what a tensor product of vectors is. Take one vector with components v_i from one vector space V of dimension d_V, and another with components w_j from space W of dimension d_W, and form the $d_V \times d_W$ matrix (or second rank tensor) $v_i w_j$. This is denoted $v \otimes w$, and is called the tensor product of v and w.

Now do this with all pairs of vectors forming bases in V and W. The resulting set of matrices, numbering $d_V \times d_W$, by definition span the tensor product space $V \otimes W$.

If we have a representation of a group on V and on W, then we get for free a representation on $V \otimes W$. Taking the fundamental representation as an example, this is because we know the transformation law for $v_i w_j$ from the transformation law for v and w

$$\begin{gathered} v_i \to v_i' = R_{ij} v_j, \qquad w_i \to w_i' = R_{ij} w_j \\ v_i w_j \to v_i' w_j' = R_{ik} R_{jl} v_k w_l. \end{gathered} \tag{6.33}$$

Because vectors of the form $v_i w_j$ span the tensor product space, this means that for *any* second rank tensor

$$T_{ij} \to T_{ij}' = R_{ik} R_{jl} T_{kl}, \qquad \text{or} \qquad \mathsf{T} \to \mathsf{T}' = \mathsf{R}\mathsf{T}\mathsf{R}^T. \tag{6.34}$$

However, this representation is not irreducible.

Problem 6.7

Show that this representation breaks into three:

1. Matrices proportional to the identity (1 component).
2. Antisymmetric matrices (3 components).
3. Symmetric traceless matrices (5 components).

The means that under the action Eq. (6.34), each of these three forms is preserved. Explicitly, $v_i w_j$ is decomposed as

$$v_i w_j = \frac{\mathbf{v}\cdot\mathbf{w}}{3}\delta_{ij} + \frac{1}{2}\left(v_i w_j - v_j w_i\right) + \frac{1}{2}\left(v_i w_j + v_j w_i - \frac{2\mathbf{v}\cdot\mathbf{w}}{3}\delta_{ij}\right) \tag{6.35}$$

The relationship found in Problem 6.7 can be written in shorthand as

$$\mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{3} \oplus \mathbf{5}, \tag{6.36}$$

where the number denotes the dimension of the representation (this assumes that there is not more than one inequivalent[2] representation of each dimension, which is the case here)

The three representations on the right hand side of Eq. (6.36) correspond to the $l = 0$, 1 or 2 representations. You have seen this pattern before when you discussed the addition of angular momenta: adding two $l = 1$ can give $l = 0$, 1 or 2 (see **AQP**).

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[2] **Equivalent representations** are those related by similarity transformation.

The problem of addition of angular momenta is therefore equivalent to decomposing the tensor product of representations into irreducible representations – a fine example of speaking in prose!

The fact that the irreducible unitary representations of the rotation group are finite dimensional is not obvious. It is a consequence of the group being **compact**, an idea we'll meet shortly.

$SU(2)$

As you know, *spin* angular momentum can be half odd integer, as well as integer. Spin $1/2$ is represented by the 2×2 matrices $\mathsf{S}=\frac{\hbar}{2}\boldsymbol{\sigma}$, where $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ are the Pauli matrices. Corresponding to Eq. (6.30), we expect the effect of a rotation on spin $1/2$ states to be

$$\mathsf{U}(\boldsymbol{\theta})=\exp\left(-i\boldsymbol{\theta}\cdot\mathsf{S}/\hbar\right)=\exp\left(-i\boldsymbol{\theta}\cdot\boldsymbol{\sigma}/2\right). \tag{6.37}$$

This parametrizes the most general 2×2 unitary matrix with determinant equal to 1. This is a group in its own right called $\mathbf{SU(2)}$: the group of special (unit determinant), unitary 2×2 matrices.

Problem 6.8

What property of the generators corresponds to the determinant of $\mathsf{U}(\boldsymbol{\theta})$ being equal to 1? Notice that going from $U(2)$ to $SU(2)$ reduces the dimension of the group, whereas going from $O(3)$ to $SO(3)$ does not.

Eq. (6.37) shows that there is a relationship between $SO(3)$ and $SU(2)$.

Problem 6.9

Show that if $\boldsymbol{\theta}=\theta\hat{\mathbf{n}}$

$$\mathsf{U}(\boldsymbol{\theta})=\mathbb{1}\cos\left(\theta/2\right)-i\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}\sin\left(\theta/2\right) \tag{6.38}$$

Comparing Eq. (6.38) with Eq. (6.18) we see that when $\theta=2\pi$, $\mathsf{R}=\mathbb{1}$ whereas $\mathsf{U}=-\mathbb{1}$. More generally, θ and $\theta+2\pi$ correspond to the same rotation (as should be obvious) but different $SU(2)$ matrices.

To make the relationship between these two groups explicit, consider the transformation

$$\mathsf{S}\to\mathsf{S}'=\mathsf{U}(\boldsymbol{\theta})\mathsf{S}\mathsf{U}^\dagger(\boldsymbol{\theta}) \tag{6.39}$$

Eq. (6.41) is a representation of a Lie group on its own generators called the **adjoint representation**.

Problem 6.10

Use the formula

$$\exp\left(A\right)B\exp\left(-A\right)=B+[A,B]+\frac{1}{2!}[A,[A,B]]+\frac{1}{3!}[A,[A,[A,B]]]+\cdots \tag{6.40}$$

to show

$$\mathsf{U}(\boldsymbol{\theta})\mathsf{S}\mathsf{U}^\dagger(\boldsymbol{\theta})=\mathsf{R}^{-1}(\boldsymbol{\theta})\mathsf{S} \tag{6.41}$$

Eq. (6.41) gives an explicit map from $SU(2)$ matrices to $SO(3)$ matrices which respects the group structure i.e. the rotation corresponding to $\mathsf{U}_1\mathsf{U}_2$ is $\mathsf{R}_2\mathsf{R}_1$. Such a map is called a group **homomorphism**. Since $\pm\mathsf{U}$ give rise to the same R, the map is two-to-one. Regarded as a representation of $SU(2)$, it is not faithful. Though the groups are different, they are identical in the vicinity of the identity, and thus the Lie algebras coincide: $so(3) \simeq su(2)$.

A homomorophism that is one-to-one is called an **isomorphism**.

Topological features

The elements of a Lie group are a continuum. Therefore it is appropriate to ask what kind of space – or **manifold** – they form. The dimension of the space is just the number of parameters of the group. But what about the *shape* of this space? For $SU(2)$ it is not hard to figure out. Eq. (6.38) can be written

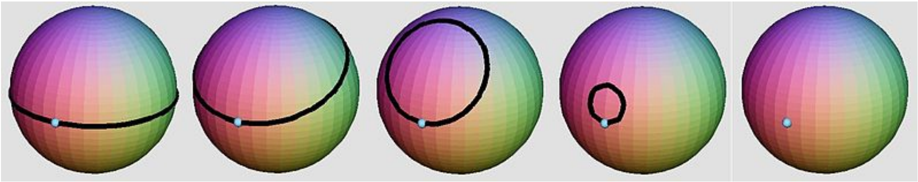
$$\mathsf{U} = a_0\mathbb{1} + \mathbf{a}\cdot\boldsymbol{\sigma} \tag{6.42}$$

subject to $a_0^2 + \mathbf{a}^2 = 1$. Thus we can identify $SU(2)$ with a **3-sphere**. What about $SO(3)$? Eq. (6.41) shows that $(a_0, \mathbf{a})$ and $(-a_0, -\mathbf{a})$ correspond to the same element of $SO(3)$. Thus $SO(3)$ is a 3-sphere *with anitpodal points identified*. Just for the record, the proper mathematical name for this space is **real projective space**, or $\mathbf{RP}^3$.

There is some potential for confusion here. What a mathematician calls a 3-sphere – denoted $\mathbf{S}^3$ – a physicist may call the surface of a four dimensional sphere. We stick with the mathematical name as it immediately conveys the dimension of the space.

If you find this idea a bit strange, the following simpler example may help. If we take a line and identify points that differ by integer multiples of some fixed amount (this is the same thing as imposing periodic boundary conditions), the result is a circle. Doing the same in two dimensions (e.g. $\mathbf{r} \simeq \mathbf{r} + p\hat{\mathbf{x}} + q\hat{\mathbf{y}}$ for p, q integer) results in a torus. These identifications do not change the space locally, but affect the global topology.

