Part II Topics in Quantum Theory

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Preface

> *"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, 2002)

The development of quantum theory during the 20^{th} 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.

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CHAPTER 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!).

1.1.1 Time Independent Case

The Hamiltonian is

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

where the position and momentum operators satisfy

$$[\hat{x}, \hat{p}] = i\hbar. \tag{1.2}$$

The state of the oscillator $\bar{\psi}$ evolves in time according to the (time dependent) Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\bar{\psi} = \hat{H}\bar{\psi}. \tag{1.3}$$

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

$$\bar{\psi}(t) = \exp\left(-i\hat{H}t/\hbar\right)\bar{\psi}(0) \equiv \hat{U}(t)\bar{\psi}(0). \tag{1.4}$$

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

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

$$\hat{U}(t) = \mathbb{I} - i\frac{\hat{H}t}{\hbar} - \frac{1}{2}\left(\frac{\hat{H}t}{\hbar}\right)^2 + \cdots . \tag{1.5}$$

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

$$\hat{U}(t) = \sum_n e^{-iE_n t/\hbar} |n\rangle \langle n| . \tag{1.6}$$

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 $\hat{p} = -i\hbar\, \mathrm{d}/\mathrm{d}x$ and study the time independent Schrödinger equation in this representation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2 \psi_n = E_n\psi_n, \tag{1.7}$$

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

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \tag{1.8}$$

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

$$\begin{aligned} \hat{a} &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right) \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right), \end{aligned} \tag{1.9}$$

which satisfy

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1. \tag{1.10}$$

The Hamiltonian is expressed as

$$\hat{H} = \frac{\hbar\omega}{2}\left[\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right] = \hbar\omega\left(N + \frac{1}{2}\right), \tag{1.11}$$

where $N \equiv \hat{a}^\dagger\hat{a}$. The commutation relation Eq. (1.10) implies

$$[N, \hat{a}] = -\hat{a}, \quad \left[N, \hat{a}^\dagger\right] = +\hat{a}^\dagger, \tag{1.12}$$

which in turn tells us that acting with $\hat{a}^\dagger(\hat{a})$ 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 $\hat{U}(t)$ indirectly, from the effect it has on operators. Recall that in the *Heisenberg picture* operators acquire a time dependence

$$\hat{\mathcal{O}}(t) = \hat{U}^\dagger(t)\hat{\mathcal{O}}\hat{U}(t), \tag{1.13}$$

equivalent to the Heisenberg equation of motion

$$\frac{\mathrm{d}\hat{\mathcal{O}}(t)}{\mathrm{d}t} = \frac{i}{\hbar}\Big[\hat{H}, \hat{\mathcal{O}}(t)\Big]. \tag{1.14}$$

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

$$\hat{H} = \hat{U}^\dagger(t)\hat{H}\hat{U}(t) = \frac{\hat{p}(t)^2}{2m} + \frac{1}{2}m\omega^2\hat{x}(t)^2. \tag{1.15}$$

We have

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{x}(t)] = \frac{\hat{p}(t)}{m} \tag{1.16}$$

$$\frac{\mathrm{d}\hat{p}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{p}(t)] = -m\omega^2\hat{x}(t). \tag{1.17}$$

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

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = \frac{\partial\hat{H}}{\partial\hat{p}} = \frac{\hat{p}}{m} \tag{1.18}$$

$$\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} = -\frac{\partial\hat{H}}{\partial\hat{x}} = -m\omega^2\hat{x}. \tag{1.19}$$

Considering the case for the more general Hamiltonian,

$$\hat{H} = \hat{T}(\hat{p}) + \hat{V}(\hat{x}) = \sum_n \frac{t_n\hat{p}^n}{n!} + \sum_n \frac{v_n\hat{x}^n}{n!}, \tag{1.20}$$

we find the Heisenberg equation of motion

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{i}{\hbar}\sum_n \left[\frac{t_n\hat{p}^n}{n!}, \hat{x}\right] = \hat{T}'(\hat{p}), \tag{1.21}$$

which corresponds to Hamilton's equation $\dot{\hat{x}} = \partial\hat{H}\big/\partial\hat{p}$. The same proof works for $\mathrm{d}\hat{p}(t)/\mathrm{d}t = -\hat{V}'(\hat{x})$.

The general solution to Eqs. (1.18) and (1.19) is

$$\hat{x}(t) = \cos(\omega t)\hat{x}(0) + \sin(\omega t)\frac{\hat{p}(0)}{m\omega} \tag{1.22}$$

$$\hat{p}(t) = \cos(\omega t)\hat{p}(0) - m\omega\sin(\omega t)\hat{x}(0), \tag{1.23}$$

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 $\hat{a}$, $\hat{a}^\dagger$ in Eq. (1.9) can be seen as complex amplitudes whose phase changes linearly in time

$$\hat{a}(t) = e^{-i\omega t}\hat{a}(0), \quad \hat{a}^\dagger(t) = e^{+i\omega t}\hat{a}^\dagger(0). \tag{1.24}$$

This follows by writing the Hamiltonian as $\hat{H} = \omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$, such that $\dot{\hat{a}}(t) = -i\omega(t)$, which can be integrated to yield $\hat{a}(t)\exp(-i\omega t)\hat{a}(0)$.

1.1.2 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[1]

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - F(t)\hat{x}. \tag{1.25}$$

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

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}(t)|\psi\rangle \tag{1.26}$$

is *not*

$$\hat{U}(t) \neq \exp\Big(-i\hat{H}(t)t/\hbar\Big). \tag{1.27}$$

Let's consider the situation described by

$$F(t) = \begin{cases} F_1 & 0 \leq t < t_1 \\ F_2 & t_1 \leq t < t_2 \end{cases}. \tag{1.28}$$

The evolution operator is

$$\hat{U}(t) = \begin{cases} U_1(t) & 0 \leq t < t_1 \\ U_2(t-t_1)U_1(t_1) & t_1 \leq t < t_2 \end{cases}, \tag{1.29}$$

where $U_i = e^{-i\hat{H}_i t/\hbar}$ and $\hat{H}_i = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - F_i\hat{x}$. It's important to realise that $\hat{H}_1$ and $\hat{H}_2$ don't commute with each other,

$$[\hat{H}_1, \hat{H}_2] = -i\hbar\frac{\hat{p}}{m}(F_1 - F_2), \tag{1.30}$$

thus U_1 and U_2 don't commute and the product of U_1 and U_2 in Eq. (1.29) 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

$$\begin{aligned}
\hat{U}(t) &= \lim_{\Delta t\to 0} e^{-i\hat{H}(t-\Delta t)\Delta t/\hbar}e^{-i\hat{H}(t-2\Delta t)\Delta t/\hbar}\cdots e^{-i\hat{H}(\Delta t)\Delta t/\hbar}e^{-i\hat{H}(0)\Delta t/\hbar} \\
&= \lim_{\Delta t\to 0}\left(1 - \frac{i\hat{H}(t-\Delta t)\Delta t}{\hbar}\right)\left(1 - \frac{i\hat{H}(t-2\Delta t)\Delta t}{\hbar}\right)\cdots\left(1 - \frac{i\hat{H}(0)\Delta t}{\hbar}\right) \\
&= 1 - \frac{i}{\hbar}\int_0^t \mathrm{d}t_1\,\hat{H}(t_1) - \frac{1}{\hbar^2}\int_0^t \mathrm{d}t_2\int_0^{t_2}\mathrm{d}t_1\,\hat{H}(t_2)\hat{H}(t_1) + \cdots.
\end{aligned} \tag{1.31}$$

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

$$\mathcal{T}[\hat{H}(t_1)\hat{H}(t_2)] = \begin{cases} \hat{H}(t_1)\hat{H}(t_2) & t_1 \geq t_2 \\ \hat{H}(t_2)\hat{H}(t_1) & t_2 > t_1 \end{cases}, \tag{1.32}$$

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

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

$$\hat{U}(t) = 1 - \frac{i}{\hbar}\int_0^t \mathrm{d}t_1\, \hat{H}(t_1) - \frac{1}{2\hbar^2}\int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1\, \mathcal{T}[\hat{H}(t_1)\hat{H}(t_2)] + \cdots . \tag{1.33}$$

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

$$\hat{U}(t) = \mathcal{T}\exp\Big(-\frac{i}{\hbar}\int_0^t \mathrm{d}t'\, \hat{H}(t')\Big) \tag{1.34}$$

This expression should be handled with extreme care! It evidently reduces to $e^{-i\hat{H}t/\hbar}$ in the case of a time-independent Hamiltonian. In the general case, it is only really useful in the form of the expansion Eq. (1.33).

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

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{x}(t)] = \frac{\hat{p}(t)}{m} \tag{1.35}$$

$$\frac{\mathrm{d}\hat{p}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{p}(t)] = -\, m\omega^2\hat{x}(t) + F(t). \tag{1.36}$$

In terms of $\hat{a}$ and $\hat{a}^\dagger$

$$\hat{H}(t) = \frac{\hbar\omega}{2}\Big(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\Big) - F(t)\sqrt{\frac{\hbar}{2m\omega}}\Big(\hat{a} + \hat{a}^\dagger\Big), \tag{1.37}$$

and we have

$$\frac{\mathrm{d}\hat{a}}{\mathrm{d}t} = -i\omega\hat{a} + iF(t)\sqrt{\frac{1}{2m\hbar\omega}}. \tag{1.38}$$

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

$$\frac{\mathrm{d}\tilde{\hat{a}}}{\mathrm{d}t} = +i\frac{F(t)e^{i\omega t}}{\sqrt{2m\hbar\omega}}, \tag{1.39}$$

with general solution

$$\tilde{\hat{a}}(t) = \tilde{\hat{a}}(0) + \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega t'}\,\mathrm{d}t'\,, \tag{1.40}$$

and similarly

$$\tilde{\hat{a}}^\dagger(t) = \tilde{\hat{a}}^\dagger(0) - \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{-i\omega t'}\,\mathrm{d}t'\,. \tag{1.41}$$

From this we have

$$\hat{x}(t) = \frac{1}{2}\sqrt{\frac{2\hbar}{m\omega}}\Big(\hat{a}(t) + \hat{a}^\dagger(t)\Big) = \hat{x}(0) - \frac{1}{m\omega}\int_0^t F(t')\sin(\omega t')\,\mathrm{d}t'\,, \tag{1.42}$$

this is the same as for a classical harmonic oscillator (in the rotating frame).

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

$$\hat{a}\,|0\rangle = 0. \tag{1.43}$$

Since $\hat{a}(t)\hat{U}^\dagger(t)\hat{a}\hat{U}(t)$ we have $\hat{a}\hat{U}(t) = \hat{U}(t)\hat{a}(t)$ and thus

$$\hat{a}\hat{U}(t)\,|0\rangle = \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}\,\mathrm{d}t'\,\hat{U}(t)\,|0\rangle\,, \tag{1.44}$$

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

$$\frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}\,\mathrm{d}t'\,, \tag{1.45}$$

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

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle\,. \tag{1.46}$$

The explicit form of a normalised coherent state is

$$|\alpha\rangle = e^{-|\alpha|^2/2}e^{\alpha\hat{a}^\dagger}\,|0\rangle\,, \tag{1.47}$$

where both the property Eq. (1.46) and the normalisation follow from the fundamental commutator $[\hat{a},\hat{a}^\dagger] = 1$. Given Eq. (1.47),

$$\hat{a}\,|\alpha\rangle = e^{-|\alpha|^2/2}\left[\hat{a}, e^{\alpha\hat{a}^\dagger}\right]|0\rangle = \alpha\,|\alpha\rangle\,. \tag{1.48}$$

For the normalisation, we have

$$\langle\alpha|\alpha\rangle = e^{-|\alpha|^2}\sum_{n,m}\langle 0|\frac{(\alpha^*\hat{a})^n}{n!}\frac{\left(\alpha\hat{a}^\dagger\right)^m}{m!}|0\rangle = e^{-|\alpha|^2}\sum_n\frac{|\alpha|^2}{n!} = 1. \tag{1.49}$$

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

Time-dependent perturbation theory (see AQP notes) gives

$$c_n^{(1)} = -\frac{i}{\hbar}\int_{t_0}^t \mathrm{d}t'\,e^{i\omega_{n,i}t'}V_{n,i}(t'). \tag{1.50}$$

In our case the energy different between $|0\rangle$ and $|1\rangle$ is $\hbar\omega$, and the matrix element $V_{1,0}(t') = -F(t')\hbar/(2m\omega)$. This coincides with (1.45), because

$$\langle 1|\hat{U}(t)|0\rangle = \langle 0|\hat{U}(t)\hat{a}(t)|0\rangle = \langle 0|\hat{U}(t)|0\rangle\,\frac{i}{\sqrt{2m\hbar\omega}}\int_0^t F(t')e^{i\omega(t'-t)}\,\mathrm{d}t'\,. \tag{1.51}$$

Then $\langle 0|\hat{U}(t)|0\rangle = 1 + \mathcal{O}(F^2)$.

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 $\hat{S}_i = \frac{1}{2}\hat{\sigma}_i$ as

$$\hat{H}(t) = \mathbf{H}(t) \cdot \hat{\mathbf{S}}, \tag{1.52}$$

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

$$\hat{H}(t) = \frac{1}{2}\begin{pmatrix} H_z(t) & H_x(t) - iH_y(t) \\ H_x(t) + iH_y(t) & -H_z(t) \end{pmatrix}. \tag{1.53}$$

The Schrödinger equation corresponding to Eq. (1.52) is

$$i\hbar \frac{\mathrm{d}\,|\Psi\rangle}{\mathrm{d}t} = \hat{H}(t)\,|\Psi\rangle\,, \tag{1.54}$$

where $|\Psi\rangle = (\psi_\uparrow, \psi_\downarrow)$.

As before, the formal solution to Eq. (1.54) can be written as

$$|\Psi(t)\rangle = \hat{U}(t,t')\,|\Psi(t')\rangle\,, \tag{1.55}$$

In the present case, $\hat{U}(t,t')$ 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 $\hat{H}(t)$ and $\hat{U}(t,t')$. If we think of $\hat{U}(t,t')$ as representing a kind of rotation in Hilbert space, $\hat{H}(t)$ 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 $\hat{\mathbf{S}}(t) = \hat{U}^\dagger(t,t')\hat{\mathbf{S}}(t')\hat{U}(t,t')$, which take the form

$$\begin{aligned} \frac{\mathrm{d}\hat{\mathbf{S}}}{\mathrm{d}t} &= \frac{i}{\hbar}[\mathbf{H}(t), \hat{\mathbf{S}}] \\ &= \frac{1}{\hbar}\mathbf{H}(t) \times \hat{\mathbf{S}} \end{aligned} \tag{1.56}$$

by virtue of the spin commutation relations $[\hat{S}_i, \hat{S}_j] = i\varepsilon_{ijk}\hat{S}_k$.[2] Thus $\hat{\mathbf{S}}$ 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

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

the solution must be expressible in the form of a matrix connecting the initial and final operators

$$\hat{\mathbf{S}}(t) = \mathrm{R}(t,t')\hat{\mathbf{S}}(t'). \tag{1.57}$$

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

$$\mathrm{R}(t,t') = \mathcal{T}\exp\left(\int_{t'}^{t} \Omega(t_i)\,\mathrm{d}t_i\right), \tag{1.58}$$

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

$$\Omega(t) = \begin{pmatrix} 0 & -H_z(t) & H_y(t) \\ H_z(t) & 0 & -H_x(t) \\ -H_y(t) & H_x(t) & 0 \end{pmatrix}. \tag{1.59}$$

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

To find the $t \to t'$ time-evolution matrix for a magnetic field in the z-direction, and the matrix that maps the Heisenberg spin operator at time t' to the Heisenberg spin operator at t, we start from Eq. (1.53) to first yield the Hamiltonian

$$\hat{H} = \begin{pmatrix} H/2 & 0 \\ 0 & H/2 \end{pmatrix}. \tag{1.60}$$

This is independent of time, and therefore the time-ordered exponential is just an ordinary matrix exponential because the Hamiltonian cannot fail to commute with itself when evaluated at different times. Moreover it is diagonal in this basis and so the matrix exponential is also easily evaluated:

$$\begin{aligned} \hat{U}(t,t') &= \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_{t'}^{t} H(t_i)\,\mathrm{d}t_i\right) \\ &= \exp\left(-\frac{i}{\hbar}\begin{pmatrix} H(t-t')/2 & 0 \\ 0 & -H(t-t')/2 \end{pmatrix}\right) \\ &= \begin{pmatrix} \exp\left(-\frac{i}{\hbar}H(t-t')/2\right) & 0 \\ 0 & \exp\left(\frac{i}{\hbar}H(t-t')/2\right) \end{pmatrix}. \end{aligned} \tag{1.61}$$