To quantify how the identification of antipodal points alters the 3-sphere, we need to introduce one of the most basic notions of topology. We say that a space is **simply connected** if any closed path in that space can be continuously contracted to nothing. Evidently this is possible for paths on the 2-sphere, and it probably won't surprise you to learn that the same holds for the 3-sphere.



TANGENT The **Poincaré conjecture** stated that every simply connected, closed three dimensional manifold is **homeomorphic** (roughly: equivalent if we allow space to be smoothly deformed) to a 3-sphere. I say 'stated' because after roughly a century of effort this conjecture was proven in 2002-2003 by the Russian mathematician Grigori Perelman. The Poincaré conjecture was of such fundamental importance in topology, and so stubbornly resistant to proof[3], that it was offered as one of the Millenium Prize Problems by the Clay Mathematics Institute, with a prize of one million dollars. You might suppose, given the timing, that the money played a decisive role, but in fact Perelman declined the prize when it was offered in 2010, having already refused the Fields Medal (a.k.a. the Nobel Prize of

[3] As is often the case, the higher and lower dimensional analogs turned out to be easier. The four dimensional case was proven in 1982 by Michael Freedman.

mathematics) in 2006.

What about $SO(3)$? It's not hard to see that there are closed paths that *cannot* be contracting to nothing, namely those joining two antipodal points on the 3-sphere: remember that these are the *same* point in $SO(3)$.

What is the implication for the rotations? Consider a rotation unfolding as a function of time (or some other parameter), with the rotation angle increasing smoothly from 0 to 2π, whereupon a body would be returned to its original position. This sequence of transformations – a closed path in $SO(3)$ – cannot be smoothly deformed to a trivial sequence where the body remains unrotated. However, if the angle increases from 0 to 4π, the resulting path can be deformed to nothing.

This fact is sufficiently surprising that it demands a visual proof that makes no use of the machinery of matrices and groups. The following one is due to Hermann Weyl. As a warm up, consider one coin rolling around the circumference of another fixed coin of equal size. If you haven't seen this problem before, you should convince yourself that in rolling once around the circumference of the fixed coin, the rolling coin rotates twice.

A somewhat similar example comes from astronomy: the Earth rotates on its axis $366\frac{1}{4}$ times in one year.

Now imagine two cones in contact: one fixed in space and the other free to roll on the first. Let the half angle of the cones increase from zero to $\pi/2$. When the angle is small, the situation is almost identical to the two coin problem: the rolling cone rotates by (almost) 4π when it rolls once around the fixed cone. As the half angle increases to $\pi/2$, the cones become almost flat surfaces, and the motion is reduced to a wobble, with vanishing rotation. This shows that a 4π rotation can be smoothly reduced to no rotation.

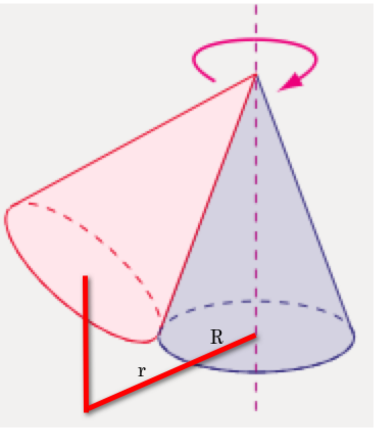


Figure 6.1: Weyl's demonstration.

One possible source of confusion in all of this is linguistic. When we say *rotation*, we may envisage a rotation unfolding in time i.e. a path in the group starting at the identity and finishing at some final rotation, or we may envisage only the final rotation. In the latter sense, there is of course no difference between a 2π rotation and no rotation.

Two more notions of topology are useful, but a bit more technical, so the following is only a rough discussion. We say that a space is **connected** if any two points can be connected by a path. As an example of a space that is not connected, consider the group $O(3)$. This includes one component, the subgroup $SO(3)$ of proper rotations, and another component consisting of the improper rotations (it's not a subgroup, as it does not contain the identity, and the composition of two improper rotations is proper). There is evidently no path starting in one component and ending in the other.

Finally, the notion of **compactness** roughly translates as *finite*. Thus $SU(2)$ and $SO(3)$ are compact groups, while the Lorentz group, which we'll meet in the next chapter, is not.

6.3 *How Pauli solved the Hydrogen atom*

In 1926, Erwin Schrödinger published his equation and showed that it gave the correct energy levels for the Hydrogen atom. Almost simultaneously, Wolfgang Pauli showed that the same result could be obtained using Heisenberg's *matrix mechanics* (see Section 2.1). You know how Schrödinger did it, but what about Pauli? It turns out that there is a higher symmetry hiding under our noses that allows a complete solution of the problem.

Before we get started, let's note the following fact, which seems to demand explanation. The energy levels of the Hydrogen Hamiltonian

This is in Gaussian units, so you won't see any factors of $4\pi\varepsilon_0$.

$$H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{|\mathbf{r}|}, \tag{6.43}$$

are

$$E_{nlm} = -\frac{me^4}{2\hbar^2}\frac{1}{n^2}. \tag{6.44}$$

We have labelled the eigenvalue by the **principal** (n), the **azimuthal** (l) and the **magnetic** (m) quantum numbers, but you will notice that the energy only depends on the first of these. An absence of dependence upon the magnetic quantum number is a natural consequence of rotational invariance, which one would expect to lead to a $(2l+1)$-fold degeneracy. The absence of any dependence on l is however surprising, and special to the case of a Coulomb potential. Since $l = 0, \ldots, n-1$, the result is that the overall degeneracy of each energy level is n^2, with $n = 1, 2, \ldots$. Since we know that degenerate multiplets can arise from symmetry, it's natural to ask whether this unexpectedly large degeneracy is the result of some 'hidden' symmetry, or what is the same thing, some extra conserved quantity.

In the Schrödinger picture, the solution of the radial equation involves the generalized Laguerre polynomials of order $n-l-1$, so that $n > l-1$.

In fact, an extra conservation law for the *classical* Hamiltonian was already well known to Pauli, and is called the **Runge–Lenz vector**

The Hamiltonian Eq. (6.43) is also known as the **Kepler problem**, for obvious reasons. In this context, the Runge–Lenz vector was discovered repeatedly over the years. For the somewhat murky history, see (**??**)

$$\mathbf{K} = \frac{1}{me^2}\mathbf{L}\times\mathbf{p} + \frac{\mathbf{r}}{|\mathbf{r}|}, \tag{6.45}$$

Problem 6.11

Use conservation of angular momentum and the equation of motion $m\dot{\mathbf{v}} = -e^2\mathbf{r}/|\mathbf{r}|^3$, to show that $d\mathbf{K}/dt = 0$. Show also that

$$\begin{aligned} \mathbf{K}\cdot\mathbf{L} &= 0 \qquad \text{and,} \\ \mathbf{K}^2 &= \frac{2H\mathbf{L}^2}{me^4} + 1 \end{aligned} \tag{6.46}$$

TANGENT That's all very well, but probably you find this a bit unsatisfactory. Where did $\mathbf{K}$ come from? What does it mean? The following picture, due to Hamilton, sheds a lot of light on the matter. In plane polar coordinates, the angular momentum perpendicular to the plane of motion is

$$L = mr^2\dot{\theta}. \tag{6.47}$$

We use this expression, and the equation of motion, to obtain the rate of change of the velocity with angle

$$\frac{d\mathbf{v}}{d\theta} = \frac{\dot{\mathbf{v}}}{\dot{\theta}} = -\frac{e^2}{L}\frac{\mathbf{r}}{|\mathbf{r}|} = -\frac{e^2}{L}\left(\cos\theta, \sin\theta\right). \tag{6.48}$$

This equation can be integrated to give

$$\mathbf{v}(\theta) = \mathbf{v}_0 - \frac{e^2}{L}\left(\sin\theta, -\cos\theta\right), \tag{6.49}$$

where $\mathbf{v}_0$ is a constant of integration. The motion in velocity space is even simpler than the motion in real space: the velocity vector moves on a circle of radius e^2/L centered on $\mathbf{v}_0$. The three possible motions are then:

Elliptic The origin (zero velocity) lies inside the circle, and the velocity vector performs complete circuits (at the same angular velocity as the position vector).

Hyperbolic The origin lies outside the circle, and the velocity vector moves on an arc of the circle, tending to the endpoints of the arc as $t \to \pm\infty$ and the particle move to infinity.

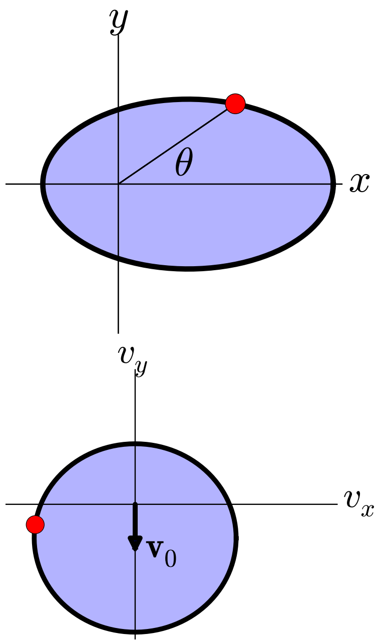


Figure 6.2: (Top) Elliptical orbit and (Bottom) hodograph indicating the direction of $\mathbf{v}_0$

Parabolic The intermediate case. The origin lies *on* the circle, and the velocity tends to zero as the particle escapes to infinity.

To find the relationship between the trajectory in velocity space – called the **hodograph** – and the Runge–Lenz vector, we first note that $\mathbf{v}_0$ and the maximum and minimum velocities are all collinear. The maximum velocity is achieved at the minimum distance, and vice versa. At these points the velocity and position are perpendicular, so the two terms of Eq. (6.45) point along the major axis, and are perpendicular to $\mathbf{v}_0$.

Problem 6.12

Use energy conservation at the maximum and minimum distances to show

$$\mathbf{v}_0 = -\frac{L}{e^2}\hat{\mathbf{z}} \times \mathbf{K} \tag{6.50}$$

$\mathbf{L}$, $\mathbf{K}$ and H subject to Eq. (6.46) represent five independent conserved quantities. Since phase space is six dimensional, fixing these five means motion is restricted to one dimension. In particular, all orbits are closed, a property that is special to the $1/r$ and r^2 potentials (this result is known as **Bertrand's theorem**).

Now, what about quantum mechanics? We have a small problem in that Eq. (6.45) is not Hermitian, but Pauli rectified that with the guess

Note that this isn't an issue for $\mathbf{L}$ itself.

$$\mathbf{K} = \frac{1}{2me^2}\left[\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}\right] + \frac{\mathbf{r}}{|\mathbf{r}|}, \tag{6.51}$$

which indeed commutes with the Hamiltonian. The next problem is to determine the *algebra* of these conserved quantities. We already know that

$$[L_k, L_l] = i\hbar\varepsilon_{klm}L_m. \tag{6.52a}$$

Furthermore, since $\mathbf{L}$ generates the rotations

$$[L_k, K_l] = i\hbar\varepsilon_{klm}K_m, \tag{6.52b}$$

as you can verify by direct calculation (generally, any vector operator will have this commutation relation with $\mathbf{L}$). Finally, and least trivially

$$[K_k, K_l] = i\hbar\varepsilon_{klm}L_m\left(\frac{-2H}{me^4}\right) \tag{6.52c}$$

Note that since $\mathbf{L}$ commutes with the Hamiltonian, it doesn't matter where we put H – we can think of it just as a number in these expressions.

Problem 6.13

[*Hard*] Prove Eq. (6.52c). Show further that the first of Eq. (6.46) continues to hold, while the second becomes

$$\mathbf{K}^2 = \frac{2H}{me^4}\left[\mathbf{L}^2 + \hbar^2\right] + 1 \tag{6.53}$$

Eqs. (6.52) can be put in a more symmetrical form by defining

$$\mathbf{L}^{\pm} = \frac{1}{2}\left(\mathbf{L} \pm \sqrt{\frac{me^4}{-2E}}\mathbf{K}\right), \tag{6.54}$$

(we assume that the energy – to be determined – is negative as we are interested in bound states) which satisfy

$$\begin{aligned}\left[L_k^+, L_l^+\right] &= i\hbar\varepsilon_{klm}L_m^+\\ \left[L_k^-, L_l^-\right] &= i\hbar\varepsilon_{klm}L_m^-.\\ \left[L_k^+, L_l^-\right] &= 0.\end{aligned} \tag{6.55}$$

We see that there are not one but *two* $su(2)$ algebras, whose generators commute with the Hamiltonian. The degenerate multiplets will then be tensor product representations characterized by a pair (s_+, s_-) of spin quantum numbers. Bearing in mind that $s_\pm$ can be integer or half integer, we instead define $n_\pm = 2s_\pm + 1$. The degeneracy of a multiplet is then n_+n_-. But then we notice that the condition $\mathbf{K}\cdot\mathbf{L} = 0$ implies

$$\left(\mathbf{L}^+ + \mathbf{L}^-\right)\cdot\left(\mathbf{L}^+ - \mathbf{L}^-\right) = 0, \tag{6.56}$$

or $\left(\mathbf{L}^+\right)^2 = \left(\mathbf{L}^-\right)^2$. Thus $n_+ = n_-$ and we have proved the existence of degenerate multiplets of size n^2 with $n = 1, 2, \ldots$. If we wish, these representations can be split up into irreducible representations of the angular momentum $\mathbf{L}^+ + \mathbf{L}^-$, using the usual addition rules

$$\mathbf{n}\otimes\mathbf{n} = (\mathbf{2n-1})\oplus(\mathbf{2n-3})\oplus\cdots\mathbf{1} \tag{6.57}$$

We are almost done: it remains only to find the eigenenergies.

Problem 6.14

Use Eq. (6.53) to find the energy levels Eq. (6.44).

$SO(4)$

It turns out that the sum of two $su(2)$ algebras Eq. (6.55) is isomorphic to another Lie algebra called $so(4)$. The corresponding group, $SO(4)$, is the group of rotations in four dimensions.

Although we've seen $su(2) \simeq so(3)$ and now $su(2)\oplus su(2) \simeq so(4)$, don't get the idea that this happens all the time. The list of isomorphisms between Lie algebras is actually rather short.

To see this relationship, we consider rotations in 4D in analogy with our treatment of $SO(3)$ in Section 6.2. The generators are the antisymmetric 4×4 matrices, and any such matrix may be expressed in terms of the six generators

$$\mathsf{L}_x = \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&-1\\0&0&1&0\end{pmatrix},\ \mathsf{L}_y = \begin{pmatrix}0&0&0&0\\0&0&0&1\\0&0&0&0\\0&-1&0&0\end{pmatrix},\ \mathsf{L}_z = \begin{pmatrix}0&0&0&0\\0&0&-1&0\\0&1&0&0\\0&0&0&0\end{pmatrix}$$
$$\mathsf{K}_x = \begin{pmatrix}0&-1&0&0\\1&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix},\ \mathsf{K}_y = \begin{pmatrix}0&0&-1&0\\0&0&0&0\\1&0&0&0\\0&0&0&0\end{pmatrix},\ \mathsf{K}_z = \begin{pmatrix}0&0&0&-1\\0&0&0&0\\0&0&0&0\\1&0&0&0\end{pmatrix}. \tag{6.58}$$

For $SO(3)$, Eq. (6.17) had an interpretation in terms of rotation axis, but this is special to three dimensions. The matrices of Eq. (6.58) generate rotations in planes specified by *pairs* of coordinates. Only in 3D does such a plane define a unique direction perpendicular to it.

The algebra of these generators is

$$\begin{aligned}[\mathsf{L}_k, \mathsf{L}_l] &= \varepsilon_{klm}\mathsf{L}_m\\ [\mathsf{L}_k, \mathsf{K}_l] &= \varepsilon_{klm}\mathsf{K}_m\\ [\mathsf{K}_k, \mathsf{K}_l] &= \varepsilon_{klm}\mathsf{L}_m.\end{aligned} \tag{6.59}$$

Eq. (6.52) coincides with this algebra after the redefinition

$$\begin{aligned}\mathbf{L} &\longrightarrow \frac{1}{i\hbar}\mathbf{L}\\ \mathbf{K} &\longrightarrow \frac{1}{i\hbar}\sqrt{\frac{me^4}{-2E}}\mathbf{K}.\end{aligned} \tag{6.60}$$

Eq. (6.53) becomes

$$\mathbf{L}^2+\mathbf{K}^2=\hbar^2+\frac{me^4}{2H}, \tag{6.61}$$

which plays the role of the conserved quantity $\mathbf{L}^2$ for $SO(3)$. The ground state is therefore an $SO(4)$ singlet, where the right hand side vanishes.