Since $\Omega_{jk} = -H_i\varepsilon_{ijk}$ and $H_i = \delta_{iz}H$ we find that

$$\Omega(t) = \begin{pmatrix} 0 & -H & 0 \\ H & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{1.62}$$

which is not diagonal and therefore not trivial to exponentiate even though there is no problem time-ordering. We could perform a diagonalisation, but it is nicer to notice that $\Omega = iH\sigma_y \oplus 0$, and use $e^{i\theta\sigma_a} = \cos\theta + i\sigma_a\sin\theta$ (to prove this,use $\sigma_a^2 = 1$). Then

$$\begin{aligned} \mathrm{R}(t,t') &= \exp(iH(t-t')\sigma_y) \oplus \exp(0) \\ &= (\cos(H(t-t')) + i\sigma_y\sin(H(t-t'))) \oplus 1, \end{aligned} \tag{1.63}$$

with the matrix explicitly

$$\mathrm{R}(t,t') = \begin{pmatrix} \cos(H(t-t')) & -\sin(H(t-t')) & 0 \\ \sin(H(t-t')) & \cos(H(t-t')) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{1.64}$$

1.2.1 Rabi Oscillations

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

$$\hat{\mathbf{H}}(t) = \begin{pmatrix} \hat{H}_R \cos(\omega t) \\ \hat{H}_r \sin(\omega t) \\ \hat{H}_0 \end{pmatrix}, \tag{1.65}$$

corresponding to the Hamiltonian

$$\hat{H}(t) = \hat{H}_0 \hat{S}_z + \frac{\hat{H}_R}{2}\left(\hat{S}_+ e^{-i\omega t} + \hat{S}_- e^{i\omega t}\right), \tag{1.66}$$

where $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$. The key to solving the problem is to transform the Schrödinger equation Eq. (1.54) by multiplying by $\exp\left(i\omega t\hat{S}_z\right)$. Define

$$|\Psi_R(t)\rangle \equiv \exp\left(i\omega t\hat{S}_z\right)|\Psi(t)\rangle\,. \tag{1.67}$$

This transformed state satisfies

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi_R\rangle &= i\hbar e^{i\omega t\hat{S}_z}\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle - \hbar\omega\hat{S}_z|\Psi_R\rangle \\ &= e^{i\omega t\hat{S}_z}\hat{H}(t)|\Psi\rangle - \hbar\omega\hat{S}_z|\Psi_R\rangle \\ &= e^{i\omega t\hat{S}_z}\hat{H}(t)e^{-i\omega t\hat{S}_z}|\Psi_R\rangle - \hbar\omega\hat{S}_z|\Psi_R\rangle \\ &= \hat{H}_{\mathrm{Rabi}}|\Psi_R\rangle\,. \end{aligned} \tag{1.68}$$

In the last line we defined

$$\hat{H}_{\mathrm{Rabi}} \equiv e^{i\omega t\hat{S}_z}\hat{H}(t)e^{-i\omega t\hat{S}_z} - \hbar\omega\hat{S}_z = (\hat{H}_0 - \hbar\omega)\hat{S}_z + \hat{H}_R\hat{S}_x. \tag{1.69}$$

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 $(\hat{H}_R, 0, \hat{H}_0 - \hbar\omega)$ at the **Rabi frequency**,

$$\omega_R = \frac{1}{\hbar}\sqrt{(\hat{H}_0 - \hbar\omega)^2 + \hat{H}_R^2}. \tag{1.70}$$

The amplitude of the oscillations in $\hat{S}_z$ due to this precession is maximal when $\hat{H}_0 = \hbar\omega$. In this case the rotation frequency of the field matches the frequency of precession about the z-axis that would occur if $\hat{H}_R = 0$.

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 adiabatic approximation is a special case of this idea. Let's suppose that in our two level system, the field $\hat{\mathbf{H}}(t)$ 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

$$\hat{H}(t)\left|\pm_t\right\rangle = E_\pm(t)\left|\pm_t\right\rangle. \tag{1.71}$$

We put the t in a subscript on the states to emphasise that they depend on time as a *parameter*. We refer to the $|\pm_t\rangle$ as the **instantaneous energy eigenstates**. Although we can always define these states for any $\hat{\mathbf{H}}(t)$, 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 $\hat{H}(t)$ 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

$$|\Psi(t)\rangle = c_+(t)\left|+_t\right\rangle + c_-(t)\left|-_t\right\rangle. \tag{1.72}$$

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 $\mathrm{d}\left|\pm_t\right\rangle/\mathrm{d}t$.

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 $\mathrm{d}\left|\pm_t\right\rangle/\mathrm{d}t$ as an exercise in *time independent* perturbation theory.[3] Going from t to $t+\delta t$ changes the Hamiltonian by an amount

$$\delta\hat{H}(t) = \frac{\mathrm{d}\hat{H}(t)}{\mathrm{d}t}\delta t. \tag{1.73}$$

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

$$\delta\left|+_t\right\rangle = \frac{\langle -_t|\delta\hat{H}(t)|+_t\rangle}{E_+(t)-E_-(t)}\left|-_t\right\rangle, \tag{1.74}$$

so that

$$\frac{\mathrm{d}\left|+_t\right\rangle}{\mathrm{d}t} = \frac{\langle -_t|\dot{\hat{H}}(t)|+_t\rangle}{E_+(t)-E_-(t)}\left|-_t\right\rangle. \tag{1.75}$$

Using Eq. (1.75) and the corresponding result for $\mathrm{d}\left|-_t\right\rangle/\mathrm{d}t$, we find that the Schrödinger equation gives the following pair of equations for the $c_\pm(t)$

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} E_+(t) & i\hbar\frac{\langle +_t|\dot{\hat{H}}(t)|-_t\rangle}{E_+-E_-} \\ i\hbar\frac{\langle -_t|\dot{\hat{H}}(t)|+_t\rangle}{E_--E_+} & E_-(t) \end{pmatrix}\begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}. \tag{1.76}$$

[3] It's a bit like the interaction representation in time dependent perturbation theory.

If $\hat{H}(t)$ is changing slowly enough, the off-diagonal terms can be neglected and the solution is[4]

$$\boxed{c_{\pm}(t) = \exp\left(-\frac{i}{\hbar}\int_0^t E_{\pm}(t')\,\mathrm{d}t'\right)c_{\pm}(0).} \tag{1.77}$$

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. (1.76) must be small compared to $E_1(t) - E_2(t)$, which corresponds to the condition

$$\hbar\left|\langle -_t|\dot{\hat{H}}|+_t\rangle\right| \ll \left[E_+(t) - E_-(t)\right]^2. \tag{1.78}$$

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 $\hbar$.

1.3.0.1 Adiabatic [*non-examinable*]

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").

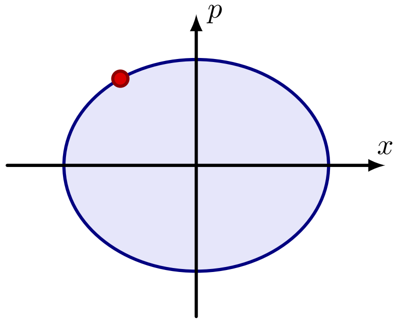

Fig. 1.1: The action of a periodic trajectory is equal to the area enclosed in the phase plane. For a simple harmonic oscillator the curve is an ellipse and the action is the product of the energy and the period. If the period of the oscillator is altered slowly (by changing the length of a pendulum,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

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**

$$S = \oint p\,\mathrm{d}x\,. \tag{1.79}$$

($\oint$ 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

[4] 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.

that predated Schrödinger, Heisenberg, et al.. If the motion of a system is quantised, 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 quantisation condition**

$$\oint p\,\mathrm{d}x = nh, \quad n \in \mathbb{N}. \tag{1.80}$$

1.3.1 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. (1.78) is not satisfied. Let's consider time evolution with the Hamiltonian

$$\hat{H}(t) = \begin{pmatrix} \beta t & \Delta \\ \Delta & -\beta t \end{pmatrix}. \tag{1.81}$$

The instantaneous eigenvalues are

$$E_\pm(t) = \pm\sqrt{(\beta t)^2 + \Delta^2}. \tag{1.82}$$

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

$$\exp\left(-\frac{i}{\hbar}\int_0^t E_-(t')\,\mathrm{d}t'\right)|-_t\rangle\,, \tag{1.83}$$

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.

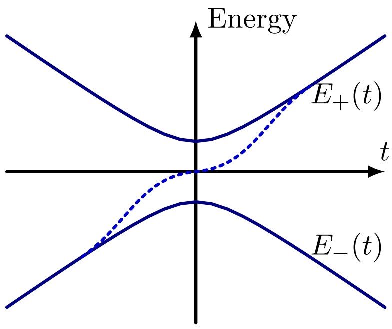

Fig. 1.2: Instantaneous eigenvalues of the Landau–Zener problem. The dotted line schematically illustrates what happens when we pass over the branch point.

How small should β be? We use the condition Eq. (1.78), and the fact that the minimum splitting of the energy levels is 2Δ to arrive at the requirement

$$\frac{\hbar\beta}{\Delta^2} \ll 1. \tag{1.84}$$

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

1.3.1.1 Arbitrary Contour [*non-examinable*]

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.

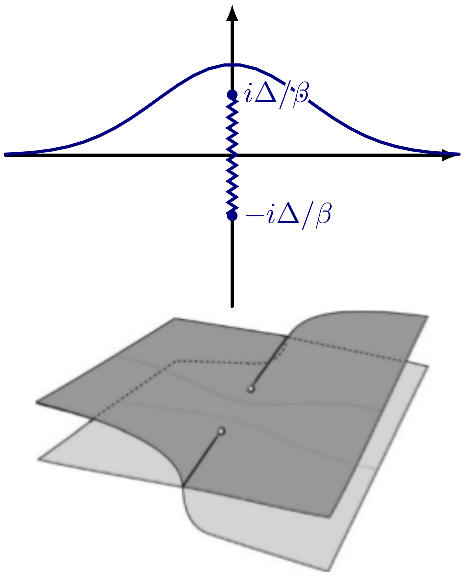

Fig. 1.3: (Top) Branch cut and contour of time evolution in the complex t plane. (Bottom) Riemann surface of $\sqrt{(\beta t)^2 + \Delta^2}$ (real part).

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. (1.83): 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. (1.83). The real part of the exponent arising during evolution from $t = -\infty$ to $t = +\infty$ can then be written

$$\frac{2i}{\hbar}\int_0^{i\Delta/\beta} \sqrt{(\beta t)^2 + \Delta^2}\,\mathrm{d}t = -\frac{\pi\Delta^2}{2\hbar\beta}, \tag{1.85}$$

giving the modulus of the amplitude

$$|c_-(-\infty \to +\infty)| = \exp\left(-\frac{\pi\Delta^2}{2\hbar\beta}\right). \tag{1.86}$$

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. (1.86) actually gives the probability to make the transition to the upper state. The probability to remain in the lower state is therefore

$$\boxed{P_{\text{ground}} = 1 - \exp\left(-\frac{\pi\Delta^2}{2\hbar\beta}\right).} \tag{1.87}$$

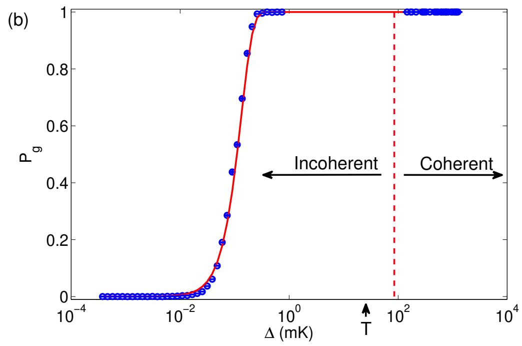

Fig. 1.4: Comparison of Eq. (1.87) with the probability of a superconducting qubit to remain in the ground state. The two states correspond to different values of the magnetic flux trapped in a superconducting ring, and the bias is provided by ramping another flux.[1]

To verify the Landau-Zener result to lowest non-vanishing order in time-dependent perturbation theory, since the result is perturbative in Δ, so we take for our unperturbed Hamiltonian $\hat{H}_0$

$$\hat{H}_0 = \begin{pmatrix} \beta t & 0 \\ 0 & \beta t \end{pmatrix}, \tag{1.88}$$

and our perturbation $\hat{V}$

$$\hat{V} = \begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix}. \tag{1.89}$$

Since our unperturbed Hamiltonian carries an explicit time dependence, we have to remember to integrate it up when converting between the interaction and Schrödinger pictures:

$$\hat{V}_I(t) = \exp\left(i \int_{t_0}^{t} \hat{H}_0(t')\,\mathrm{d}t' / \hbar \right) \hat{V}_S(t_0) \exp\left(-i \int_{t_0}^{t} \hat{H}_0(t')\,\mathrm{d}t' / \hbar \right). \tag{1.90}$$

The Landau-Zener tunnelling appears in this formulation as the transition from the $-\beta t$ eigenstate to the $+\beta t$ eigenstate. Using the result of first-order time dependent perturbation theory

$$c_+^{(1)} = -\frac{i}{\hbar} \int_{-\infty}^{\infty} \exp\left(i \int_0^{t'} \left(E_0^+(t'') - E_0^-(t'') \right) \mathrm{d}t'' \right) V_{+-}(t')\,\mathrm{d}t'\,, \tag{1.91}$$

we find

$$\begin{aligned} c_+^{(1)} &= -\frac{i\Delta}{\hbar} \int_{-\infty}^{\infty} e^{i(\beta-(-\beta))t'^2/2}\,\mathrm{d}t' \\ &= -\frac{i\Delta}{\hbar} \sqrt{\frac{\pi\hbar}{i\beta}}. \end{aligned} \tag{1.92}$$

Therefore the transition probability $P_{-\to+}$ is given by

$$\left| c_+^{(1)} \right|^2 = \frac{\pi\Delta^2}{\beta\hbar}, \tag{1.93}$$

in agreement with the Landau-Zener result to order Δ^2.

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

$$\delta\left|+_t\right\rangle = \frac{\langle -_t|\delta\hat{H}(t)|+_t\rangle}{E_+(t)-E_-(t)}\left|-_t\right\rangle. \tag{1.94}$$

This change is in the direction of $\left|-_t\right\rangle$ i.e. *orthogonal* to $\left|+_t\right\rangle$. The usual justification for this in the context of perturbation theory is that any change parallel to $\left|+_t\right\rangle$ 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 $\left|+_t\right\rangle$ gives

$$\left|+_t\right\rangle \to e^{i\delta\theta}\left|+_t\right\rangle \sim (1+i\delta\theta)\left|+_t\right\rangle. \tag{1.95}$$

Suppose now that $\hat{H}(t)$ is subject to some adiabatic *cyclic* change around some closed path γ in the space of matrices. If after time T we have $\hat{H}(T)=\hat{H}(0)$, then after evolving $\left|+_t\right\rangle$ according to Eq. (1.94) it would be natural to expect that it will return to its original value. That is,

$$\left|+_T\right\rangle \stackrel{?}{=} \left|+_0\right\rangle. \tag{1.96}$$

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

$$\left|+_T\right\rangle = e^{i\theta_B[\gamma]}\left|+_0\right\rangle, \tag{1.97}$$

where the phase $\theta_B[\gamma]$ 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. (1.52)) is parametrised in terms of the field $\mathbf{H}(t)$. Suppose we fix the states $\left|\mathbf{H},\pm\right\rangle$ for each value of the field at the outset. That is, there is no ambiguity in the phase as in Eq. (1.97). We can then use these states to write the state of the system in the instantaneous eigenbasis (c.f. Eq. (1.72))

$$\left|\Psi(t)\right\rangle = c_+(t)\left|\mathbf{H}(t),+\right\rangle + c_-(t)\left|\mathbf{H}(t),-\right\rangle. \tag{1.98}$$

If $\left|\mathbf{H},+\right\rangle$ changes smoothly as $\mathbf{H}$ changes, we will see that Eq. (1.94) cannot be obeyed: there is always some contribution in the direction of $\left|\mathbf{H},+\right\rangle$ corresponding to a change of phase. This defines a vector field in the space of $\mathbf{H}$ by

$$\mathbf{A}_+(\mathbf{H}) \equiv -i\left\langle \mathbf{H},+\right|(\boldsymbol{\nabla}_{\mathbf{H}}\left|\mathbf{H},+\right\rangle), \tag{1.99}$$

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

To show that using normalised states guarantees $\mathbf{A}_+(\mathbf{H})$ is real, we start by considering the norm of the state $\left|\mathbf{H}+\delta\mathbf{H},+\right\rangle$:

$$\langle \mathbf{H}+\delta\mathbf{H},+|\mathbf{H}+\delta\mathbf{H},+\rangle = \langle \mathbf{H},+|\mathbf{H},+\rangle + \delta\mathbf{H}\cdot\Big(\boldsymbol{\nabla}(\langle \mathbf{H},+|)\left|\mathbf{H},+\right\rangle + \langle \mathbf{H},+|\,\boldsymbol{\nabla}(\left|\mathbf{H},+\right\rangle)\Big) + \mathcal{O}\Big(\delta^2\Big), \tag{1.100}$$

which vanishes to $\mathcal{O}(\delta^2)$ if

$$0 = \Big(\boldsymbol{\nabla}\left\langle \mathbf{H},+\right|\Big)\left|\mathbf{H},+\right\rangle + \left\langle \mathbf{H},+\right|\Big(\boldsymbol{\nabla}\left|\mathbf{H},+\right\rangle\Big). \tag{1.101}$$

Now using the definition of $\mathbf{A}_+ = -i \langle \mathbf{H}, + | \left(\boldsymbol{\nabla} | \mathbf{H}, + \rangle \right)$ we find that

$$\begin{aligned} \mathbf{A}_+^* &= \mathbf{A}_+^\dagger \\ &= i \Big(\boldsymbol{\nabla} \langle \mathbf{H}, + | \Big) | \mathbf{H}, + \rangle \\ &= -i \langle \mathbf{H}, + | \Big(\boldsymbol{\nabla} | \mathbf{H}, + \rangle \Big) \\ &= \mathbf{A}_+. \end{aligned} \tag{1.102}$$

This reflects the anti-Hermitian nature of the gradient operator.