The $SO(4)$ symmetry turns out to have a remarkable *geometrical* significance. The motion in momentum space can be mapped to free motion on the 3-sphere, and $SO(4)$ is the symmetry group of this space. Furthermore, taking the energy to be *positive* has the effect of changing the signature of the metric from $(+,+,+,+)$ to $(-,+,+,+)$ (c.f. Eq. (6.60)), so the symmetry group becomes the **Lorentz group** of special relativity, which is the subject of the next chapter. These developments are described in (**??**).

Note that Eq. (6.61) is not satisfied by the matrices Eq. (6.59), but rather by their representations matrices, just as $\mathbf{L}^2=\hbar^2 l(l+1)$, with different l values for different representations. Eq. (6.59) is the fundamental representation, and has $\mathsf{L}^2+\mathsf{K}^2=-3$.

7
Relativistic quantum mechanics

Though relativity was still a young theory, it weighed heavily on the minds of the early quantum mechanics. In Schrödinger's notebooks from 1925, there appears the equation now known as the **Klein–Gordon equation**

Oskar Klein and Walter Gordon were two of the numerous people to rediscover it the following year.

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2c^2}{\hbar^2}\right]\Psi(\mathbf{r},t) = 0. \tag{7.1}$$

It's not hard to see the motivation for this equation. We can find plane wave solutions

$$\Psi(\mathbf{r},t) = \exp\left(i\left[\mathbf{p}\cdot\mathbf{r} - Et\right]/\hbar\right), \tag{7.2}$$

where the energy and momentum satisfy the familiar relativistic relationship

More formally, one can show that Eq. (7.1) is invariant under Lorentz transformations.

$$E^2 = \mathbf{p}^2c^2 + m^2c^4. \tag{7.3}$$

Eq. (7.1) therefore seems like a good candidate to replace the Schrödinger equation, which has free particle solutions satisfying $E = \mathbf{p}^2/2m$.

Schrödinger abandoned the Klein–Gordon equation after realising that it does not predict the fine structure of Hydrogen correctly – not least because the spin of the electron is not included. The success of Dirac's theory of the relativistic electron of 1928 seemed to confirm that Eq. (7.1) was not part of Nature's plan.

As we'll see below, there are other *conceptual* difficulties with the interpretation of the Klein–Gordon equation, and other relativistic wave equations (including the Dirac equation), as equations for the wavefunctions of single particles. The first of these is that Eq. (7.3) has both positive and negative energy solutions. The same could be said of *classical* relativistic particles, of course, but if such a particle had positive energy at one time, there is no way for it to evolve into one with negative energy at a later time. When we add external potentials to Eq. (7.1), however, it is possible for negative frequency components to be generated even if none are present initially, and the physical significance of these is unclear.

As we will see, relativistic wave equations are more properly understood as the equations of motion of quantum *fields* describing a system of many particles, just as in our discussion of second quantization in Chapter 4. Furthermore, this interpretation demands that each type of particle is associated with an **antiparticle**, a twin with the same mass but opposite charge.

This is only in the relativistic case. Antiparticles are not mandated by nonrelativistic case we discussed in Chapter 4.

Properly reinterpreted, Eq. (7.1) is understood as the equation of motion of a spin-0 boson field. This means that it describes composite particles like the pions. The only elementary particle that *might* be described by the Klein–Gordon equation is the **Higgs boson**.

7.1 Antiparticles

This section overlaps with Sections 3.8 and 4.7 of the **TP1** lecture notes.

Let's compare the mathematical structure of the Klein–Gordon equation and the Schrödinger equation. One is first order in time, and the other second. This is not a minor difference: the equivalence of the Schrödinger and Heisenberg pictures, and our whole understanding of time evolution in quantum mechanics, rests upon the unitary transformation

$$|\Psi(t)\rangle = \exp\left(-iHt/\hbar\right)|\Psi(0)\rangle\,. \tag{7.4}$$

However, to propagate a second order equation forward in time requires that we know not just $\Psi(\mathbf{r},t)$, but also $\partial_t\Psi(\mathbf{r},t)$, just as we must know positions and velocities to solve Newton's equation.

This is after all the whole idea of Hamiltonian mechanics.

From a purely mathematical standpoint, we can easily replace Eq. (7.1) with a system of first order equations by introducing a new field $\Pi(\mathbf{r},t)$

$$\begin{aligned}\partial_t\Psi(\mathbf{r},t) &= \Pi(\mathbf{r},t)\\ \partial_t\Pi(\mathbf{r},t) &= -\left[m^2-\nabla^2\right]\Psi(\mathbf{r},t).\end{aligned} \tag{7.5}$$

(Here and in the rest of this chapter, we are going to work in units where $\hbar = c = e = 1$). This is not particularly satisfactory, though: what is the meaning of $\Pi(\mathbf{r},t)$? Is $|\Psi(\mathbf{r},t)|^2$ still the probability density for the particle?

The resolution of this difficulty is rather drastic. We are going to abandon the interpretation of Eq. (7.1) as a wave equation for the wave function of a single particle. Instead, we will interpret it as the Heisenberg equation of motion of a field operator describing a many particle system. We have met this other interpretation already in Chapter 4 (c.f. Eq. (4.53)). There, because we dealt with non-relativistic physics, both interpretations – single particle and many particle – were possible. In the relativistic case the latter interpretation is the only one that makes sense. Bear in mind, then, that what follows is not a *derivation*, starting from the one particle picture, but rather a heuristic explanation of new physical laws.

How can we obtain Eq. (7.5) as a Heisenberg equation of motion? Evidently, the commutation relations that we found in Chapter 4

$$\left[\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right] = \delta(\mathbf{r}-\mathbf{r}') \tag{7.6}$$

will not do the trick. Instead, we need something that resembles the familiar commutation relation $[q,p]=i$ of position and momentum

$$\left[\psi(\mathbf{r}),\pi^\dagger(\mathbf{r}')\right] = \left[\psi^\dagger(\mathbf{r}),\pi(\mathbf{r}')\right] = i\delta(\mathbf{r}-\mathbf{r}'), \tag{7.7}$$

together with the Hamiltonian

$$H_{\text{KG}} = \int d\mathbf{r}\left[\nabla\psi^\dagger\cdot\nabla\psi + m^2\psi^\dagger\psi + \pi^\dagger\pi\right] \tag{7.8}$$

Problem 7.1

Check that Eqs. (7.7) and Eq. (7.8) give Eq. (7.5)

To get a feel for what is going on here, let's compare the two systems

$$\begin{aligned} H_{\mathrm{NR}} &= \omega a^\dagger a, & \left[a, a^\dagger\right] &= 1 \\ H_R &= p^\dagger p + \omega^2 z^\dagger z, & \left[z, p^\dagger\right] &= \left[z^\dagger, p\right] = i. \end{aligned} \tag{7.9}$$

H_{NR} is analogous to a non-relativistic system with the commutation relation Eq. (7.6). The real and imaginary parts of a are conjugate to one another, and the time evolution is $a(t) = \exp(-i\omega t)\, a(0)$. If we were talking about classical variables, we would say that the plane of complex a was the phase plane, and we can only move in a clockwise direction as t increases.

H_{R} is analogous to the relativistic system. It describes a 2D harmonic oscillator, as we can see if we write the (non-Hermitian) z and p variables in terms of the (Hermitian) Cartesian components

$$\begin{aligned} z &= \frac{1}{\sqrt{2}}(x + iy) \\ p &= \frac{1}{\sqrt{2}}(p_x + ip_y)\,. \end{aligned} \tag{7.10}$$

Thus, though z is complex it commutes with $z^\dagger$. If we want to describe this system in terms of creation and annihilation operators we have to introduce two pairs. We could do this separately for x and y or instead use complex z and p to define

$$\begin{aligned} a &= \sqrt{\frac{\omega}{2}} z + \frac{i}{\sqrt{2\omega}} p \\ b^\dagger &= \sqrt{\frac{\omega}{2}} z - \frac{i}{\sqrt{2\omega}} p, \end{aligned} \tag{7.11}$$

in which case

$$H_{\mathrm{R}} = \omega\left[a^\dagger a + b^\dagger b\right] + \text{const.} \tag{7.12}$$

The time evolution is then

$$\begin{aligned} a(t) &= \exp(-i\omega t)\, a(0) \\ b(t) &= \exp(-i\omega t)\, b(0). \end{aligned} \tag{7.13}$$

Note, however, that

$$\begin{aligned} z(t) &= \sqrt{\frac{1}{2\omega}}\left[a(t) + b^\dagger(t)\right] \\ &= \sqrt{\frac{1}{2\omega}}\left[a(0)\exp(-i\omega t) + b^\dagger(0)\exp(i\omega t)\right], \end{aligned} \tag{7.14}$$

so that the time dependence of $z(t)$ contains *both positive and negative frequencies*. From the point of view of a 2D oscillator this is perfectly natural: the general motion will be one with elliptic polarisation. To interpret this doubling of the degrees of freedom from a particle point of view, it's natural to suppose that a and b describe *distinct* particles.

Before continuing, let's quickly run through the same analysis for the Klein–Gordon Hamiltonian Eq. (7.8). We expand $\psi(\mathbf{r})$ and $\pi(\mathbf{r})$ in Fourier modes as

$$\begin{aligned} \psi(\mathbf{r}) &= \sum_{\mathbf{k}} \sqrt{\frac{1}{2\omega_{\mathbf{k}}}}\left[a_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r}) + b_{\mathbf{k}}^\dagger \exp(-i\mathbf{k}\cdot\mathbf{r})\right] \\ \pi(\mathbf{r}) &= -i\sum_{\mathbf{k}} \sqrt{\frac{\omega_{\mathbf{k}}}{2}}\left[a_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r}) - b_{\mathbf{k}}^\dagger \exp(-i\mathbf{k}\cdot\mathbf{r})\right]. \end{aligned} \tag{7.15}$$

These fields satisfy Eq. (7.7) for any $\omega_{\mathbf{k}}$. The choice of $\omega_{\mathbf{k}}$ is suggested by the Hamiltonian. If we take

$$\omega_{\mathbf{k}} = \sqrt{\mathbf{k}^2 + m^2}, \tag{7.16}$$

then cross terms involving $a_{\mathbf{k}} b_{-\mathbf{k}}$ and $a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}}$ disappear and the Hamiltonian is the sum of terms describing the two particle types

$$H_{\text{KG}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left[a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + b^\dagger_{\mathbf{k}} b_{\mathbf{k}} \right]. \tag{7.17}$$

Problem 7.2

When the modes evolve as in Eq. (7.13), so that

$$\psi(\mathbf{r}, t) = \sum_{\mathbf{k}} \sqrt{\frac{1}{2\omega_{\mathbf{k}}}} \left[a_{\mathbf{k}} \exp\left(i\left[\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t\right]\right) + b^\dagger_{\mathbf{k}} \exp\left(-i\left[\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t\right]\right) \right] \tag{7.18}$$

verify that the Klein–Gordon equation is obeyed.

When we interpret $\psi(\mathbf{r}, t)$ as an operator, with contributions from particle annihilation and antiparticle creation modes, the negative frequencies are no longer mysterious.

What can we say about the two types of particles? Evidently they have the same mass, as the dispersion relation Eq. (7.16) is the same for both a's and b's. To find out their charge we add a vector potential, which appears in H_{KG} as

$$H_{\text{KG}} = \int d\mathbf{r} \left[(\nabla + i\mathbf{A})\, \psi^\dagger \cdot (\nabla - i\mathbf{A})\, \psi + m^2 \psi^\dagger \psi + \pi^\dagger \pi \right]. \tag{7.19}$$

Taking $\mathbf{A}$ to be constant for simplicity, we find that Eq. (7.19) is solved by a simple generalisation of Eq. (7.15)

$$\begin{aligned}
\psi(\mathbf{r}) &= \sum_{\mathbf{k}} \sqrt{\frac{1}{2\omega_{\mathbf{k}}}} \left[a_{\mathbf{k}} \exp\left(i\left[\mathbf{k}+\mathbf{A}\right]\cdot\mathbf{r}\right) + b^\dagger_{\mathbf{k}} \exp\left(-i\left[\mathbf{k}-\mathbf{A}\right]\cdot\mathbf{r}\right) \right] \\
\pi(\mathbf{r}) &= -i \sum_{\mathbf{k}} \sqrt{\frac{\omega_{\mathbf{k}}}{2}} \left[a_{\mathbf{k}} \exp\left(i\left[\mathbf{k}+\mathbf{A}\right]\cdot\mathbf{r}\right) - b^\dagger_{\mathbf{k}} \exp\left(-i\left[\mathbf{k}-\mathbf{A}\right]\cdot\mathbf{r}\right) \right].
\end{aligned} \tag{7.20}$$

Since $\mathbf{A} = -\int^t \mathbf{E}(t')dt'$, we see that an electric field pulse shifts the momenta of the two types of particles in opposite directions, showing that they have opposite charge.

TANGENT If this was all there was to it, antiparticles might still be a curiosity, akin to the negative energy solutions of $E^2 = \mathbf{p}^2 + m^2$. After all, Eq. (7.17) conserves the two types of particles separately, so maybe there are just no b particles in the universe. This would be rather asymmetric, and in fact the imbalance between matter and antimatter in the observable universe *is* a big mystery.

However, there are mechanisms that create antiparticles, or rather **particle-antiparticle pairs**. The most famous example is the decay of an energetic photon, clearly visible in cloud or bubble chambers, which can occur when the energy of the photon exceeds twice the rest mass energy of an electron. Describing this process requires us to consider the *interaction* of the quantum field of the photon with the field of the charged particles, which goes beyond the scope of this course.

Pair production can also occur in strong electric fields, which may be treated by introducing the classical vector potential into the Hamiltonian as in Eq. (7.19). In

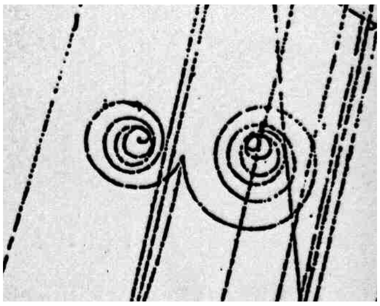


Figure 7.1: Electron-positron pair production in a bubble chamber. The two particles move in helical paths in the presence of a magnetic field, with opposite senses indicating their opposite charges.

writing Eq. (7.20) we assumed that **A** was not only constant in space but also in time, so linking an expression valid for *static* **A** to an electric field pulse was a piece of sleight of hand that turns out to be only justified for adiabatic changes in **A**, corresponding to low fields.

Let's discuss this problem a little more quantitatively, restricting ourselves to one spatial dimension. In a spatially constant but time varying vector potential, a particular plane wave component ψ_k of the Klein–Gordon field satisfies

$$\ddot{\psi}_k(t) + \omega^2_{k-A(t)}\psi_k(t) = 0, \tag{7.21}$$

which is just the equation of a (2D) oscillator with a time dependent frequency. For a constant electric field we have $\mathbf{A} = -\mathbf{E}t$ and so

$$\omega^2(t) \equiv \omega^2_{k-A(t)} = (k+Et)^2 + m^2. \tag{7.22}$$

When E is small we expect the oscillator to adiabatically follow the changing frequency, so that

Notice the resemblance to the WKB wavefunction, which arises because Eq. (7.21) can be interpreted as a 1D Schrödinger equation, with time playing the role of space.

$$\psi_k(t) = \frac{1}{\sqrt{2\omega(t)}}\left[a_k \exp\left(-i\int^t \omega(t')dt'\right) + b^\dagger_{-k}\exp\left(i\int^t \omega(t')dt'\right)\right]. \tag{7.23}$$

When **E** is not small, adiabaticity is violated and the amplitudes of the two components are mixed. Using the analogy to the Schrödinger equation, the result is expressed in terms of a transfer matrix

$$\begin{pmatrix} a_{k,\text{init}} \\ b^\dagger_{-k,\text{init}} \end{pmatrix} = \begin{pmatrix} u & v \\ v^* & u^* \end{pmatrix}\begin{pmatrix} a_{k,\text{final}}(\infty) \\ b^\dagger_{-k,\text{final}}(\infty) \end{pmatrix}, \tag{7.24}$$

where

$$|u|^2 - |v|^2 = 1 \tag{7.25}$$

If you are wondering where this parametrisation comes from, look back at Problem 3.2. Note that the same transformations appear in Problem 4.9.