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

$$\hat{\mathbf{n}} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}. \tag{1.103}$$

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

$$\hat{H} = \frac{H_0}{2} \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}. \tag{1.104}$$

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

$$|\mathbf{H}, +\rangle = \begin{pmatrix} \cos(\theta/2) e^{-i\phi/2} \\ \sin(\theta/2) e^{i\phi/2} \end{pmatrix}. \tag{1.105}$$

Computing $\mathbf{A}_+(\mathbf{H})$ defined by Eq. (1.99) gives[5]

$$\mathbf{A}_+(\mathbf{H}) = -\hat{\boldsymbol{\phi}} \frac{\cot\theta}{2H_0}. \tag{1.107}$$

In order to find the Berry connection $\mathbf{A}_-$, we can write first down $|\mathbf{H}, -\rangle$ by demanding orthogonality with the E_+ eigenstate, so that in the basis with $\hat{S}_z$ diagonal,

$$|\mathbf{H}, -\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} e^{-i\phi/2} \\ \cos\frac{\theta}{2} e^{i\phi/2} \end{pmatrix}. \tag{1.108}$$

Taking the $\mathbf{H}$-space gradient of this state gives

$$\boldsymbol{\nabla} |\mathbf{H}, -\rangle = \frac{\hat{\boldsymbol{\theta}}}{2r} \begin{pmatrix} -\cos\frac{\theta}{2} e^{-i\phi/2} \\ -\sin\frac{\theta}{2} e^{i\phi/2} \end{pmatrix} - \frac{i\hat{\boldsymbol{\phi}}}{2r\sin\theta} \begin{pmatrix} -\sin\frac{\theta}{2} e^{-i\phi/2} \\ -\cos\frac{\theta}{2} e^{i\phi/2} \end{pmatrix}, \tag{1.109}$$

and noticing that the projection onto $\hat{\boldsymbol{\theta}}$ is proportional to $|\mathbf{H}, +\rangle$ we can write down

$$\begin{aligned} \langle \mathbf{H}, - | \boldsymbol{\nabla} | \mathbf{H}, - \rangle &= \frac{i\hat{\boldsymbol{\phi}}}{2r\sin\theta} \Big(-\sin\tfrac{\theta}{2} e^{i\phi/2}, \quad \cos\tfrac{\theta}{2} e^{-i\phi/2} \Big) \begin{pmatrix} \sin\frac{\theta}{2} e^{-i\phi/2} \\ \cos\frac{\theta}{2} e^{i\phi/2} \end{pmatrix} \\ &= i\hat{\boldsymbol{\phi}} \frac{\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}}{2r\sin\theta} \\ &= \hat{\boldsymbol{\phi}} \frac{i\cot\theta}{2r}, \end{aligned} \tag{1.110}$$

[5] The gradient operator in spherical polars is

$$\boldsymbol{\nabla} = \hat{\mathbf{r}} \partial_r + \hat{\boldsymbol{\theta}} \frac{1}{r} \partial_\theta + \hat{\boldsymbol{\phi}} \frac{1}{r\sin\theta} \partial_\phi, \tag{1.106}$$

we'll often use the notation $\partial_i = \partial/\partial x_i$, $\partial_i^2 = \partial^2 \big/ \partial x_i^2$, etc. in these notes.

and so

$$\begin{aligned}\mathbf{A}_- &= -i\,\langle \mathbf{H}, -|\boldsymbol{\nabla}|\mathbf{H}, -\rangle \\ &= +\hat{\phi}\frac{i\cot\theta}{2r}.\end{aligned} \tag{1.111}$$

We now use Eq. (1.98) in the derivation of the adiabatic theorem as before. Instead of Eq. (1.94) we get

$$\delta\,|\mathbf{H}, +\rangle = \frac{\langle \mathbf{H}, -|\delta\hat{H}|\mathbf{H}, +\rangle}{H_0}\,|\mathbf{H}, -\rangle + i\mathbf{A}_+(\mathbf{H})\cdot\delta\mathbf{H}\,|\mathbf{H}, +\rangle\,, \tag{1.112}$$

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

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} E_+(t) + \hbar\mathbf{A}_+(\mathbf{H})\cdot\dot{\mathbf{H}} & 0 \\ 0 & E_-(t) + \hbar\mathbf{A}_-(\mathbf{H})\cdot\dot{\mathbf{H}} \end{pmatrix}\begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}, \tag{1.113}$$

and the solution is now

$$c_\pm(t) = \exp\left(-\frac{i}{\hbar}\int_0^t \left[e_\pm(t') + \hbar\mathbf{A}_\pm(\mathbf{H})\cdot\dot{\mathbf{H}}\right]\mathrm{d}t'\right)c_\pm(0). \tag{1.114}$$

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

$$\boxed{\theta_{B,\pm}[\gamma] = -\oint_\gamma \mathbf{A}_\pm(\mathbf{H})\cdot\mathrm{d}\mathbf{H}\,,} \tag{1.115}$$

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

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 $\theta_{B,\pm}$ does too. However, any other choice can be obtained by multiplying $|\mathbf{H}, \pm\rangle$ by some $\mathbf{H}$ dependent phase factor. Then

$$\begin{aligned}|\mathbf{H}, \pm\rangle &\to \exp(i\Lambda_\pm(\mathbf{H}))\,|\mathbf{H}, \pm\rangle \\ \mathbf{A}_\pm(\mathbf{H}) &\to \mathbf{A}_\pm + \boldsymbol{\nabla}_{\mathbf{H}}\Lambda_\pm(\mathbf{H}),\end{aligned} \tag{1.116}$$

and the line integral in Eq. (1.115) 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 recognise Eq. (1.116) 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 $\theta_{B,\pm}$ is a gauge invariant quantity.

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

$$\mathbf{B}_\pm(\mathbf{H}) \equiv \boldsymbol{\nabla}_{\mathbf{H}} \times \mathbf{A}_\pm(\mathbf{H}) = \pm\frac{\hat{\mathbf{n}}}{2H_0^2}, \tag{1.117}$$

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

$\theta_{B,\pm}$. Using Stokes' theorem to convert the loop integral in Eq. (1.115) into a surface integral over a surface Σ bounded by γ gives

$$\boxed{\theta_{B,\pm}[\gamma] = -\sum_{\Sigma} \mathbf{B}_\pm \cdot \mathrm{d}\mathbf{S} = \mp\frac{1}{2}\Omega,} \tag{1.118}$$

where Ω is the solid angle enclosed by Σ.[6]

Note that the singularities appearing the gauge field in Eq. (1.106) 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.

1.4.1 Classical Analogue [*non-examinable*]

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.

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

$$L_{\text{axle}} \stackrel{?}{=} I\dot{\theta} = 0. \tag{1.119}$$

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 $(\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\mathbf{n}})$, where $\hat{\mathbf{n}}$ is parallel to the axle, and $\hat{\mathbf{a}} \times \hat{\mathbf{b}} = \hat{\mathbf{n}}$. The motion we just described corresponds to a rotation in the $a - b$ plane. Rotating the axle by ϕ corresponds to

$$\begin{aligned} \hat{\mathbf{a}} &\to \cos\phi \hat{\mathbf{a}} + \sin\phi + \hat{\mathbf{b}} \\ \hat{\mathbf{b}} &\to \cos\phi \hat{\mathbf{b}} - \sin\phi \hat{\mathbf{a}}. \end{aligned} \tag{1.120}$$

Now notice that

$$\mathrm{d}\phi = -\hat{\mathbf{a}} \cdot \mathrm{d}\hat{\mathbf{b}} = \hat{\mathbf{b}} \cdot \mathrm{d}\hat{\mathbf{a}}\,. \tag{1.121}$$

[6] 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.

Thus Eq. (1.119) should really be

$$\dot{\theta} + \dot{\phi} = \dot{\theta} + \frac{1}{2}\left[\hat{\mathbf{b}} \cdot \dot{\hat{a}} - \hat{\mathbf{a}} \cdot \dot{\hat{b}}\right] = 0. \tag{1.122}$$

To make the connection to Berry's phase, we introduce the complex vector $\boldsymbol{\psi} = (\hat{\mathbf{a}} + i\hat{\mathbf{b}})/\sqrt{2}$. Then Eq. (1.122) can be written

$$\dot{\theta} + i\boldsymbol{\psi}^{\dagger}\frac{\mathrm{d}\boldsymbol{\psi}}{\mathrm{d}t} = 0. \tag{1.123}$$

Now for each direction $\hat{\mathbf{n}}$, fix $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$. We have some freedom here, as we can always choose them differently by rotating in the plane normal to $\hat{\mathbf{n}}$ as in Eq. (1.120). 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

$$\Delta\theta = \int \dot{\theta}\,\mathrm{d}t = \int -i\boldsymbol{\psi}^{\dagger}\frac{\mathrm{d}\boldsymbol{\psi}}{\mathrm{d}t}\,\mathrm{d}t = \int \mathbf{A}_{\hat{\mathbf{n}}} \cdot \mathrm{d}\hat{\mathbf{n}}\,, \tag{1.124}$$

where we defined $\mathbf{A}_{\hat{\mathbf{n}}} = -i\boldsymbol{\psi}^{\dagger}\boldsymbol{\nabla}_{\hat{\mathbf{n}}}\boldsymbol{\psi}$. 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

$$\hat{\mathbf{a}} = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) \tag{1.125}$$

$$\hat{\mathbf{b}} = (-\sin\phi, \cos\phi, 0) \tag{1.126}$$

$$\hat{\mathbf{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \tag{1.127}$$

and then compute

$$\mathbf{A}_{\hat{\mathbf{n}}} = -\cos\theta\boldsymbol{\nabla}_{\hat{\mathbf{n}}}\phi. \tag{1.128}$$

We get

$$\Delta\theta = \oint \mathbf{A}_{\hat{\mathbf{n}}} \cdot \mathrm{d}\hat{\mathbf{n}} = \int (\boldsymbol{\nabla}_{\hat{\mathbf{n}}} \times \mathbf{A}_{\hat{\mathbf{n}}}) \cdot \mathrm{d}\mathbf{S} = \int \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = \Omega, \tag{1.129}$$

which is the result stated above.

$\boldsymbol{\nabla}_{\hat{\mathbf{n}}} \times \mathbf{A}_{\hat{\mathbf{n}}}$ can be found in a slicker way without introducing an explicit parametrisation of the triad. To evaluate the antisymmetric tensor

$$\partial_i\hat{\mathbf{a}} \cdot \partial_j\hat{\mathbf{b}} - \partial_j\hat{\mathbf{a}} \cdot \partial_i\hat{\mathbf{b}}, \tag{1.130}$$

we first notice that $\partial_i\hat{\mathbf{a}}$ must lie in the $b - n$ plane (to preserve normalisation) and likewise $\partial_j\hat{\mathbf{b}}$ must lie in the $a - n$ plane. Thus Eq. (1.130) can be written

$$\partial_i\hat{\mathbf{a}} \cdot \partial_j\hat{\mathbf{b}} - \partial_j\hat{\mathbf{a}} \cdot \partial_i\hat{\mathbf{b}} = (\hat{\mathbf{n}} \cdot \partial_i\hat{\mathbf{a}})\left(\hat{\mathbf{n}} \cdot \partial_j\hat{\mathbf{b}}\right) - (\hat{\mathbf{n}} \cdot \partial_j\hat{\mathbf{a}})\left(\hat{\mathbf{n}} \cdot \partial_i\hat{\mathbf{b}}\right). \tag{1.131}$$

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

$$\begin{aligned}(\hat{\mathbf{n}} \cdot \partial_i\hat{\mathbf{a}})\left(\hat{\mathbf{n}} \cdot \partial_j\hat{\mathbf{b}}\right) - (\hat{\mathbf{n}} \cdot \partial_j\hat{\mathbf{a}})\left(\hat{\mathbf{n}} \cdot \partial_i\hat{\mathbf{b}}\right) &= (\hat{\mathbf{a}} \cdot \partial_i\hat{\mathbf{n}})\left(\hat{\mathbf{b}} \cdot \partial_j\hat{\mathbf{n}}\right) - (\hat{\mathbf{n}} \cdot \partial_j\hat{\mathbf{n}})\left(\hat{\mathbf{b}} \cdot \partial_i\hat{\mathbf{n}}\right) \\ &= (\hat{\mathbf{a}} \times \hat{\mathbf{b}}) \cdot (\partial_i\hat{\mathbf{n}} \times \partial_j\hat{\mathbf{n}}) \\ &= \hat{\mathbf{n}} \cdot (\partial_i\hat{\mathbf{n}} \times \partial_j\hat{\mathbf{n}}).\end{aligned} \tag{1.132}$$

In polar coordinates,

$$\hat{\mathbf{n}} \cdot (\partial_i\hat{\mathbf{n}} \times \partial_j\hat{\mathbf{n}}) = \sin\theta\partial_i\theta\partial_j\phi, \tag{1.133}$$

which is just what we found before.

Chapter 2

Introduction to Path Integrals

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 $\hat{U}(t) \equiv e^{-i\hat{H}t/\hbar}$, where $\hat{H}$ is the Hamiltonian, as

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

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

$$\langle\Psi(t)|\hat{A}|\Phi(t)\rangle = \langle\Psi(0)|\hat{A}(t)|\Phi(0)\rangle\,, \tag{2.3}$$

where $\hat{A}(t) \equiv e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}$ defines the time evolution of $\hat{A}$. To put it another way, $\hat{A}(t)$ obeys the Heisenberg equation of motion

$$\frac{\mathrm{d}\hat{A}}{\mathrm{d}t} = \frac{i}{\hbar}\left[\hat{H}, \hat{A}\right]. \tag{2.4}$$

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

Eqs. (2.1) and (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.[1] This is **Feynman's path integral**.

[1]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.

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

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

where $|\mathbf{r}\rangle$ denotes a position eigenstate.[2] $\theta(t)$ 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 $t > t'$

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

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 both of

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

To explain why these two definitions are equivalent, if we integrate Eq. (2.8) with respect to t from $t'-\varepsilon$ to $t'+\varepsilon$ we find

$$i\hbar K(\mathbf{r},t'+\varepsilon|\mathbf{r}',t') - \int_{t'-\varepsilon}^{t'+\varepsilon} \mathrm{d}t\,\hat{H}K(\mathbf{r},t|\mathbf{r}',t') = i\hbar\delta(\mathbf{r}-\mathbf{r}'). \tag{2.9}$$

Using the fact that we know $K = 0$ for $t < t'$ we may approximate the integral for small ε as

$$K(\mathbf{r},t'+\varepsilon|\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}') - \varepsilon\frac{i}{\hbar}\hat{H}K(\mathbf{r},t|\mathbf{r}',t'). \tag{2.10}$$

We can see that this is equivalent to the first definition (2.5) by Taylor expanding (2.5) in t about t' and using the fact that $\partial_t\hat{U} = -\frac{i}{\hbar}\hat{H}\hat{U}$ as well as $\hat{U}(0) = 1$,

$$\begin{aligned} K(\mathbf{r},t'+\varepsilon|\mathbf{r}',t') &\approx \langle\mathbf{r}|\hat{U}(0)|\mathbf{r}'\rangle + \varepsilon\,\langle\mathbf{r}|\partial_t\hat{U}(0)|\mathbf{r}'\rangle \\ &\approx \delta(\mathbf{r}-\mathbf{r}') - \varepsilon\frac{i}{\hbar}\,\langle\mathbf{r}|\hat{H}\hat{U}(0)|\mathbf{r}'\rangle \\ &\approx \delta(\mathbf{r}-\mathbf{r}') - \varepsilon\frac{i}{\hbar}\hat{H}K(\mathbf{r},t'+\varepsilon|\mathbf{r}',t'). \end{aligned} \tag{2.11}$$

[2]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.

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

$$\left[\frac{\partial}{\partial t} - D\nabla_{\mathbf{r}}^2\right] K_{\text{heat}}(\mathbf{r}, t|\mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t') \tag{2.12}$$

$$K_{\text{heat}}(\mathbf{r}, t|\mathbf{r}', t') = 0 \quad \text{for} \quad t < t'. \tag{2.13}$$

To show that the fundamental solution of the heat equation is

$$K_{\text{heat}}(\mathbf{r}, t|\mathbf{r}', t') = \frac{\theta(t - t')}{(4\pi D(t - t'))^{3/2}} \exp\left(-\frac{(\mathbf{r} - \mathbf{r})^2}{4D(t - t')}\right), \tag{2.14}$$

we must first note that the Heaviside step function θ takes care of the second demanded property (2.13). We must also consider that

$$\frac{\partial}{\partial t}\theta(t - t') = \delta(t - t'), \tag{2.15}$$

which can be verified by integrating both sides with respect to time along the interaval $(-\infty, t)$. Armed with this it is a simple matter of applying the operator $\left[\frac{\partial}{\partial t} - D\nabla_{\mathbf{r}}^2\right]$ to (2.14) for K_{heat}. Doing this we find

$$\left[\frac{\partial}{\partial t} - D\nabla_{\mathbf{r}}^2\right] K_{\text{heat}}(\mathbf{r}, t|\mathbf{r}', t') = \delta(t - t')\frac{1}{(4\pi D(t - t'))^{3/2}} \exp\left(-\frac{(\mathbf{r} - \mathbf{r})^2}{4D(t - t')}\right) \tag{2.16}$$

where in the above we have made use of the identity

$$\nabla_{\mathbf{r}}^2 \exp\left(\frac{\alpha}{2}\mathbf{r}^2\right) = \left(3\alpha + \alpha^2\mathbf{r}^2\right) \exp\left(\frac{\alpha}{2}\mathbf{r}^2\right) \tag{2.17}$$

for the spatial derivatives, and we find that all of the terms involving Heaviside functions cancel.

We should now examine the right hand side of the formula (2.16) excluding the $\delta(t-t')$ term; let

$$f(\mathbf{r}, t|\mathbf{r}', t') = \frac{1}{(4\pi D(t - t'))^{3/2}} \exp\left(-\frac{(\mathbf{r} - \mathbf{r})^2}{4D(t - t')}\right). \tag{2.18}$$

We only need to worry about the case where $t - t' = 0$ since there is a temporal delta function multiplying it in (2.16). In the limit that $t - t' \to 0$ we can see that the function vanishes everywhere where $\mathbf{r} - \mathbf{r}'$ is non-zero. However, we can also see from the standard Gaussian formula

$$\int \mathrm{d}^N\mathbf{r} \exp\left(-\frac{\mathbf{r}^2}{2\sigma^2}\right) = \left(\sigma\sqrt{2\pi}\right)^N, \tag{2.19}$$

thus

$$\int f(\mathbf{r},t|\mathbf{r}',t')\,\mathrm{d}^3\mathbf{r} = 1. \tag{2.20}$$

These are the exact properties of a delta function in $\mathbf{r}-\mathbf{r}'$, so we see that

$$\lim_{t\to t'} f(\mathbf{r},t|\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}'), \tag{2.21}$$

and thus (2.14) is the fundamental solution of the heat equation.

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

$$\Theta(\mathbf{r},t) = \int \mathrm{d}\mathbf{r}'\, K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',0)\Theta(\mathbf{r},0). \tag{2.22}$$

Eqs. (2.14) and (2.22) 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. (2.14), 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.

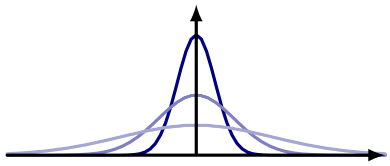

Fig. 2.1: Spreading of a hot spot.

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

$$K(\mathbf{r},t|\mathbf{r}',t') = \int \mathrm{d}^3\mathbf{r}''\, K(\mathbf{r},t|\mathbf{r}'',t'')K(\mathbf{r}'',t''|\mathbf{r}',t'). \tag{2.23}$$

To verify this for $K_{\text{heat}}(\mathbf{r},t|\mathbf{r}',t')$, we must substitute its form into (2.14) and show both sides are equivalent. If we concentrate on the exponent of the integrand, we should complete the square in order to perform the Gaussian Integral,

$$-\frac{(\mathbf{r}-\mathbf{r}'')^2}{4D(t-t'')} - \frac{(\mathbf{r}''-\mathbf{r}')^2}{4D(t''-t')} = -\frac{t-t'}{4D(t-t'')(t''-t'}\left(\mathbf{r}'' + \frac{(t''-t')\mathbf{r}-(t-t'')\mathbf{r}'}{t-t'}\right)^2 - \frac{(\mathbf{r}-\mathbf{r}')^2}{4D(t-t')}. \tag{2.24}$$

When multiplying the time-dependant prefactors of equation (2.14), we find a product of Heaviside θ functions. Since we know that $t<t''<t'$, we find

$$\theta(t-t') = \theta(t-t'')\theta(t''-t'). \tag{2.25}$$

The standard N-dimensional Gaussian integral says that

$$\int \mathrm{d}^N\mathbf{r}\exp\left(-\frac{\mathbf{r}^2}{2\sigma^2}\right) = \left(\sigma\sqrt{2\pi}\right)^N. \tag{2.26}$$

Applying this to the integrand of equation (2.23) with it's exponent in the completed square form (2.24), we find that the time-dependant prefactors cancel out. The entire RHS just simplifies down to (2.14), which is the same as the LHS.

With this in hand, it's a small leap to find the propagator for the free particle Schrödinger equation. The Hamiltonian is $\hat{H} = -\frac{\hbar^2\nabla^2}{2m}$, so by taking $D \to \frac{\hbar}{2m}$ and $t \to it$, we get[3]

$$\boxed{K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t')\left(\frac{m}{2i\pi\hbar(t-t')}\right)^{3/2} \exp\left(-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')}\right).} \tag{2.27}$$

2.2.1 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 $\hat{H} = -\frac{\hbar^2\nabla^2}{2m}$ is diagonal in momentum space, it makes sense to look at[4]

$$\begin{aligned} K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') &= \theta(t-t') \langle \mathbf{p}|\hat{U}(t-t')|\mathbf{p}'\rangle \\ &= \theta(t-t') \exp\left(-i\frac{\mathbf{p}^2}{2m}\frac{t-t'}{\hbar}\right)\delta(\mathbf{p}-\mathbf{p}') \end{aligned} \tag{2.28}$$

We can confirm that Eqs. (2.27) and (2.28) are related by a change of basis (Fourier transform) using

$$\langle \mathbf{r}|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar). \tag{2.29}$$

The definitions of the respective propagators are

$$K(\mathbf{r}, t|\mathbf{r}', t') = \langle \mathbf{r}|\hat{U}(t-t')|\mathbf{r}'\rangle \tag{2.30}$$

$$K(\mathbf{p}, t|\mathbf{p}', t') = \langle \mathbf{p}|\hat{U}(t-t')|\mathbf{p}'\rangle\,. \tag{2.31}$$

We may transform from one to the other by inserting two resolutions of the identity

$$\begin{aligned} \langle \mathbf{r}|\hat{U}(t-t')|\mathbf{r}'\rangle &= \langle \mathbf{r}|\left[\int \mathrm{d}\mathbf{p}\,|\mathbf{p}\rangle\langle\mathbf{p}|\right]\hat{U}(t-t')\left[\int \mathrm{d}\mathbf{p}'\,|\mathbf{p}'\rangle\langle\mathbf{p}'|\right]|\mathbf{r}'\rangle \\ &= \int \mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}'\,\langle\mathbf{r}|\mathbf{p}\rangle\,\langle\mathbf{p}|\hat{U}(t-t')|\mathbf{p}'\rangle\,\langle\mathbf{p}'|\mathbf{r}'\rangle \\ &= \int \frac{\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}'}{(2\pi\hbar)^3} \exp(i(\mathbf{p}\cdot\mathbf{r}-\mathbf{p}'\cdot\mathbf{r}')/\hbar)\,\langle\mathbf{p}|\hat{U}(t-t')|\mathbf{p}'\rangle\,. \end{aligned} \tag{2.32}$$

We know from Eqs. (2.27) and (2.28) that

$$K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t')\left(\frac{m}{2i\pi\hbar(t-t')}\right)^{3/2} \exp\left(-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')}\right) \tag{2.33}$$

$$K_{\text{free}}(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t')\delta(\mathbf{p}-\mathbf{p}')\exp\left(-i\frac{\mathbf{p}^2}{2m}\frac{t-t'}{\hbar}\right), \tag{2.34}$$

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

[4] Don't forget that with the normalisation 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 $\delta(x)$ in d-dimensions has units of $[\text{x}]^{-d}$.

so the answer amounts to putting expression (2.34) into the left hand side of (2.32) and showing that this is equivalent to (2.33). If we do this, we can integrate over $\mathbf{p}'$ and apply the properties of the δ-function to set $\mathbf{p}' = \mathbf{p}$. We now have an exponent in the integrand on which we may complete the square

$$i\mathbf{p} \cdot \frac{\mathbf{r}-\mathbf{r}'}{\hbar} - i\frac{\mathbf{p}^2(t-t')}{2m\hbar} = -\frac{i(t-t')}{2m\hbar}\left(\mathbf{p} - m\frac{\mathbf{r}-\mathbf{r}'}{t-t'}\right)^2 - \frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')}. \tag{2.35}$$

Now we have completed the square we may apply our N-dimensional Gaussian integral formula (2.26). Performing this gives the required LHS.

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

$$K(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t') \sum_\alpha \varphi_\alpha(\mathbf{r})\varphi_\alpha^*(\mathbf{r}')e^{-iE_\alpha(t-t')/\hbar}. \tag{2.36}$$

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.[5]

$$|\Psi(t)\rangle = \hat{U}(t,t')\,|\Psi(t')\rangle\,. \tag{2.38}$$

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

2.3 The Path Integral

By using the reproducing property of the kernel (2.23) 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 characterised by its own propagator

$$K(\mathbf{r}_\mathrm{f}, t_\mathrm{f}|\mathbf{r}_\mathrm{i}, t_\mathrm{i}) = \int \mathrm{d}\mathbf{r}_1 \cdots \mathrm{d}\mathbf{r}_{N-1}\, K(\mathbf{r}_\mathrm{f}, t_\mathrm{f}|\mathbf{r}_{N-1}, t_{N-1}) \cdots K(\mathbf{r}_1, t_1|\mathbf{r}_\mathrm{i}, t_\mathrm{i}). \tag{2.39}$$

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[6] 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.

[5]In terms of the Hamiltonian $\hat{H}(t)$, $\hat{U}(t,t')$ has the deceptively simple form,

$$\hat{U}(t,t') = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_{t'}^{t} \mathrm{d}t_i\,\hat{H}(t_i)\right), \tag{2.37}$$

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.

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

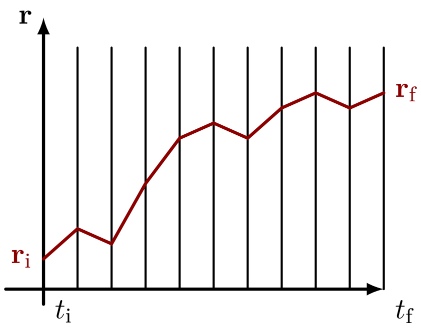

Fig. 2.2: Slicing the propagation time into many small intervals.

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. (2.27)

$$K_\mathrm{free}(\mathbf{r}, t|\mathbf{r}', t') = \theta(t-t')\left(\frac{m}{2i\pi\hbar(t-t')}\right)^{3/2} \exp\left(-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2i\hbar(t-t')} - i\frac{V_0(t-t')}{\hbar}\right), \tag{2.40}$$

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. (2.40) 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)[7].

Putting this into Eq. (2.39), for $N \to \infty$, $(\mathbf{r}_{i+1})^2/(t_{i+1} - t_i) \to \dot{\mathbf{r}}^2 \Delta t$,

$$\boxed{K(\mathbf{r}_\mathrm{f}, t_\mathrm{f}|\mathbf{r}_\mathrm{i}, t_\mathrm{i}) = \int_{\substack{\mathbf{r}(t_\mathrm{f})=\mathbf{r}_\mathrm{f} \\ \mathbf{r}(t_\mathrm{i})=\mathbf{r}_\mathrm{i}}} \mathcal{D}\mathbf{r}(t) \exp\left(\frac{i}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \left[\frac{m\dot{\mathbf{r}}^2}{2} - V(\mathbf{r}(t))\right] \mathrm{d}t\right).} \tag{2.41}$$

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 $\left(\frac{m}{2i\pi\hbar\Delta t}\right)^{3/2}$. 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. (2.41), 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 normalisation, and calculate the effect of introducing $V(\mathbf{r})$ relative to this

2.3.1 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. (2.41) represents the first appearance in quantum mechanics of the *Lagrangian*

$$L(\mathbf{r}, \dot{\mathbf{r}}) \equiv \frac{m\dot{\mathbf{r}}^2}{2} - V(\mathbf{r}), \tag{2.42}$$

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

and its time integral, the *action*[8]

$$S[\mathbf{r}(t)] \equiv \int_{t_\mathrm{i}}^{t_\mathrm{f}} L(\mathbf{r}(t), \dot{\mathbf{r}}(t))\, \mathrm{d}t\,. \tag{2.43}$$

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

$$\frac{\partial L}{\partial \mathbf{r}} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\mathbf{r}}}\right) = 0. \tag{2.44}$$

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

$$L_\mathrm{SHO}(x, \dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2. \tag{2.45}$$

The propagator is therefore expressed as the path integral

$$K_\mathrm{SHO}(x_\mathrm{f}, t_\mathrm{f}|x_\mathrm{i}, t_\mathrm{i}) = \int_{\substack{x(t_\mathrm{f})=x_\mathrm{f}\\ x(t_\mathrm{i})=x_\mathrm{i}}} \mathcal{D}x(t) \exp\left(\frac{i}{\hbar}\overbrace{\int_{t_\mathrm{i}}^{t_\mathrm{f}} \left[\frac{m\dot{x}^2}{2} - \frac{m\omega^2 x^2}{2}\right] \mathrm{d}t}^{S_\mathrm{SHO}[x(t)]}\right). \tag{2.46}$$

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

$$S_\mathrm{SHO}[x_0(t) + \eta(t)] = S_\mathrm{SHO}[x_0(t)] + S_\mathrm{SHO}[\eta(t)] + \int_{t_\mathrm{i}}^{t_\mathrm{f}} \left[m\dot{x}_0(t)\dot{\eta}(t) - m\omega^2 x_0(t)\eta(t)\right] \mathrm{d}t\,. \tag{2.47}$$

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

$$-\int_{t_\mathrm{i}}^{t_\mathrm{f}} \left[m\ddot{x}_0(t) + m\omega^2 x_0(t)\right]\eta(t)\, \mathrm{d}t\,. \tag{2.48}$$

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.

[8] 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

(2.47) vanishes[9] and the propagator takes the from

$$K_{\mathrm{SHO}}(x_{\mathrm{f}}, t_{\mathrm{f}}|x_{\mathrm{i}}, t_{\mathrm{i}}) = \exp\left(\frac{i}{\hbar} S_{\mathrm{SHO}}[x_0(t)]\right) \times \int_{\eta(t_{\mathrm{f}})=\eta(t_{\mathrm{i}})=0} \mathcal{D}\eta(t) \exp\left(\frac{i}{\hbar}\int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}} \left[\frac{m\dot{\eta}^2}{2} - \frac{m\omega^2\eta^2}{2}\right] \mathrm{d}t\right). \quad (2.49)$$

To find the classical action of the trajectory of a harmonic oscillator with $x(t_{\mathrm{i}}) = x_{\mathrm{i}}$ and $x(t_{\mathrm{f}}) = x_{\mathrm{f}}$, we first let $T \equiv t_{\mathrm{f}} - t_{\mathrm{i}}$ and shift things to be symmetrical around $t = 0$. Then we can write the classical motion as

$$x(t) = A\cos\omega t + B\sin\omega t \quad (2.50)$$

with

$$A = \frac{x_{\mathrm{f}} + x_{\mathrm{i}}}{2\cos\omega T}, \quad B = \frac{x_{\mathrm{f}} - x_{\mathrm{i}}}{2\sin\omega T}. \quad (2.51)$$

Evaluating the Lagrangian gives

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2\Big[\Big(B^2 - A^2\Big)\cos 2\omega T + 2AB\sin 2\omega T\Big]. \quad (2.52)$$

When we calculate the action integral the term in AB vanishes (being odd), leaving

$$\begin{aligned} S_{\mathrm{SHO}} = \int_{-T/2}^{T/2} L\,\mathrm{d}t &= \frac{1}{2}m\omega\Big(B^2 - A^2\Big)\sin\omega T \\ &= \frac{m\omega}{2\sin\omega T}\Big[\Big(x_{\mathrm{i}}^2 + x_{\mathrm{f}}^2\Big)\cos\omega(t_{\mathrm{f}} - t_{\mathrm{i}})) - 2x_{\mathrm{i}}x_{\mathrm{f}}\Big]. \end{aligned} \quad (2.53)$$

As a check, let $\omega \to 0$ and see that the free particle action is recovered.