We have already calculated this effect twice: in the Landau–Zener problem (Section 1.3) and the quantum point contact (Section 3.C). As in the latter case, $|v|^2$ is the ratio of reflection to transmission coefficients, and is given by

$$|v|^2 = \exp\left(-\frac{\pi m^2}{E}\right). \tag{7.26}$$

Remember that we are using the Heisenberg picture, where the states do not evolve. A vacuum state for the initial a and b particles

$$a_{k,\text{init}}|\text{VAC}\rangle = b_{-k,\text{init}}(-\infty)|\text{VAC}\rangle = 0, \tag{7.27}$$

therefore satisfies

$$\left(u a_{k,\text{final}} + v b^\dagger_{-k,\text{final}}\right)|\text{VAC}\rangle = 0. \tag{7.28}$$

In terms of $a_{k,\text{final}}$ and $b_{k,\text{final}}$ $|\text{VAC}\rangle$ therefore contains a factor

$$\exp\left(-(v/u)a^\dagger_{k,\text{final}}b^\dagger_{-k,\text{final}}\right)|N_a = 0, N_b = 0\rangle. \tag{7.29}$$

Problem 7.3

Show that in the state described by Eq. (7.29) the probability of finding n $(k,-k)$ pairs is

$$P_n = (1-\rho)\rho^n, \qquad \rho = \left|\frac{v}{u}\right|^2 = \frac{1}{1+\exp\left(\pi m^2/E\right)}, \tag{7.30}$$

with an average $\bar{n} = \rho$.

It's straightforward to turn this into a calculation of a rate, by remembering that in a system of length L with periodic boundary conditions, the spacing of k states is $2\pi/L$, and the wavevectors of individual modes are increasing at a rate E. Thus

$$\text{Rate} = \frac{EL}{2\pi}\frac{1}{1+\exp\left(\pi m^2/E\right)}, \tag{7.31}$$

which is proportional to the system size, so the meaningful quantity is the rate of pair production per unit volume.

This process of pair production is known as the **Schwinger mechanism**. Though we discussed the case of bosons described by the Klein–Gordon field, the same process occurs for all relativistic fields. Conceptually, it is the simplest demonstration that antiparticles are real and may be created. Practically, the colossal fields[1] required to tear particle-antiparticle pairs out of the vacuum have never been realised, though experiments continue with high intensity lasers.

7.2 The Lorentz group

Including spacetime translations as well as transformations that preserve the origin leads to the **Poincaré group**.

The Lorentz group is closely related to the group $SO(4)$ that we met at the end of the last chapter. Instead of considering rotations that preserve the squared length of a 4D vector, leading to the orthogonality condition, we look for linear transformations that preserve the squared **spacetime interval**

$$s^2 = (ct)^2 - \mathbf{x}^2. \tag{7.32}$$

We introduce some standard notation for 4-vectors. $x^\mu \equiv (ct, x, y, z)$ is the position 4-vector. Greek indices indicate that all four entries are included (e.g. $\mu = 0, 1, 2, 3$), while Roman indices include only spatial coordinates (e.g. $i = 1, 2, 3$). The squared spacetime interval is then

$$g_{\mu\nu}x^\mu x^\nu = x_\mu x^\mu \tag{7.33}$$

$$x_\mu x^\mu = x_0^2 - x_1^2 - x_2^2 - x_3^2, \tag{7.34}$$

where the **metric tensor** is

$$g = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{7.35}$$

and indices are raised and lowered by contraction with $g_{\mu\nu} = g^{\mu\nu}$ i.e. $x_\mu = g_{\mu\nu}x^\nu$. The scalar product $g_{\mu\nu}x^\mu y^\nu$ is preserved by a linear transformation $\Lambda : x^\mu \to \Lambda^\mu{}_\nu x^\nu$ if

$$\Lambda^T g \Lambda = g, \tag{7.36}$$

which replaces the orthogonality condition. This defines a group called $O(1,3)$, which reflects the signature of the metric.

As in the case of $O(3)$, the Lorentz group consists of more than one connected component. Eq. (7.36) implies

$$(\det \Lambda)^2 = 1, \tag{7.37}$$

so we can again distinguish transformations based on the sign of the determinant, with those transformations having $\det\Lambda = -1$ being disconnected

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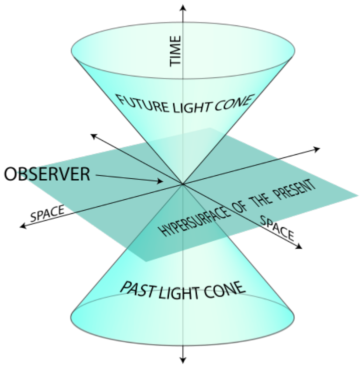
[1] The scale set by the exponent in Eq. (7.31) corresponds to a variation of electric potential energy by mc^2 over the Compton wavelength h/mc of the particles.

from the identity, and those with $\det \Lambda = 1$ forming a subgroup denoted $SO(1,3)$.

There is, however, another distinction to be made, that does not arise in the case of the rotations. The past and future light cones separate 4-vectors with positive squared length (time-like, with our choice of signs) from those with negative squared length (space-like). Because the two cones touch only at the origin, we can distinguish transformations based on whether they take a 4-vector to another within the same light cone, or to the opposite light cone. It's not hard to see that these two cases are distinguished by the sign of Λ^0_0, with the case $\Lambda^0_0 > 0$ corresponding to those transformations that preserve the direction of time (called **orthochronous**) and $\Lambda^0_0 < 0$ describing those that don't.

So $O(1,3)$ has four disconnected components. The subgroup of proper ($\det \Lambda = 1$), orthochronous Lorentz transformations is denoted $SO^+(1,3)$ and is called the **restricted Lorentz group**.



Lie algebra

Working out the Lie algebra of $so(1,3)$ is a small variation on the case of $so(4)$ discussed in Chapter 6. Writing a transformation in terms of a generator (a.k.a. member of the Lie algebra) λ

$$\Lambda = \exp\left(\lambda\right), \tag{7.38}$$

we find that the condition Eq. (7.36) on Λ means that the generator satisfies

$$\lambda^T g + g\lambda = 0. \tag{7.39}$$

The left hand side is a symmetric matrix, so this gives 10 linear conditions on the 16 elements of λ, leaving a 6 dimensional space of solutions. Within the 3×3 block corresponding to the spatial coordinates, λ is antisymmetric, just as in the case of $so(3)$ (which is of course a subalgebra). The difference from $so(4)$ is that

$$\lambda_{0i} = \lambda_{i0}, \qquad i = 1, 2, 3. \tag{7.40}$$

A complete basis is provided by

$$\mathsf{J}_x = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \ \mathsf{J}_y = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \ \mathsf{J}_z = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$
$$\mathsf{K}_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \ \mathsf{K}_y = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \ \mathsf{K}_z = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{7.41}$$

and the algebra of these generators is

$$\begin{aligned} \left[\mathsf{J}_k, \mathsf{J}_l\right] &= \varepsilon_{klm}\mathsf{J}_m \\ \left[\mathsf{J}_k, \mathsf{K}_l\right] &= \varepsilon_{klm}\mathsf{K}_m \\ \left[\mathsf{K}_k, \mathsf{K}_l\right] &= -\varepsilon_{klm}\mathsf{J}_m. \end{aligned} \tag{7.42}$$

The only difference from $so(4)$ is the minus sign in the last of these.