Now we turn our attention to the η path integral in Eq. (2.49). 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

$$\eta(t) = \sum_{n=1}^{\infty} \eta_n \sin\left(\frac{\pi n(t - t_{\mathrm{i}})}{t_{\mathrm{f}} - t_{\mathrm{i}}}\right). \quad (2.54)$$

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

$$S_{\mathrm{SHO}}[\eta(t)] = \frac{m(t_{\mathrm{f}} - t_{\mathrm{i}})}{4}\sum_{n=1}^{\infty}\left[\frac{\pi^2 n^2}{(t_{\mathrm{f}} - t_{\mathrm{i}})^2} - \omega^2\right]\eta_n^2. \quad (2.55)$$

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

The Gaussian integral we can do

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-bx^2/2} = \sqrt{\frac{2\pi}{b}}. \quad (2.56)$$

[9] 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.

So we take a wild guess and write

$$K_{\mathrm{SHO}}(x_{\mathrm{f}}, t_{\mathrm{f}}|x_{\mathrm{i}}, t_{\mathrm{i}}) \stackrel{?}{=} \exp\left(\frac{i}{\hbar}S_{\mathrm{SHO}}[x_0(t)]\right) \times \prod_{n=1}^{\infty}\sqrt{\frac{4\pi i\hbar}{m}\frac{(t_{\mathrm{f}}-t_{\mathrm{i}})}{\pi^2 n^2 - \omega^2(t_{\mathrm{f}}-t_{\mathrm{i}})^2}}. \tag{2.57}$$

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. (2.27) to one dimension, we find

$$K_{\mathrm{SHO}}(x_{\mathrm{f}}, t_{\mathrm{f}}|x_{\mathrm{i}}, t_{\mathrm{i}}) = \left(\frac{m}{2i\pi\hbar(t_{\mathrm{f}}-t_{\mathrm{i}})}\right)^{1/2} \exp\left(\frac{i}{\hbar}S_{\mathrm{SHO}}[x_0(t)]\right) \times \prod_{n=1}^{\infty}\left(1-\frac{\omega^2(t_{\mathrm{f}}-t_{\mathrm{i}})^2}{\pi^2 n^2}\right)^{-1/2}. \tag{2.58}$$

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

$$\prod_{n=1}^{\infty}\left(1-\frac{\omega^2(t_{\mathrm{f}}-t_{\mathrm{i}})^2}{\pi^2 n^2}\right) = \frac{\sin(\omega(t_{\mathrm{f}}-t_{\mathrm{i}}))}{\omega(t_{\mathrm{f}}-t_{\mathrm{i}})}. \tag{2.59}$$

We arrive at the final result

$$\boxed{K_{\mathrm{SHO}}(x_{\mathrm{f}}, t_{\mathrm{f}}|x_{\mathrm{i}}, t_{\mathrm{i}}) = \left(\frac{m\omega}{2i\pi\hbar\sin(\omega(t_{\mathrm{f}}-t_{\mathrm{i}}))}\right)^{1/2} \exp\left(\frac{i}{\hbar}S_{\mathrm{SHO}}[x_0(t)]\right).} \tag{2.60}$$

To show that Eq. (2.60) satisfies the free particle Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}K = -\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 K, \tag{2.61}$$

for short times, $\omega(t_{\mathrm{f}}-t_{\mathrm{i}}) \ll 1$, we may use the short time approximation to simplify the form of K_{SHO}. Working to first order in $\omega(t_{\mathrm{f}}-t_{\mathrm{i}})$, we may simplify the cosine and sine terms to give

$$K_{\mathrm{SHO}}(x_{\mathrm{f}}, t_{\mathrm{f}}|x_{\mathrm{i}}, t_{\mathrm{i}}) = \left(\frac{m\omega}{2i\pi\hbar\omega(t_{\mathrm{f}}-t_{\mathrm{i}})}\right)^{1/2} \exp\left(\frac{i}{\hbar}S_{\mathrm{SHO}}[x_0(t)]\right), \tag{2.62}$$

where we expand the action detailed in equation (2.53) to first order in $\omega(t_{\mathrm{f}}-t_{\mathrm{i}})$,

$$\begin{aligned} S_{\mathrm{SHO}}[x_0(t)] &= \frac{m\omega}{2\sin(\omega(t_{\mathrm{f}}-t_{\mathrm{i}}))}\left[\left(x_{\mathrm{i}}^2+x_{\mathrm{f}}^2\right)\cos(\omega(t_{\mathrm{f}}-t_{\mathrm{i}})) - 2x_{\mathrm{i}}x_{\mathrm{f}}\right] \\ &= \frac{m\omega(x_{\mathrm{i}}-x_{\mathrm{f}})^2}{2\omega(t_{\mathrm{f}}-t_{\mathrm{i}})}. \end{aligned} \tag{2.63}$$

If we apply this reduced form of K_{SHO} to the free-particle Schrödinger equation (2.61), where the $\nabla_{\mathbf{r}}^2$ is interpreted to act on x_{f}, we can see that (2.61) is satisfied.

2.4.1 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[10]. 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 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 discretisation of time that we used to derive it. For Eq. (2.41) 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 (2.14). 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.

[10]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!).

2.5.1 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 $\lambda = \frac{h}{p} = \frac{h}{mv}$ 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

$$\psi(x) = Ae^{\pm ikx} \tag{2.64}$$

$$k = \frac{\sqrt{2m(E-V)}}{\hbar}. \tag{2.65}$$

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

$$\psi(x) = Ae^{\pm Kx} \tag{2.66}$$

$$K = \frac{\sqrt{2m(V-E)}}{\hbar}. \tag{2.67}$$

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.

2.5.2 Derivation

We seek to solve

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + k^2(x)\psi(x) = 0 \tag{2.68}$$

$$k^2(x) = \frac{2m}{\hbar^2}(E - V(x)) \tag{2.69}$$

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,

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = iS' e^{iS} \tag{2.70}$$
$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = (iS'' - S'^2)e^{iS}, \tag{2.71}$$

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

$$\begin{aligned} S' &= \pm\sqrt{k^2(x) + iS''(x)} \\ &= \pm k(x)\sqrt{1 + iS''(x)/k^2} \end{aligned} \tag{2.72}$$

(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

$$\begin{aligned} S' &= \pm k\sqrt{1 \pm ik'(x)/k^2} \\ &\approx k\left(1 \pm \frac{i}{2}\frac{k'(x)}{k^2}\right) \\ &\approx \pm k + \frac{i}{2}\frac{k'(x)}{k} \end{aligned} \tag{2.73}$$

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

$$\begin{aligned} \frac{\mathrm{d}S}{\mathrm{d}x} &= \pm k + \frac{i}{2}\frac{k'}{k} \\ S(x) &\sim \pm \int^x k(x')\,\mathrm{d}x' + \frac{i}{2}\int^x \frac{k'(x')}{k(x')}\,\mathrm{d}x' + c \end{aligned} \tag{2.74}$$

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

$$\begin{aligned} S(x) &= \pm \int^x k(x')\,\mathrm{d}x' + \frac{i}{2}\ln k + c \\ \psi &= e^{iS} \\ &= Ce^{\pm i\int^x k(x')\mathrm{d}x'}e^{-\frac{1}{2}\ln k} \\ &= \frac{C}{\sqrt{k(x)}}e^{\pm i\int^x k(x')\mathrm{d}x'} \end{aligned} \tag{2.75}$$

Note that in making the expansion, we have assumed that $\frac{k'}{k^2} \ll 1$ or $\frac{\lambda}{2\pi}\frac{\mathrm{d}k}{\mathrm{d}x} \ll k$, i.e. that the change in k in one wavelength is much smaller than k. Alternatively, one has $\lambda\frac{\mathrm{d}V}{\mathrm{d}x} \ll \frac{\hbar^2k^2}{m}$ 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

$$\psi(x) = \frac{C}{\sqrt{K(x)}}e^{\pm i\int^x K(x')\mathrm{d}x'} \tag{2.76}$$
$$K^2 = \frac{2m}{\hbar^2}(V - E) > 0. \tag{2.77}$$

2.5.3 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

$$k^2(x) = \frac{2m}{\hbar^2}\left(-\frac{\mathrm{d}V}{\mathrm{d}x}\right)_{x=a}(x-a). \tag{2.78}$$

The Schrödinger equation near the turning point becomes

$$\psi'' - \left.\frac{\mathrm{d}V}{\mathrm{d}x}\right|_{x=a}\frac{2m}{\hbar^2}(x-a)\psi = 0. \tag{2.79}$$

If we let

$$z = \alpha(x-a) \tag{2.80}$$

$$\alpha^3 = \frac{2m}{\hbar^2}\frac{\mathrm{d}V}{\mathrm{d}x} \geq 0, \tag{2.81}$$

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

$$f''(z) - zf(z) = 0. \tag{2.82}$$

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

$$i'(k) + k^2\tilde{f}(k) = 0 \tag{2.83}$$

is *first* order, and may be solved easily

$$\tilde{f}(k) = A\exp\Big(ik^3/3\Big), \tag{2.84}$$

with A some constant. Thus all we have to do to find the solution $f(z)$ is compute the Fourier integral[11]

$$f(z) = \frac{1}{2\pi}\int e^{ikz}\tilde{f}(k)\,\mathrm{d}k = \frac{A}{2\pi}\exp\Big(ik^3/3 + ikz\Big)\,\mathrm{d}k\,. \tag{2.85}$$

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. (2.85), and our freedom to choose this allows us to generate more than one solution.

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

To show that $f(z)$ defined by Eq. (2.85) satisfies Airy's equation , we have

$$\begin{aligned} f''(x) - xf(x) &= A\int \left(-k^2 - x\right)\exp\left(ik^3/3 + ikx\right)\mathrm{d}k \\ &= iA\int \frac{\mathrm{d}}{\mathrm{d}k}\exp\left(ik^3/3 + ikx\right)\mathrm{d}k \\ &= 0, \end{aligned} \tag{2.86}$$

as long as the integrand vanishes at the endpoints.

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

$$\mathrm{I}: \quad 0 < \theta < \pi/3 \tag{2.87}$$

$$\mathrm{II}: \quad 2\pi/3 < \theta < \pi \tag{2.88}$$

$$\mathrm{III}: \quad 4\pi/3 < \theta < 5\pi/3. \tag{2.89}$$

$$\tag{2.90}$$

Different choices for the starting and ending wedge give different solutions[12].

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

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[13] satisfy $k^2 + z = 0$ and lie at

$$k_{\mathrm{sp}} = \begin{cases} \pm i\sqrt{z} & \text{for} z > 0 \\ \pm\sqrt{|z|} & \text{for} z < 0, \end{cases} \tag{2.91}$$

with the integrand taking the values

$$\exp\left(ik_{\mathrm{sp}}^3/3 + ik_{\mathrm{sp}}z\right) = \begin{cases} \exp\left(\mp\frac{2}{3}z^{3/2}\right) & \text{for} z > 0 \\ \exp\left(\mp i\frac{2}{3}|z|^{3/2}\right) & \text{for} z < 0. \end{cases} \tag{2.92}$$

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[14] value gives

$$\exp\left(ik^3/3 + ikz\right) \sim \exp\left(\mp\frac{2}{3}z^{3/2}\right)\exp\left(\mp\sqrt{z}(k - k_{\mathrm{sp}})^2\right), \tag{2.93}$$

where the $\pm$ 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

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

[13] Why do we look at a stationary point if we only want to maximise the real part of the exponent? Think about the Cauchy-Riemann equations.

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

the integrand decays fastest. For $-i\sqrt{z}$, the steepest descent direction is parallel to the imaginary axis.

Eq. (2.93) 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. (2.85) is then approximately

$$f(z) \sim \frac{A}{2\pi}\frac{\pi^{1/2}}{z^{1/4}}\exp\left(-\frac{2}{3}z^{3/2}\right) \quad \text{as} \quad z\to\infty. \tag{2.94}$$

The **Airy function** $\mathrm{Ai}(z)$ is defined by this contour,[15] with the (arbitrary) choice $A=1$. Thus we have

$$\mathrm{Ai}(z) \sim \frac{1}{2\pi^{1/2}z^{1/4}}\exp\left(-\frac{2}{3}z^{3/2}\right) \quad \text{as} \quad z\to\infty. \tag{2.95}$$

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. (2.93))

$$\exp\left(ik^3/3+ikz\right) \sim \exp\left(\mp\frac{2}{3}|z|^{3/2}\right)\exp\left(\pm i\sqrt{|z|}(k-k_{\mathrm{sp}})^2\right). \tag{2.96}$$

Fig. 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 give

$$\mathrm{Ai}(z) \sim \frac{1}{\pi^{1/2}|z|^{1/4}}\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right) \quad \text{as} \quad z\to\infty. \tag{2.97}$$

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

$$\oint p(x)\,\mathrm{d}x = h\left(n+\frac{1}{2}\right), \quad n\in\mathbb{N}, \tag{2.98}$$

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

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. (2.41) is

$$\exp\left(\frac{i}{\hbar}S[\mathbf{r}(t)]\right), \tag{2.99}$$

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

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.[16] 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

$$K(\mathbf{r},t;\mathbf{r}',t') \sim (\text{Gaussian integral}) \times \exp\left(\frac{i}{\hbar}S[\mathbf{r}_{\text{cl}}(t)]\right). \tag{2.100}$$

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

2.6.0.1 van Vleck Propagator [*non-examinable*]

Unfortunately we don't have time to make Eq. (2.100) precise. The result of evaluating the Gaussian path integral is the **van Vleck propagator**. In three dimensions, this is

$$K_{\text{vV}}(\mathbf{r},t;\mathbf{r}',t') = \sum_{\substack{\text{classical}\\ \text{paths}}} \left(\frac{1}{2\pi i\hbar}\right)^{3/2} \det\left(-\frac{\partial^2 S}{\partial\mathbf{r}\partial\mathbf{r}'}\right)^{-1/2} \exp\left(\frac{i}{\hbar}S[\mathbf{r}_{\text{cl}}(t)]\right). \tag{2.101}$$

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. (2.53)). 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,[17] just as when we evaluated the Airy function for $x < 0$.

[16] Such approximations are usually called semiclassical. The WKB method is another example.

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

Chapter 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**);
- 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 generalisation 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.

Fig. 3.1: Schematic view of scattering in one dimension.

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 $\pm\infty$.

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 localised potential brings the wonderful simplification that outside of 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

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

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.

For a δ-function potential $V = g\delta(x)$, to find the scattering matrix $\mathrm{S}(k)$, we first know the wave function (3.1) has to be continuous at the origin,

$$a_+ + a_- = b_+ + b_-. \tag{3.2}$$

Integrating the Schrödinger equation across the origin gives us the second condition,

$$\begin{aligned} \int_{-\varepsilon}^{\varepsilon} \left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + g\delta(x)\Psi \right) \mathrm{d}x &= \int_{-\varepsilon}^{\varepsilon} E\Psi \, \mathrm{d}x \\ \int_{-\varepsilon}^{\varepsilon} \left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi \right) \mathrm{d}x + g\Psi(0) &= 0 \\ \frac{\hbar^2}{2m} \left(\left. \frac{\partial \Psi}{\partial x} \right|_{\varepsilon} - \left. \frac{\partial \Psi}{\partial x} \right|_{-\varepsilon} \right) + g\Psi(0) &= 0 \end{aligned} \tag{3.3}$$

where we have assumed that $\int_{-\varepsilon}^{\varepsilon} E\Psi \, \mathrm{d}x \to 0$ for $\varepsilon \to 0$. This gives

$$\frac{\hbar^2}{2m} ik(b_+ - b_- - (a_+ - a_-)) + g(a_+ + a_-) = 0 \tag{3.4}$$

Combined with equation (3.2) this gives

$$a_+ = \frac{g}{ik\hbar^2/m - g} a_- + \frac{ik\hbar^2/m}{ik\hbar^2/m - g} b_+ \tag{3.5}$$

$$b_- = \frac{g}{ik\hbar^2/m - g} b_+ + \frac{ik\hbar^2/m}{ik\hbar^2/m - g} a_-. \tag{3.6}$$

And so it is clear that the relationship between the coefficients in Eq. (3.1) may be written in terms of the **scattering matrix** $\mathrm{S}(k)$,

$$\begin{pmatrix} a_- \\ b_+ \end{pmatrix} = \overbrace{\begin{pmatrix} r_{\mathrm{LL}} & t_{\mathrm{RL}} \\ t_{\mathrm{LR}} & r_{\mathrm{RR}} \end{pmatrix}}^{\mathrm{S}(k)} \begin{pmatrix} a_+ \\ b_- \end{pmatrix}, \tag{3.7}$$

where the reflection and transmission coefficients have the form

$$r_{\mathrm{LL}} = r_{\mathrm{RR}} = \frac{g}{i\hbar^2 k/m - g}, \quad t_{\mathrm{RL}} = t_{\mathrm{LR}} = \frac{i\hbar^2 k/m}{i\hbar^2 k/m - g}. \tag{3.8}$$

The property responsible for $r_{\mathrm{LL}} = r_{\mathrm{RR}}$, $t_{\mathrm{RL}} = t_{\mathrm{LR}}$ is that the potential is symmetric.