A general $SO^+(1,3)$ transformation can then be written as

$$\Lambda(\boldsymbol{\theta},\boldsymbol{\phi}) = \exp\left(\boldsymbol{\theta}\cdot\mathsf{J} + \boldsymbol{\phi}\cdot\mathsf{K}\right). \tag{7.43}$$

To check that this chimes with what you already know, consider the transformation corresponding to $\boldsymbol{\theta} = 0$, $\boldsymbol{\phi} = (\phi, 0, 0)$. Then it's easy to show

$$\Lambda = \begin{pmatrix} \cosh\phi & \sinh\phi & 0 & 0 \\ \sinh\phi & \cosh\phi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{7.44}$$

which in more elementary notation is

$$\begin{aligned} x &= \gamma\left(x + vt\right) \\ t &= \gamma\left(t + vx\right), \end{aligned} \tag{7.45}$$

with $\gamma = (1-v^2)^{-1/2} = \cosh\phi$. Eq. (7.45) corresponds to a boost to a reference frame moving with velocity $(-v, 0, 0)$.

The appearance of hyperbolic rather than trigonometric functions is an indicator that we are dealing with a noncompact group. One other feature worth remarking on, not obvious in elementary treatments of Lorentz transformations, is that the generators of boosts in different directions do not commute with each other. The consequence is that a sequence of boosts around a closed path in velocity space is associated with a rotation. This is the phenomenon of **Thomas precession**, which plays a role in the spin-orbit interaction (see **AQP**). Since Thomas precession is built into the Dirac equation we won't discuss it further.

$SL(2,\mathbb{C})$ and spinors

In Chapter 6 we saw that the rotations were realised on spin $1/2$ states by the elements of $SU(2)$. A relativistic theory of spin $1/2$ particles requires that we find how this transformation law is extended to include the Lorentz transformations. This turns out to be remarkably painless. The relevant transformations are those of the group $SL(2,\mathbb{C})$, the **special linear group** of degree 2. This is the group of complex matrices (that's what the $\mathbb{C}$ indicates) of unit determinant.

Before seeing how this group is related to $SO^+(1,3)$, let's introduce it in a little more detail. A general element has the form

$$\mathsf{S} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad ad - bc = 1. \tag{7.46}$$

The condition of unit determinant means that the elements of the Lie algebra are defined only by the property that they are traceless. A complete basis is provided by the six matrices

$$\mathsf{J}_i = -\frac{i}{2}\sigma_i, \qquad \mathsf{K}_i = \frac{1}{2}\sigma_i \tag{7.47}$$

Problem 7.4

Of course, the notation is not an accident. Verify that these satisfy Eq. (7.42).

The $SL(2,\mathbb{C})$ transformation corresponding to Eq. (7.43) is then

$$\mathsf{S} = \exp\left(\boldsymbol{\theta}\cdot J + \boldsymbol{\phi}\cdot\mathsf{K}\right). \tag{7.48}$$

To make this map explicit we need the generalisation of Eq. (6.41), which provides the (two-to-one) homomorphism of $SU(2)$ to $SO(3)$. In the present case, we have

$$\mathsf{S}(\boldsymbol{\theta},\boldsymbol{\phi})\sigma^{\mu}\mathsf{S}^{\dagger}(\boldsymbol{\theta},\boldsymbol{\phi}) = \left([\Lambda(\boldsymbol{\theta},\boldsymbol{\phi})]^{-1}\right)^{\mu}{}_{\nu}\sigma^{\nu}, \tag{7.49}$$

where $\sigma^{\mu} = (\sigma^0,\sigma^1,\sigma^2,\sigma^3)$, and $\sigma^0 = \mathbb{1}$ (we put the indices upstairs because this quantity transforms as a 4-vector). Once again the map is two-to-one.

Problem 7.5

Show that this holds for $\boldsymbol{\theta} = 0$. You will need the analog of Eq. (6.40) for $e^A B e^A$.

There is, however, an inequivalent way to relate the two groups

$$\left[\mathsf{S}^{\dagger}(\boldsymbol{\theta},\boldsymbol{\phi})\right]^{-1}\bar{\sigma}^{\mu}\left[\mathsf{S}(\boldsymbol{\theta},\boldsymbol{\phi})\right]^{-1} = \left([\Lambda(\boldsymbol{\theta},\boldsymbol{\phi})]^{-1}\right)^{\mu}{}_{\nu}\bar{\sigma}^{\nu}, \tag{7.50}$$

where $\bar{\sigma}^{\mu} = (\sigma^0,-\sigma^1,-\sigma^2,-\sigma^3)$. The two component complex vectors on which S acts are called **spinors**, and the two representations corresponding to Eq. (7.49) and Eq. (7.50) are called **right handed** and **left handed Weyl spinors**

$$\begin{aligned}\Lambda(\boldsymbol{\theta},\boldsymbol{\phi}) :&\psi_+ \longrightarrow S(\boldsymbol{\theta},\boldsymbol{\phi})\psi_+\\ \Lambda(\boldsymbol{\theta},\boldsymbol{\phi}) :&\psi_- \longrightarrow \left[S^{\dagger}(\boldsymbol{\theta},\boldsymbol{\phi})\right]^{-1}\psi_-.\end{aligned} \tag{7.51}$$

7.3 *The Dirac equation*

Eq. (7.49) and Eq. (7.50) immediately suggest a possible wave equation – or in fact two – for spin $1/2$ particles

$$\begin{aligned}\bar{\sigma}^{\mu}\partial_{\mu}\psi_+ &= 0\\ \sigma^{\mu}\partial_{\mu}\psi_- &= 0,\end{aligned} \tag{7.52}$$

known as **Weyl equations**. The amazing thing about these equations is that, by virtue of the transformation property Eq. (7.49) and Eq. (7.50), they are Lorentz invariant despite being first order in space and time derivatives. It's easy to verify that if $\psi_+(x^{\mu})$ is a solution, then so is $\mathsf{S}\psi_+(\Lambda^{\mu}{}_{\nu}x^{\nu})$.

However, the Weyl equations suffer from a serious shortcoming. By applying the operator $\bar{\sigma}_{\nu}\partial^{\nu}$ to the first and $\sigma_{\nu}\partial^{\nu}$ to the second, you can see that they both satisfy the *massless* Klein–Gordon equation

$$\partial^{\mu}\partial_{\mu}\psi_{\pm} = 0. \tag{7.53}$$

Thus, they are of no use in describing massive particles . Adding a mass

The Weyl equations describe neutrinos in the original Standard Model of particle physics, although neutrinos are now known to have (tiny) masses.

term in the obvious way

$$\bar{\sigma}^{\mu}\partial_{\mu}\psi_{+} \overset{?}{=} m\psi_{+}, \tag{7.54}$$

violates Lorentz invariance. However, the combination

$$\begin{aligned} i\bar{\sigma}^{\mu}\partial_{\mu}\psi_{+} &= m\psi_{-} \\ i\sigma^{\mu}\partial_{\mu}\psi_{-} &= m\psi_{+}, \end{aligned} \tag{7.55}$$

is Lorentz invariant. We can present these as a single equation by assembling our two component Weyl spinors into four component **Dirac** spinors

$$\Psi = \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} \tag{7.56}$$

and defining the **gamma matrices**

$$\gamma^0 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} 0 & -\sigma^i \\ \sigma^i & 0 \end{pmatrix}. \tag{7.57}$$

The gamma matrices obey the anticommutation relations

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu}\mathbb{1}. \tag{7.58}$$

We can finally write the **Dirac equation** for massive spin $1/2$ particles as

$$\boxed{(i\gamma^{\mu}\partial_{\mu} - m)\Psi = 0} \tag{7.59}$$

Figure 7.2: Plaque commemorating Dirac and his equation before installation in Westminster Abbey.

The Dirac equation explains a number of properties that had to be included in an ad hoc way in the nonrelativistic theory of the electron, most notably that the gyromagnetic ratio (or g-factor) of the electron is 2 (give or take corrections due to QED, which require the theory of interacting quantum fields).

Like the Klein–Gordon equation, it has negative frequency solutions, which were the cause of much head-scratching at the time. As we discussed earlier, the way out is provided by reinterpreting Eq. (7.59) as a Heisenberg equation of motion of the electron field, which necessitates the existence of anti-electrons, or **positrons**. Interestingly, it is not possible to quantise a spin $1/2$ – or generally half odd integer spin – field using commutation relations. Anticommutation relations must be used instead, meaning that such particles are fermions. The correspondence

Dirac initially suggested that the anti-electron might be the proton, the only positively charged particle known at the time, but Weyl pointed out that they had to have the same mass.

$$\begin{aligned} \text{Integer spin} &\longleftrightarrow \text{Bosons} \\ \text{Half odd integer spin} &\longleftrightarrow \text{Fermions.} \end{aligned} \tag{7.60}$$

is known as the **spin statistics connection**.