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

$$\Psi_k(x) = \begin{cases} e^{ikx} + r_{\mathrm{LL}} e^{-ikx} & x \ll 0 \\ t_{\mathrm{LR}} e^{ikx} & x \gg 0, \end{cases} \tag{3.9}$$

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** $\mathrm{T}(k)$, which expresses the amplitudes on one side of the scatterer in terms of those on the other

$$\begin{pmatrix} b_+ \\ b_- \end{pmatrix} = \mathrm{T}(k) \begin{pmatrix} a_+ \\ a_- \end{pmatrix} = \begin{pmatrix} t_{\mathrm{LR}} - r_{\mathrm{RR}} r_{\mathrm{LL}}/t_{\mathrm{RL}} & r_{\mathrm{RR}}/t_{\mathrm{RL}} \\ -r_{\mathrm{LL}}/t_{\mathrm{RL}} & 1/t_{\mathrm{RL}} \end{pmatrix} \begin{pmatrix} a_+ \\ a_- \end{pmatrix} \tag{3.10}$$

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 $\mathrm{S}(k)$ exists for any potential $V(x)$, being defined by the relation Eq. (3.7) 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.[1] The goal of scattering theory is to find $\mathrm{S}(k)$ given $V(x)$, or at least to deduce its general properties. Let us discuss some of these properties now.

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

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

$$\partial_t P(x,t) + \partial_x J(x,t) = 0, \tag{3.11}$$

where the probability current is

$$J(x,t) = -\frac{i\hbar}{2m}[\Psi^* \partial_x \Psi - \Psi \partial_x \Psi^*]. \tag{3.12}$$

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

$$\partial_x J(x) = 0. \tag{3.13}$$

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

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

$$J(-L) = J(L). \tag{3.14}$$

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

$$\frac{\hbar k}{m}\left[|a_+|^2 - |a_-|^2\right] = \frac{\hbar k}{m}\left[|b_+|^2 - |b_-|^2\right] \tag{3.15}$$

(happily the cross terms vanish). Eq. (3.15) 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.

To prove that Eq. (3.15) implies that $\mathrm{S}(k)$ is a *unitary* matrix, we must prove that $\mathrm{S}(k)^\dagger = \mathrm{S}(k)^{-1}$, i.e. $\mathrm{S}^\dagger\mathrm{S} = \mathbb{I}$. We have from Eq. (3.7) that

$$\begin{pmatrix} a_- \\ b_+ \end{pmatrix} = \mathrm{S}(k)\begin{pmatrix} a_+ \\ b_- \end{pmatrix}, \tag{3.16}$$

now multiply both sides by their conjugate to give

$$\begin{aligned} |a_-|^2 + |b_+|^2 &= \begin{pmatrix} a_+ \\ b_- \end{pmatrix}^\dagger \mathrm{S}(k)^\dagger\mathrm{S}(k)\begin{pmatrix} a_+ \\ b_- \end{pmatrix} \\ &= |a_+|^2 + |b_-|^2, \end{aligned} \tag{3.17}$$

which is true only if $\mathrm{S}^\dagger\mathrm{S} = \mathbb{I}$. For checking that Eq. (3.7) is unitary, we simply calculate $\mathrm{S}(k)^\dagger$,

$$\begin{pmatrix} \frac{g}{-ik\hbar^2/m-g} & \frac{-ik\hbar^2/m}{-ik\hbar^2/m-g} \\ \frac{-ik\hbar^2/m}{-ik\hbar^2/m-g} & \frac{g}{-ik\hbar^2/m-g} \end{pmatrix} \tag{3.18}$$

and check that $\mathrm{S}^\dagger\mathrm{S} = \mathbb{I}$.

From the unitarity of the S-matrix we can obtain $\mathrm{T}_{12}^* = \mathrm{T}_{21}$ and $\mathrm{T}_{21}^* = \mathrm{T}_{12}$. The determinant of the T-matrix is 1 for a symmetric potential.

3.1.2 Channels and Phase Shifts

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

$$\mathrm{USU}^\dagger = \begin{pmatrix} e^{2i\delta_1} & 0 \\ 0 & e^{2i\delta_2} \end{pmatrix}, \tag{3.19}$$

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

$$\begin{aligned} \begin{pmatrix} a_+ \\ b_- \end{pmatrix} &= \mathrm{U}^\dagger\begin{pmatrix} c_1^{\mathrm{in}} \\ c_2^{\mathrm{in}} \end{pmatrix} \\ \begin{pmatrix} a_- \\ b_+ \end{pmatrix} &= \mathrm{U}^\dagger\begin{pmatrix} c_1^{\mathrm{out}} \\ c_2^{\mathrm{out}} \end{pmatrix} \end{aligned} \tag{3.20}$$

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

$$c_{1,2}^{\text{out}} = e^{2i\delta_{1,2}} c_{1,2}^{\text{in}}. \tag{3.21}$$

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.

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. (3.20) as

$$\begin{aligned} \begin{pmatrix} a_+ \\ b_- \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} c_{\text{even}}^{\text{in}} \\ c_{\text{odd}}^{\text{in}} \end{pmatrix} \\ \begin{pmatrix} a_- \\ b_+ \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} c_{\text{even}}^{\text{out}} \\ c_{\text{odd}}^{\text{out}} \end{pmatrix} \end{aligned} \tag{3.22}$$

In this basis Eq. (3.1) takes the form

$$\Psi_k(|x| \gg 0) = c_{\text{even}} \cos(k|x| + \delta_{\text{even}}) + \operatorname{sgn}(x) c_{\text{odd}} \cos(k|x| + \delta_{\text{odd}}), \tag{3.23}$$

where for convenience we have defined $c_{\text{even,odd}} = e^{i\delta_{\text{even,odd}}} c_{\text{even,odd}}^{\text{in}}/\sqrt{2}$.

The eigenvalues of the S-matrix as given in Eq. (3.7) are

$$\lambda_{1,2} = -1, \; \frac{ik\hbar^2/m + g}{ik\hbar^2/m - g}. \tag{3.24}$$

This gives δ_{even} and $\tan(\delta_{\text{odd}}) = (2gk\hbar/m)(g^2 + (k\hbar^2/m)^2)$. One of the two phase shifts is thus independent of the strength of the interaction.

3.1.3 Integral Equation for Scattering Amplitude

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

$$-\frac{\hbar^2}{2m} \partial_x^2 \Psi(x) + v(x)\Psi(x) = E_k \Psi(x), \tag{3.25}$$

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. (3.9) (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

$$\Psi_k(x) = e^{ikx} + \Psi_k^{\text{scatt}}(x). \tag{3.26}$$

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. (3.9), $\Psi_k^{\text{scatt}}(x)$ has the explicit form

$$\Psi_k^{\text{scatt}}(x) = \begin{cases} r_{\text{LL}} e^{-ikx} & x \ll 0 \\ (r_{\text{LR}} - 1) e^{ikx} & x \gg 0. \end{cases} \tag{3.27}$$

With the definition Eq. (3.26), we can rewrite Eq. (3.25) as

$$\left[E_k + \frac{\hbar^2}{2m}\partial_x^2\right]\Psi_k^{\text{scatt}}(x) = V(x)\Psi_k(x). \tag{3.28}$$

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

$$\left[E_k + \frac{\hbar^2}{2m}\partial_x^2\right]G_k(x, x') = \delta(x - x') \tag{3.29}$$

(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. (3.28) as

$$\Psi_k^{\text{scatt}}(x) = \int \mathrm{d}x'\, G_k(x, x')V(x')\Psi_k(x'). \tag{3.30}$$

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

$$\boxed{\Psi_k(x) = e^{ikx} + \int \mathrm{d}x'\, G_k(x, x')V(x')\Psi_k(x').} \tag{3.31}$$

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. (3.31) is by iteration

$$\begin{aligned}\Psi_k(x) = e^{ikx} &+ \int \mathrm{d}x'\, G_k(x, x')V(x')e^{ikx'} \\ &+ \int \mathrm{d}x'\,\mathrm{d}x''\, G_k(x, x')V(x')G_k(x', x'')V(x'')e^{ikx''} + \cdots,\end{aligned} \tag{3.32}$$

which generates the **Born series**.

Now let's discuss the Green's function. From Eq. (3.29) we can see that this satisfies the free particle Schrödinger equation with energy E_k when $x \neq x'$. Therefore it has the form

$$G_k(x, x') = \begin{cases} g_+^< e^{ikx} + g_-^< e^{-ikx} & x < x' \\ g_+^> e^{ikx} + g_-^> e^{-ikx} & x > x'. \end{cases} \tag{3.33}$$

To fix the form uniquely we specify:

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

- At $x = x'$ the derivative jumps

$$\partial_x G_k(x,x')\Big|_{x=x'-\varepsilon}^{x=x'+\varepsilon} = \frac{2m}{\hbar^2}. \tag{3.34}$$

These two conditions follow from the defining Eq. (3.29).

- In order to generate a solution of the form Eq. (3.9), we must have

$$g_+^< = g_-^> = 0, \tag{3.35}$$

which corresponds to only "outgoing" waves being generated by the scattering potential.[2]

Imposing these conditions gives

$$G_k^+(x,x') = -i\frac{m}{\hbar^2 k}e^{ik|x-x'|}. \tag{3.36}$$

We have added a + to indicate this is a *particular* Green's function obeying certain boundary conditions[3] – 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.

Let us now consider the example of solving the Lippman-Schwinger equation for the δ-function potential to show that Eq. (3.9) is reproduced.

The Lippman-Schwinger equation for the delta-function potential is

$$\Psi_k(x) = e^{ikx} + \int \mathrm{d}x'\, G_k(x,x') g\delta(x')\Psi(x'), \tag{3.38}$$

where we insert G from equation (2.34) in the notes and perform the integration over x':

$$\Psi_k(x) = e^{ikx} - i\frac{gm}{\hbar^2 k}e^{ik|x|}\Psi(0). \tag{3.39}$$

Thus for $x = 0$, we can solve this to obtain $\Psi(0)$:

$$\Psi(0) = \frac{i\hbar^2 k/m}{i\hbar^2 k/m - g}. \tag{3.40}$$

We can then insert this back into equation (3.39):

$$\Psi(0) = \begin{cases} e^{-ikx} + \dfrac{g}{ik\hbar^2/m - g}e^{ikx} & x \ll 0 \\ \dfrac{ik\hbar^2/m}{ik\hbar^2/m - g}e^{ikx} & x \gg 0, \end{cases} \tag{3.41}$$

which gives the required result cf. equation (3.9).

[2] 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.

[3] 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:

$$\lim_{|x-x'|\to\infty} \left[\partial_{|x-x'|} - ik\right] G(x,x') = 0. \tag{3.37}$$

However, this **radiation condition** has the same content as Eq. (3.35).

3.1.4 Quantum Wires [*non-examinable*]

Fig. 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.

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

$$\mathsf{S} = \begin{pmatrix} r_{\mathrm{LL}} & t_{\mathrm{RL}} \\ t_{\mathrm{LR}} & r_{\mathrm{RR}} \end{pmatrix}. \tag{3.42}$$

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*

$$\boxed{G = G_0 \sum_n T_n,} \tag{3.43}$$

where $G_0 = 2e^2/\hbar \sim 7.75 \times 10^{-5}\Omega^{-1}$ is the **quantum of conductance**.

3.2 The Scattering Problem in Three Dimension

We are now ready to begin our assault on three dimensions. We will see that all[4] of the concepts we introduced in studying the one dimensional problem have natural counterparts in 3D.

3.2.1 The Scattering Amplitude and Cross Section

We first seek an analog of Eq. (3.9), in which the wavefunction is written in terms of an incoming plane wave and transmitted and reflected waves. Like Eq. (3.9), 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.

[4]With the exception of the transfer matrix.

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

$$\boxed{\Psi_k(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{ikz} + \frac{f(\theta,\phi)}{r}e^{ikr},} \tag{3.44}$$

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 e^{ikr} and not e^{-ikr}.

The main difference from Eq. (3.9) is that Eq. (3.44) 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 $|\mathbf{r}| \to \infty$.

Nevertheless, inserting (3.44) into the free Schrödinger equation, and using

$$\nabla^2 \frac{e^{ikr}}{r} = -k^2 \frac{e^{ikr}}{r} \tag{3.45}$$

$$\nabla^2 e^{ikz} = -k^2 e^{ikz}, \tag{3.46}$$

we obtain

$$-k^2\Psi_k(r) + \frac{e^{ikr}}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f(\theta,\phi)}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 f(\theta,\phi)}{\partial\phi^2}\right) = -k^2\Psi_k(r) \tag{3.47}$$

and so for equation (3.44) to be a solution, we would need

$$\lim_{r\to\infty}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f(\theta,\phi)}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 f(\theta,\phi)}{\partial\phi^2}\right\} \to 0. \tag{3.48}$$

Since this term decays as $1/r^3$, equation (3.44) works asymptotically in the large r limit.

You might argue that Eq. (3.26) is a closer analog of Eq. (3.44) than Eq. (3.9), because of it represents a division into incoming and scattered waves, and we would not disagree. But Eq. (3.26) was defined everywhere, rather than just outside the interaction region. We'll introduce the corresponding expression in the 3D case shortly.

Eq. (3.44) 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

$$\mathbf{J}(\mathbf{r}) = -\frac{i\hbar}{2m}[\Psi^*\boldsymbol{\nabla}\Psi - \Psi\boldsymbol{\nabla}\Psi^*]. \tag{3.49}$$

Calculating the current using Eq. (3.44) gives

$$\mathbf{J}(\mathbf{r}) \xrightarrow[r\to\infty]{} \frac{\hbar k}{m}\left[\hat{\mathbf{z}} + \frac{|f(\theta,\phi)|^2}{r^2}\hat{\mathbf{r}}\right] + (\text{cross terms with } \exp(\pm ik[r-z]) \text{ factors}). \tag{3.50}$$

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).

But what about the cross terms? The presence of the rapidly oscillating factors $\exp(\pm ik[r-z]) = \exp(\pm ikr[1-\cos\theta])$ 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 $1/(kr)$, 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. (3.44) is not normalised. In an infinite system one can normalise states according to the flux they carry. This gives

$$\mathbf{J}(\mathbf{r}) \xrightarrow[r\to\infty]{} \mathbf{J}\left[\hat{\mathbf{z}} + \frac{|f(\theta,\phi)|^2}{r^2}\hat{\mathbf{r}}\right]. \tag{3.51}$$

The result is a simple picture of the flow of the probability current due to scattering.[5] The probability per unit time for a *scattered* particle to pass through a solid angle element $\mathrm{d}\Omega$ at coordinates (θ,ϕ) is

$$\text{probability / time} = J|f(\theta,\phi)|^2\,\mathrm{d}\Omega\,. \tag{3.52}$$

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**

$$\boxed{\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\mathrm{d}\Omega \equiv \frac{\text{probability / time}}{\text{flux}} = |f(\theta,\phi)|^2\,\mathrm{d}\Omega\,.} \tag{3.53}$$

$\mathrm{d}\sigma/\mathrm{d}\Omega$ is a function of θ and ϕ, though those arguments are normally omitted because $\mathrm{d}\sigma/\mathrm{d}\Omega$ looks like a mess. The notation $\mathrm{d}\sigma/\mathrm{d}\Omega$ 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 $\mathrm{d}\Omega$. Integrating over all solid angles gives the **total cross section**

$$\sigma_{\text{tot}} = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\,\mathrm{d}\Omega = \int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\sin\theta\,\mathrm{d}\theta\,\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \tag{3.54}$$

3.2.2 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. (3.51) over a sphere centred on the origin. For a stationary state, we should expect to get zero

[5] 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. (3.52) will have to remain heuristic.

net flux (c.f. Eq. (3.14)). The plane wave contribution, represented by the first term, gives zero, as anything passing in through one hemisphere leaves through the other. So Eq. (3.51) implies

$$\int |f(\theta,\phi)|^2 \, d\Omega = \sigma_{\text{tot}} = 0. \tag{3.55}$$

Which doesn't sound good. The problem is that we have been too cavalier with the cross terms in Eq. (3.50). 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**.

Fig. 3.3: Finding the intensity of the wavefunction on a screen.

In Fig. 3.3 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. (3.44), we find the square modulus of the wavefunction to be

$$|\Psi_k(\mathbf{r})|^2 = 1 + \frac{2\,\mathrm{Re}\left\{f(\theta,\phi)e^{ik(r-z)}\right\}}{r} + \frac{|f(\theta,\phi)^2|}{r^2}. \tag{3.56}$$

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

$$r = \sqrt{x^2+y^2+z^2} \sim z + \frac{x^2+y^2}{2z}, \quad z \gg x, y. \tag{3.57}$$

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

$$|\Psi_k(\mathbf{r})|^2 \sim 1 + \frac{2\,\mathrm{Re}\left\{f(\theta=0)e^{ik(x^2+y^2)/2z}\right\}}{z}. \tag{3.58}$$

Integrating over the screen gives

$$\begin{aligned}\int_{\text{Screen}} dA\, |\Psi_k(\mathbf{r})|^2 &= \int_0^R dr\, 2\pi r \left[1 + \frac{2\,\mathrm{Re}\left\{f(\theta=0)e^{ik(x^2+y^2)/2z}\right\}}{z}\right] \\ &= \pi R^2 - \frac{4\pi}{k}\,\mathrm{Im}\{f(\theta=0)\}. \end{aligned} \tag{3.59}$$

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

$$\boxed{\sigma_{\text{tot}} = \frac{4\pi}{k}\,\mathrm{Im}\{f(\theta=0)\},} \tag{3.60}$$

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.

Thus our original expression Eq. (3.51) 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.

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.

3.2.3 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. (3.31)

$$\boxed{\Psi_k(\mathbf{r}) = e^{ikz} + \int \mathrm{d}\mathbf{r}'\, G_k^+(\mathbf{r}, \mathbf{r}') V(\mathbf{r}') \Psi_k(\mathbf{r}').} \tag{3.61}$$

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

$$\left[E_k + \frac{\hbar^2}{2m}\nabla^2\right] G_k^+(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'), \tag{3.62}$$

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

$$\boxed{G_k^+(\mathbf{r}, \mathbf{r}') = -\frac{m}{2\pi\hbar^2} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}.} \tag{3.63}$$

As in the 1D case, you can verify directly that Eq. (3.63) 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

$$G_k^+ \to -\frac{m}{2\pi\hbar^2} \frac{1}{|\mathbf{r} - \mathbf{r}'|}. \tag{3.64}$$

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

$$\nabla^2 G_L(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \tag{3.65}$$

is just

$$G_L(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|}. \tag{3.66}$$

The E_k term in Eq. (3.62) is not involved in producing the δ-function, and therefore we have verified that Eq. (3.63) 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. (3.61) has the asymptotic behaviour given by Eq. (3.44). To do this, we'll need to investigate the behaviour of the Green's function at large distances. First note that, if $|\mathbf{r}| \gg |\mathbf{r}'|$

$$|\mathbf{r} - \mathbf{r}'| \sim r - \hat{\mathbf{r}} \cdot \mathbf{r}'. \tag{3.67}$$

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

$$G^+(\mathbf{r}, \mathbf{r}') \to -\frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r} e^{-i\mathbf{k}_\mathrm{f} \cdot \mathbf{r}'}, \tag{3.68}$$

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

$$\Psi_k(\mathbf{r}) \xrightarrow[r \to \infty]{} e^{ikz} - \frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int \mathrm{d}\mathbf{r}'\, e^{-i\mathbf{k}_\mathrm{f} \cdot \mathbf{r}'} V(\mathbf{r}') \Psi_k(\mathbf{r}'). \tag{3.69}$$

Comparison with Eq. (3.44) allows us to identify

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int \mathrm{d}\mathbf{r}' \exp(-i\mathbf{k}_\mathrm{f} \cdot \mathbf{r}') V(\mathbf{r}') \Psi_k(\mathbf{r}'). \tag{3.70}$$

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.

3.2.4 The Born Approximation

As we already discussed in Subsection 3.1.3, one way to solve the Lippmann–Schwinger equation is by iteration, generating the Born series (c.f. Eq. (3.32)). The lowest order approximation amounts to replacing $\Psi_k(\mathbf{r}')$ in Eq. (3.70) with the unscattered plane wave, yielding the (**first**) **Born approximation** to the scattering amplitude

$$\boxed{f_\mathrm{Born}(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int \mathrm{d}\mathbf{r}' \exp(-i\mathbf{q} \cdot \mathbf{r}') V(\mathbf{r}'),} \tag{3.71}$$

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 q. Eq. (3.71) gives the differential cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}_\mathrm{Born} = \left| \frac{m}{2\pi\hbar^2} \int \mathrm{d}\mathbf{r}' \exp(-i\mathbf{q} \cdot \mathbf{r}') V(\mathbf{r}') \right|^2. \tag{3.72}$$

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.

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[6]

$$V_c \ll \frac{\hbar^2}{mr_c^2}, \tag{3.73}$$

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

$$V_c \ll kr_c\frac{\hbar^2}{mr_c^2}, \tag{3.74}$$

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 $\exp(i\mathbf{k}_\mathrm{i}\cdot\mathbf{r})$ and $\exp(i\mathbf{k}_\mathrm{f}\cdot\mathbf{r})$ as

$$\Gamma_{\mathrm{i}\to\mathrm{f}} = \frac{2\pi}{\hbar}|\langle\mathbf{k}_\mathrm{f}|V|\mathbf{k}_\mathrm{f}\rangle|^2\delta(E_{\mathbf{k}_\mathrm{i}} - E_{\mathbf{k}_\mathrm{f}}). \tag{3.75}$$

It is instructive to compare the two derivations.

As an illustrative example, let us find the scattering amplitude within the lowest Born approximation for the spherical potential

$$V(\mathbf{r}) = \begin{cases} -V_0 & |\mathbf{r}| < a_\circ \\ 0 & |\mathbf{r}| > a_\circ \end{cases}. \tag{3.76}$$

The scattering amplitude in the Born approximation is given by Eq. (3.71). For spherically symmetric potentials $V(\mathbf{r}) = V(r)$,

$$\begin{aligned} f(\theta) &= -\frac{m}{2\pi\hbar^2}\int_0^\infty \mathrm{d}r'\int_0^{2\pi}\mathrm{d}\phi'\int_{-1}^{1}\mathrm{d}(\cos\theta')\,e^{iqr'\cos\theta'}V(r')r'^2 \\ &= -\frac{m}{\hbar^2}\int_0^\infty \mathrm{d}r\,r^2V(r)\underbrace{\int_{-1}^{1}\mathrm{d}x\,e^{iqrx}}_{\frac{2\sin qr}{qr}} \\ &= -\frac{2m}{q\hbar^2}\int_0^\infty \mathrm{d}r\,rV(r)\sin qr. \end{aligned} \tag{3.77}$$

Substituting the potential for a spherically symmetric square well

$$V(r) = \begin{cases} -V_0 & 0 \le r \le a \\ 0 & \text{otherwise} \end{cases}, \tag{3.78}$$

we find that

$$f(\theta) = \frac{2mV_0}{q\hbar^2}\int_0^a \mathrm{d}r\,r\sin qr, \tag{3.79}$$

from which we obtain the result

$$\boxed{f(\theta) = \frac{2mV_0}{q^3\hbar^2}(\sin qa - qa\cos qa).} \tag{3.80}$$

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

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

$$\Psi_k(|x| \gg 0) = c_{\text{even}} \cos(k|x| + \delta_{\text{even}}) + \text{sgn}(x) c_{\text{odd}} \cos(k|x| + \delta_{\text{odd}}). \tag{3.81}$$

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"[7] 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

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + V(r)\Psi(\mathbf{r}) = E_k\Psi(\mathbf{r}). \tag{3.82}$$

We are going to seek a solution of the form

$$\Psi(\mathbf{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{lm} Y_{lm}(\theta, \phi) R_l(r). \tag{3.83}$$

The terms in the expansion are the **partial waves** that give this technique its name. Substitution in Eq. (3.82) yields an equation for $R_l(r)$[8]

$$\frac{\mathrm{d}^2 R_l}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}R_l}{\mathrm{d}r} + \left[k^2 - \frac{l(l+1)}{r^2}\right] R_l = \frac{2mV(r)}{\hbar^2} R_l. \tag{3.86}$$

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. (3.86) with zero on the right hand side. Writing $R_l(r) = r_l(kr)$ gives the equation

$$\rho^2 \frac{\mathrm{d}^2 r_l}{\mathrm{d}\rho^2} + 2\rho\frac{\mathrm{d}r_l}{\mathrm{d}\rho} + \left[\rho^2 - l(l+1)\right] r_l = 0. \tag{3.87}$$

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

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

[8] The Laplacian can be written

$$\nabla^2 = \frac{1}{r^2}\partial_r\left(r^2\partial_r\right) - \frac{\mathbf{L}^2}{\hbar^2 r^2} \tag{3.84}$$

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

$$(\mathbf{r} \times \mathbf{p})^2 = x_j p_k x_j p_k - x_j p_k x_k p_j \tag{3.85}$$

and then using the canonical commutation relations.

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

l) respectively.[9] 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

$$\frac{\mathrm{d}^2 r_0}{\mathrm{d}\rho^2} + \frac{2}{\rho}\frac{\mathrm{d}r_0}{\mathrm{d}\rho} + r_0 = 0 \tag{3.90}$$

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

$$u'' + u = 0. \tag{3.91}$$

Then we have

$$j_0(\rho) = \frac{\sin\rho}{\rho}, \quad n_0(\rho) = -\frac{\cos\rho}{\rho}. \tag{3.92}$$

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

Fig. 3.4: The first two spherical Bessel and Neumann functions.

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

$$\begin{aligned} h_l^{(1)}(\rho) &= j_l(\rho) + i n_l(\rho) \\ h_l^{(2)}(\rho) &= \left[h_l^{(1)}(\rho)\right]^* \end{aligned} \tag{3.93}$$

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

$$h_0^{(1)}(\rho) = \frac{e^{i\rho}}{i\rho}. \tag{3.94}$$

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

$$\boxed{\begin{aligned} j_l &= (-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\sin\rho}{\rho} \\ n_l(\rho) &= -(-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\cos\rho}{\rho}. \end{aligned}} \tag{3.95}$$

From the Rayleigh formula we can deduce the series expansion of j_l via the series expansion of

$$\frac{\sin\rho}{\rho} = \sum_{n=0}^{\infty} \frac{(-1)^n \rho^{2n}}{(2n+1)!} \tag{3.96}$$

[9]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**

$$\rho^2 J_\alpha'' + \rho J_\alpha' + \left(\rho^2 - \alpha^2\right) J_\alpha = 0. \tag{3.88}$$

The two are in fact related

$$j_l(\rho) = \sqrt{\frac{\pi}{2\rho}} J_{l+1/2}(\rho) \tag{3.89}$$

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. (3.95) makes clear.

and by noticing that acting with the operator $\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}$ multiplies equation (3.96) with the exponent of ρ and decreases this exponent by 2, such that

$$\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)\frac{\sin\rho}{\rho} = \sum_{n=0}^{\infty}\frac{(-1)^n 2n\rho^{2n-2}}{(2n+1)!} \tag{3.97}$$

$$\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l\frac{\sin\rho}{\rho} = \sum_{n=0}^{\infty}\frac{(2n)!!}{(2n-2l)!!}\frac{(-1)^n\rho^{2n-2l}}{(2n+1)!}. \tag{3.98}$$

This leads to

$$j_l(\rho) = \sum_{n=0}^{\infty}\frac{(-1)^{(n+l)}\rho^{2n-l}}{(2n-2l)!!(2n+1)!!}. \tag{3.99}$$

We could now put this directly into the differential equation for the spherical Bessel function

$$\rho^2\frac{\mathrm{d}^2 j_l}{\mathrm{d}\rho^2} + 2r\frac{\mathrm{d}j_l}{\mathrm{d}\rho} + \left[\rho^2 - l(l+1)\right]j_l = 0, \tag{3.100}$$

and obtain that this equation does satisfy the differential equation.

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

In order to show the asymptotic behaviour at small arguments we try to find the leading term in the expansion (3.99). For j_l, this term corresponds to $n = l$ (terms with $n < l$ will have disappeared when differentiating l times as visible from Rayleigh's formulas), such that

$$j_l(\rho) \to \frac{(-1)^{2l}\rho^l}{(2l+1)!!} = \frac{\rho^l}{(2l+1)!!}. \tag{3.101}$$

For the Neumann function, the previous procedure can be done analagously using

$$\frac{\cos\rho}{\rho} = \sum_{n=0}^{\infty}\frac{(-1)^n\rho^{2n-1}}{(2n)!} \tag{3.102}$$

It is easiest to notice here that for small ρ, the $n = 0$ term will give the leading contribution, and just keep this term.

$$\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l\frac{1}{\rho} = (-1)^l(2l+1)!!\rho^{-1-2l} \tag{3.103}$$

such that

$$n_l(\rho) \to -\frac{(2l+1)!!}{\rho^{l+1}} \tag{3.104}$$

for small arguments.

And thus the asymptotic behaviour at small arguments is

$$\boxed{\begin{aligned} j_l(\rho) &\to \frac{\rho^l}{(2l+1)!!} \\ n_l(\rho) &\to -\frac{(2l-1)!!}{\rho^{l+1}}. \end{aligned}} \tag{3.105}$$

We notice that for large arguments the derivative with respect to ρ in the Rayleigh formula

$$\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\frac{f(\rho)}{\rho} \to \frac{1}{\rho}\frac{f'(\rho)}{\rho}, \tag{3.106}$$

since the derivative of the $1/\rho$ terms can be neglected. Thus, we obtain

$$\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{f(\rho)}{\rho} \to \frac{1}{\rho^{l+1}}\frac{\mathrm{d}^l f(\rho)}{\mathrm{d}\rho^l} \tag{3.107}$$

and

$$(-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{f(\rho)}{\rho} \to \frac{(-1)^l}{\rho}\frac{\mathrm{d}^l f(\rho)}{\mathrm{d}\rho^l}. \tag{3.108}$$

If now for example $f(\rho) = \sin\rho$, $-f'(\rho) = -\cos\rho = \sin(\rho - \pi/2)$ and $f''(\rho) = -\sin\rho = \sin(\rho - 2\pi/2)$ etc. Thus, we realise that we can write

$$j_l(\rho) \to \frac{\sin\left(\rho - \frac{l\pi}{2}\right)}{\rho} \tag{3.109}$$

and analagously for the other functions to see that the asymptotic behaviour at large arguments is

$$\boxed{\begin{aligned} j_l(\rho) &\to \frac{1}{\rho}\sin\left(\rho - \frac{l\pi}{2}\right) \\ n_l(\rho) &\to -\frac{1}{\rho}\cos\left(\rho - \frac{l\pi}{2}\right) && (3.110) \\ h_l^{(1)}(\rho) &\to -\frac{i}{\rho}\exp\left(i\left[\rho - \frac{l\pi}{2}\right]\right). && (3.111) \end{aligned}}$$

Eq. (3.110) 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 $h_l^{(2)}(\rho)$) that form the partial wave outside of the interaction region, we are going to appeal to the intuition provided by Eq. (3.23). 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[10]

$$h_l^{(1)}(|rho)e^{i\delta_l} + h_l^{(2)}(|rho)e^{-i\delta_l} \xrightarrow[r\to\infty]{} \frac{2}{\rho}\sin\left(\rho - \frac{l\pi}{2} + \delta_l\right). \tag{3.112}$$

This defines the phase shifts in the 3D case.

[10] 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.