A

Operator Kung Fu

Time for a workout!

A.1 General operator algebra

Some properties of the **commutator** $[A, B] = AB - BA$ of operators A and B

$$\begin{aligned} [A, BC] &= [A, B]C + B[A, C], && \text{'chain rule'}, \\ [A, [B, C]] + [B, [C, A]] + [C, [A, B]] &= 0, && \text{Jacobi identity} \end{aligned} \tag{A.1}$$

In **AQP** operators wore hats: we'll omit them unless there is a danger of ambiguity

Problem A.1

Suppose $[A, B] = \alpha$, a constant (or if you prefer $[A, B] = \alpha\mathbb{1}$, a multiple of the identity operator)

1. Find $[A, B^n]$.
2. Find $[A, e^B]$. *Hint:* write the operator exponential as a power series.
3. Find $[A, f(B)]$, where $f(B)$ is some function of B defined by its power series.

The following formula is frequently useful[1]

$$\begin{aligned} e^A B e^{-A} &= B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \cdots \\ &\equiv e^{[A, \cdot]} B \end{aligned} \tag{A.2}$$

where the second line is just shorthand for the first.

Problem A.2

Prove this. *Hint:* consider the differential equation in x obeyed by $e^{xA} B e^{-xA}$.

Problem A.3

Show that $e^{iPy/\hbar} f(X) e^{-iPy/\hbar} = f(X + y)$, where $[P, X] = -i\hbar$

[1] It sometimes goes by the name **Hadamard lemma**.

Problem A.4

For $[A, B] = \alpha$

1. Show that
$$e^A e^B = e^{A+B} e^{\alpha/2} = e^B e^A e^\alpha \tag{A.3}$$
2. *[Gluttons for punishment only]* Show that
$$[A^m, B^n] = \sum_{k=1}^{\min(n,m)} \alpha^k k! \binom{m}{k} \binom{n}{k} B^{n-k} A^{m-k}. \tag{A.4}$$

Hint: Find $[e^{\alpha A}, e^{\beta B}]$ and compare coefficients in the Taylor series.

A.2 *Differential operators*

Problem A.5

The 3D Laplacian can be written

$$\nabla^2 = \frac{1}{r^2} \partial_r \left(r^2 \partial_r \right) - \frac{\mathbf{L}^2}{\hbar^2 r^2}$$

where $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the orbital angular momentum. Check this directly starting from

$$(\mathbf{r} \times \mathbf{p})^2 = x_j p_k x_j p_k - x_j p_k x_k p_j$$

and then using the canonical commutation relations. *Hint:* $\mathbf{r} \cdot \nabla = r \frac{\partial}{\partial r}$.

A.3 *Angular momentum algebra*

The operators $\mathbf{J}$ could be orbital angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, spin angular momentum $\mathbf{S}$, or a combination of the two

Recall that the vector of angular momentum operators $\mathbf{J}$ satisfy

$$[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k. \tag{A.5}$$

Problem A.6

For a spin in a magnetic field $H = -\gamma \mathbf{B} \cdot \mathbf{S}$ find the form of the Heisenberg equations of motion $\frac{d\mathbf{S}}{dt} = \frac{i}{\hbar}[H, \mathbf{S}]$ obeyed by $\mathbf{S}(t) = e^{iHt/\hbar} \mathbf{S} e^{-iHt/\hbar}$.

Problem A.7

For $\mathbf{B} = B\hat{\mathbf{z}}$, find $\mathbf{S}(t) = e^{iHt/\hbar} \mathbf{S} e^{-iHt/\hbar}$ explicitly using the Hadamard lemma Eq. (A.2) and check that it obeys the equation of motion from the previous problem.

A.4 *Oscillator algebra*

We'll use the term **oscillator variables** to describe a pair of a, $a^\dagger$ of operators satisfying $[a, a^\dagger] = 1$. When you met the quantum harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{A.6}$$

you will have defined the pair

$$\begin{aligned} a &= \sqrt{\frac{m\omega}{2\hbar}}\left(x + i\frac{p}{m\omega}\right) \\ a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(x - i\frac{p}{m\omega}\right), \end{aligned} \tag{A.7}$$

which satisfy this basic relation. This in turn leads to

$$[N, a] = -a \qquad [N, a^\dagger] = +a^\dagger \tag{A.8}$$

where $N = a^\dagger a$ is the **number operator**. Summarizing the results of **AQP**, Eq. (A.8) tells us that if $|n\rangle$ is an eigenstate of N with eigenvalue n, $a^\dagger |n\rangle$ is an eigenstate with eigenvalue $n+1$. Starting from the state $|0\rangle$, we can construct an orthonormal eigenbasis

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle\,. \tag{A.9}$$

These states obey the fundamental relations

$$a^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad a\,|n\rangle = \sqrt{n}\,|n-1\rangle\,. \tag{A.10}$$

Problem A.8

Suppose the Hamiltonian Eq. (A.6) is abruptly changed to

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \alpha x. \tag{A.11}$$

That is, a linear potential (constant force) is introduced, which shifts the minimum of the overall potential by $x_0 = -2\alpha/m\omega^2$.

We can write the eigenstates of the *new* Hamiltonian as a translation of those of the *old* Hamiltonian $|n_{\text{new}}\rangle = e^{-ipx_0/\hbar}|n_{\text{old}}\rangle$. If the system is initially in its ground state, the amplitude to find the system in one of the excited states of the new Hamiltonian is then

$$\langle n_{\text{new}}|0_{\text{old}}\rangle = \langle n_{\text{old}}|\,e^{ipx_0/\hbar}\,|0_{\text{old}}\rangle$$

1. By writing p in the exponent in terms of a and $a^\dagger$, evaluate the amplitude. *Hint:* first *normal order* the exponential, which means to put all the occurrences of a to the right of occurrences of $a^\dagger$. This can be done using the result of Problem A.4.
2. What is the probability distribution of excited states?

Note that the new Hamiltonian in Problem A.8 is naturally written in terms of new oscillator variables

$$\begin{aligned} a_{x_0} &= a + \sqrt{\frac{m\omega}{2\hbar}} x_0 \\ a^\dagger_{x_0} &= a^\dagger + \sqrt{\frac{m\omega}{2\hbar}} x_0. \end{aligned} \tag{A.12}$$

The shift leaves the commutation relations unchanged.

Problem A.9

Verify that Eq. (A.12) is the result of applying the unitary transformation used in Problem A.8 to the oscillator variables, i.e.

$$\begin{aligned} a_{x_0} &= e^{-ipx_0/\hbar} a e^{ipx_0/\hbar} \\ a^\dagger_{x_0} &= e^{-ipx_0/\hbar} a^\dagger e^{ipx_0/\hbar} \end{aligned} \tag{A.13}$$

Another commonly occurring transformation of oscillator variables that preserves the commutation relations may be found by observing that $[a, a^\dagger] = 1$ for *any* ω in the original definition Eq. A.7. For the harmonic oscillator, there was a natural choice, as the Hamiltonian takes on a simple form when ω is the natural frequency of the oscillator. But from a purely algebraic point of view any member of the family of operators parametrized by α

$$\begin{aligned} a_\alpha &= \frac{1}{\sqrt{2\hbar}} \left(\alpha x + i\frac{p}{\alpha} \right) \\ a^\dagger_\alpha &= \frac{1}{\sqrt{2\hbar}} \left(\alpha x - i\frac{p}{\alpha} \right) \end{aligned} \tag{A.14}$$

has the same properties.

Problem A.10

1. Find the linear transformation that connects the oscillator variables at two different values of α
2. Show that this transformation can be effected by a unitary transformation of the form

$$U_\kappa = \exp(\kappa[a^\dagger a^\dagger - aa]) \tag{A.15}$$

   for some choice of κ.
3. What is the effect of this transformation on the variables x and p?

Problem A.11

[Harder] Adapting the method of Problem A.8, find the probability to be in each of the excited states after the *frequency* of the oscillator is shifted from $\omega_i \to \omega_f$.