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

$$\Psi(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\theta, \phi) \left[c_{lm}^{\text{out}} h_l^{(1)}(kr) + c_{lm}^{\text{in}} h_l^{(2)}(kr) \right], \tag{3.113}$$

Use the asymptotic form Eq. (3.110) and the orthogonality relation for the spherical harmonics,

$$\int \mathrm{d}\Omega \, Y_{lm}^*(\theta, \phi) Y_{l'm'}(\theta, \phi) = \delta_{ll'} \delta_{mm'}. \tag{3.114}$$

The flux is defined as

$$\text{Flux} = \int \mathrm{d}\mathbf{r} \, J(r), \tag{3.115}$$

where we know

$$J(r) = -\frac{i\hbar}{2m} \left(\Psi^*(r) \boldsymbol{\nabla} \Psi(r) - \Psi(r) (\boldsymbol{\nabla} \Psi(r))^* \right) \tag{3.116}$$

Defining

$$R_{lm}(r) = c_{lm}^{\text{out}} h_l^{(1)}(kr) + c_{lm}^{\text{in}} h_l^{(2)}(kr), \tag{3.117}$$

we have

$$\text{Flux} = -\frac{i\hbar}{2m} \int r^2 \, \mathrm{d}r \, \mathrm{d}\Omega \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{l'=0}^{\infty} \sum_{m=-l'}^{l'} (Y_{lm}^*(\theta, \phi) Y_{l'm'}(\theta, \phi)) (R_{lm}^* \boldsymbol{\nabla} R_{l'm'} - R_{lm} (\boldsymbol{\nabla} R_{l'm'})^*) \tag{3.118}$$

which after using the orthogonality relation for the spherical harmonics gives

$$\text{Flux} = -\frac{i\hbar}{2m} \int r^2 \, \mathrm{d}r \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (R_{lm}^* \boldsymbol{\nabla} R_{lm} - R_{lm} (\boldsymbol{\nabla} R_{lm})^*) \tag{3.119}$$

Since, there is no angular dependence, we only need the radial derivatives of the Hankel functions,

$$h_l^{(1)\prime}(r) = \left(\frac{i}{kr^2} + \frac{1}{r} \right) e^{i(kr - l\pi/2)} h_l^{(2)\prime}(r) = \left(h_l^{(1)\prime} \right)^* (r) \tag{3.120}$$

We notice that because $h_l^{(2)} = \left(h_l^{(1)\prime} \right)^*$ and the same for the derivative, the cross terms cancel and we get

$$\text{Flux} = -\frac{i\hbar}{2m} \int r^2 \, \mathrm{d}r \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{2i}{kr^2} \left(\left| c_{lm}^{\text{out}} \right|^2 - \left| c_{lm}^{\text{in}} \right|^2 \right) \tag{3.121}$$

which simplifies to

$$\text{Flux} = \frac{\hbar}{km} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(\left| c_{lm}^{\text{out}} \right|^2 - \left| c_{lm}^{\text{in}} \right|^2 \right). \tag{3.122}$$

3.3.1 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

$$\Psi_k(\mathbf{r}) \xrightarrow[r \to \infty]{} e^{ikz} + \frac{f(\theta, \phi)}{e}^{ikr}. \tag{3.123}$$

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

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} a_l j_l(kr) P_l(\cos\theta). \tag{3.124}$$

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

$$Y_{l0}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \tag{3.125}$$

by virtue of azimuthal symmetry. The functions $P_l(\cos\theta)$ are l^{th} order polynomials called the **Legendre polynomials**.[11] Now it is straightforward to fix 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. (3.105)). 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,

$$a_l = i^l(2l+1) \tag{3.127}$$

3.3.2 Adding the Phase Shifts

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

$$e^{ikr\cos\theta} = \frac{1}{2}\sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta)\Big[h_l^{(1)}(kr) + h_l^{(2)}(kr)\Big]. \tag{3.128}$$

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 modified, and hence

$$\Psi_k(\mathbf{r}) = \frac{1}{2}\sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta)\Big[e^{2i\delta_l}h_l^{(1)}(kr) + h_l^{(2)}(kr)\Big]. \tag{3.129}$$

The scattered wave can then be found by subtracting off the plane wave contribution. In the asymptotic region where Eq. (3.44) is valid, the yields the desired relation between $f(\theta, \phi)$ and the phase shifts

$$\boxed{f(\theta, \phi) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\Big[e^{2i\delta_l} - 1\Big]P_l(\cos\theta).} \tag{3.130}$$

[11] The Legendre polynomials can be generated from **Rodrigues' formula**

$$P_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(x^2-1\right)^n, \tag{3.126}$$

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: $P_n(1) = 1$, resulting from the normalising factor $1/2^n n!$.

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

$$\int_{-1}^{1} \mathrm{d}x\, P_l(x) P_{l'}(x) = \frac{2}{2l+1}\delta_{ll'}, \tag{3.131}$$

to give

$$\boxed{\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\theta_l.} \tag{3.132}$$

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

$$\sigma_l \leq \frac{4\pi}{k^2}(2l+1), \tag{3.133}$$

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

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

$$\mathrm{Im}\{f(\theta = 0)\} = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l = \frac{k\sigma_{\text{tot}}}{4\pi}, \tag{3.134}$$

(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.

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

$$V(\mathbf{r}) = \begin{cases} \infty & r < a_\circ \\ 0 & r > a_\circ \end{cases}, \tag{3.135}$$

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

The phase shift is related to the coefficients of the incoming and the scattered wave. To see this, we look at equation (3.129)which introduces the phase shift,

$$\Psi_k(\mathbf{r}) = \frac{1}{2}\sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta)\Big[e^{2i\delta_l}h_l^{(1)}(kr) + h_l^{(2)}(kr)\Big]. \tag{3.136}$$

and express the Hankel functions in terms of j_l and n_l again,

$$\begin{aligned}\Psi_k(r) &= \sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta)\frac{1}{2}\Big[j_l(kr)\Big(e^{2i\delta_l}+1\Big) + i n_l(kr)\Big(e^{2i\delta_l}-1\Big)\Big] \\ &= \sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta) \times e^{i\delta_l}[j_l(kr)\cos\delta_l - n_l(kr)\sin\delta_l].\end{aligned} \tag{3.137}$$

We note that the radial part for a particular l is $R_l'(kr) = e^{i\delta_l}\cos\delta_l[(-\cot\delta_l)j_l(kr) + n_l(kr)]$.

Now we notice that for the hard-sphere potential, the Schrödinger equation is solvable and the radial part becomes for large r

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{l(l+1)}{r^2}\right)R_l(r)=ER_l(r)\\
\Longrightarrow\quad & r^2\frac{\mathrm{d}^2R_0(r)}{\mathrm{d}r^2}+2r\frac{\mathrm{d}R_0(r)}{\mathrm{d}r}-l(l+1)R_l(r)+\frac{2mE}{\hbar^2}R_0(r)=0\\
\Longrightarrow\quad & R_l(r)=Aj_l(kr)+Bn_l(kr)\\
\Longrightarrow\quad & R_l(r)=B\left(\frac{A}{B}j_l(kr)+n_l(kr)\right).
\end{aligned}
\tag{3.138}
$$

Comparing this to R', we can notice that the fraction of these two coefficients can be related to the phase shift,

$$\tan\delta_l=-\frac{B}{A}. \tag{3.139}$$

Now we just need to find B/A for the hard-sphere potential. Since we have

$$\Psi(r=a_\circ)=0, \tag{3.140}$$

this gives

$$Aj_l(ka_\circ)+Bn_l(ka_\circ)=0, \tag{3.141}$$

and thus

$$\tan\delta_l=\frac{j_l(ka_\circ)}{n_l(ka_\circ)}. \tag{3.142}$$

For $l=0$, we have

$$\tan\delta_l=-\frac{\sin ka_\circ}{\cos ka_\circ}=-\tan ka_\circ=\tan(\pi-ka_\circ) \tag{3.143}$$

so $\delta_0(k)=\pi-ka_\circ$. For small k, we just insert the asymptotic behaviour of the Bessel and Neumann function for small arguments and find

$$\delta_l(k)\to\frac{(ka)^{2l+1}}{(2l+1)[(2l-1)!!]^2} \tag{3.144}$$

In the small k limit,

$$\sigma_{\text{tot}}\to\text{constants}\times\frac{1}{k^2}\sum_{l=0}^{\infty}k^{4l-2} \tag{3.145}$$

and since for small k the $l=0$ term dominates

$$\sigma_{\text{tot}}\to\text{constant}. \tag{3.146}$$

Now let us consider the case of the spherical potential,

$$V(\mathbf{r})=\begin{cases}V_0 & |\mathbf{r}|<a_\circ\\ 0 & |\mathbf{r}|>a_\circ\end{cases}. \tag{3.147}$$

For $l = 0$, the radial solutions satisfy

$$R_0(r) = \begin{cases} Cj_0(k'r) & r \leq a \\ Aj_0(kr) + Bn_0(kr) & r > a \end{cases}, \tag{3.148}$$

where $k' = \sqrt{2m(E - V_0)}/\hbar$. Continuity of $R_0(r)$ and $R_0'(r)$ at $r = a$ implies that

$$Cj_0(k'a) = Aj_0(ka) + Bn_0(ka), \tag{3.149}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}r}[Cj_0(k'r)]\bigg|_{r=a} = \frac{\mathrm{d}}{\mathrm{d}r}[Aj_0(kr) + Bn_0(kr)]\bigg|_{r=a}. \tag{3.150}$$

Using the definitions of spherical Bessel functions $j_l(\rho)$ and von Neumann functions $n_l(\rho)$, Eq. (3.149) becomes

$$\begin{aligned} \frac{C}{A}\frac{\sin k'a}{k'a} &= \frac{\sin ka}{ka} + \tan\delta_0 \frac{\cos ka}{ka} \\ \frac{C}{A}\sin k'a &= \frac{k'}{k}[\sin ka + \tan\delta_0 \cos ka] \\ &= \frac{k'}{k}\frac{\sin(ka + \delta_0)}{\cos\delta_0}, \end{aligned} \tag{3.151}$$

where we have defined

$$\tan\delta_0 = -\frac{B}{A}. \tag{3.152}$$

Performing the differentiation in Eq. (3.150) we find that

$$\begin{aligned} \frac{B}{C}\frac{1}{k'a^2}[k'a\cos k'a - \sin k'a] &= \frac{1}{ka^2}[(ka\cos ka - \sin ka) - \tan\delta_0(ka\sin ka + \cos ka)] \\ \frac{B}{C}\frac{1}{k'}[k'a\cos k'a - \sin k'a] &= \frac{1}{k}[ka(\cos ka - \tan\delta_0 \sin ka) - (\sin ka + \cos ka\tan\delta_0)] \\ &= \frac{1}{k}\left[ka\frac{\cos(ka + \delta_0)}{\cos\delta_0} - \frac{\sin(ka + \delta_0)}{\cos\delta_0}\right] \\ \frac{B}{C}[k'a\cos k'a - \sin k'a] &= \frac{k'}{k}\frac{\sin(ka + \delta_0)}{\cos\delta_0}[ka\cot(ka + \delta_0) - 1]. \end{aligned} \tag{3.153}$$

Taking the quotient of Eq. (3.151) and Eq. (3.153) we find that

$$\begin{aligned} \frac{\sin k'a}{k'a\cos k'a - \sin k'a} &= \frac{1}{ka\cot(ka + \delta_0) - 1} \\ ka\sin k'a\cot(ka + \delta_0) - \sin k'a &= k'a\cos k'a - \sin k'a, \end{aligned} \tag{3.154}$$

and hence we obtain the result

$$\boxed{k\cot(ka + \delta_0) = k'\cot k'a.} \tag{3.155}$$

Rearranging this, we find that

$$\tan(ka + \delta_0) = \frac{k}{k'}\tan k'a, \tag{3.156}$$

from which we obtain

$$\boxed{\delta_0(k) = \tan^{-1}(\frac{k}{k'}\tan k'a) - ka.} \tag{3.157}$$

3.4 Low Energy Scattering, Bound States and Resonances

The previous results for the case of the hard sphere potential 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. (3.86) 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 $n_l(\rho)$.

Using the radial wave functions $R_l'(r)$ and $R_l(r)$, defined inside and outside the interaction region

$$R_l(r) = Aj_l(kr) + Bn_l(kr) \tag{3.158}$$

$$R_l'(r) = Cj_l(k'r) \tag{3.159}$$

(there is no wave coming out of the interacting region at the boundary). Matching the wavefunction and its derivative at the interaction boundary $r = a$ we obtain

$$Aj_l(ka) + Bn_l(ka) = Cj_l(k'a) \tag{3.160}$$

$$Akj_l'(ka) + Bkn_l'(ka) = Ck'j_l'(k'a), \tag{3.161}$$

where j_l' is the first derivative of j_l. Eliminating C gives

$$(Akj_l'(ka) + Bn_l') = \frac{j_l'(k'a)}{j_l(k'a)}(Aj_l(ka) + Bn_l(ka)) \tag{3.162}$$

$$\implies \quad \frac{B}{A} = -\frac{kj_l'(ka) - \gamma j_l(ka)}{kn_l'(ka) - \gamma n_l(ka)}, \tag{3.163}$$

where we define $\gamma = j_l'(k'a)/j_l(k'a)$. Knowing from above that $\frac{B}{A} = -\tan\delta_l$ gives the result,

$$\tan\delta_l = \frac{kj_l'(ka) - \gamma j_l(ka)}{kn_l'(ka) - \gamma n_l(ka)} \tag{3.164}$$

at the boundary. Inserting the asymptotic expansions, gives $\delta_l \to k^{2l+1}$ as $k \to 0$.

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

$$\boxed{\delta_o(k) \xrightarrow[k\to 0]{} -ka.} \tag{3.165}$$

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

$$-\frac{\hbar^2}{2m}\partial_r^2 u(r) + V(r)u(r) = E_k u(r). \tag{3.166}$$

This is just the Schrödinger equation for 1D motion. $u(r)$ obeys the boundary condition $u(0) = 0$. Now consider the limit of zero energy, when the right hand side of Eq. (3.166) vanishes. Outside of the interaction region the behaviour of $u(r)$ is extremely simple: it is just a straight line

Fig. 3.5: Zero energy wavefunction for a repulsive potential, leading to positive scattering length.

$$u(r) = A(r - a). \tag{3.167}$$

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

$$\frac{\sin(kr + \delta_0(k))}{kr} \xrightarrow[k\to 0]{} 1 - \frac{a}{r}. \tag{3.168}$$

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.

Fig. 3.6: (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.

We want to show that negative potentials lead to positive scattering lengths a and the other way round for the hard sphere potential. From Eq. (3.157) we know

$$\delta_0(k) = \tan^{-1}(\frac{k}{k'}\tan k'a_0) - ka_0, \tag{3.169}$$

where a_0 is the radius of the potential, $k = \sqrt{2mE}/\hbar$ corresponds to the momentum the particle has outside the interaction region, and $k' = \sqrt{2m(E - V_0)}/\hbar$ is the momentum inside the interaction region. Now we know that the scattering length a is defined as $\delta_0(k) \to -ka$ for $k \to 0$. We can expand equation (3.169) for $k \to 0$ to give

$$\delta_0(k \to 0) \to ka_0\left[\frac{1}{a_0 k'}\tan k'a_0 - 1\right]. \tag{3.170}$$

We note that the sign of the potential determines whether k' is imaginary or not, since we are looking at the $k = \sqrt{2mE}/\hbar$ limit, We can neglect E in this expression for $k' = \sqrt{-2mV_0}/\hbar$. If V_0 is negative, $k' = \kappa$; if V_0 is positive we have $k' = i\kappa$.

For a repulsive potential $V_0 > 0$, equation (3.170) corresponds to

$$\delta_0(k \to 0) \to ka_0\left[\frac{1}{a_0\kappa}\tanh(\kappa a_0) - 1\right], \tag{3.171}$$

for $k' \to i\kappa$. Thus, per definition

$$a = -a_0\left[\frac{1}{a_0\kappa}\tanh(\kappa a_0) - 1\right]. \tag{3.172}$$

The quantity inside the square brackets is always negative: since $\tanh(\kappa a_0) \in [-1, 1]$, this is obvious for large $a_0\kappa$ where the -1 term dominates, and for small arguments a_0 we can use a series expansion to show that this is still true. Hence repulsive potentials are associated with $a > 0$. For $V_0 \to \infty$, the scattering length of the potential corresponds to its hard core radius, $a = a_0$.

For an attractive potential, we obtain instead

$$\delta_0(k \to 0) \to k a_0 \left[\frac{1}{a_0 \kappa} \tan(\kappa a_0) - 1 \right], \tag{3.173}$$

and

$$a = -a_0 \left[\frac{1}{a_0 \kappa} \tan(\kappa a_0) - 1 \right] \tag{3.174}$$

Here, the term inside the square brackets is positive, for $\kappa a_0 < \pi/2$, which is where the first bound state of the attractive potential occurs.

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 $u(r) = e^{-\kappa r}$ outside of the interaction region, and we can identify $\kappa = a^{-1}$. Then

$$E_{\text{bound}} = -\frac{\hbar^2 \kappa^2}{2m} \sim -\frac{\hbar^2}{2ma^2}. \tag{3.175}$$

3.4.1 Resonant Scattering [*non-examinable*]

Fig. 3.7: Resonant scattering.

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**

$$-\frac{\hbar^2}{2m}\partial_x^2 \Psi(x) + t\delta(x)\psi_{\text{res}} = E_k \Psi(x) \tag{3.176}$$

$$\mathcal{E}_{\text{res}}\psi_{\text{res}} + t\Psi(0) = E_k \psi_{\text{res}}, \tag{3.177}$$

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

$$\Psi_{\text{even}}(x) = \cos(k|x| + \delta_{\text{even}}(k)) \tag{3.178}$$

Eq. (3.176) tells us that

$$\sin \delta_{\text{even}}(k) = -\frac{mt}{\hbar^2 k}\psi_{\text{res}}. \tag{3.179}$$

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

$$\tan \delta_{\text{even}}(k) = \frac{m}{\hbar^2 k}\frac{t^2}{\mathcal{E}_{\text{res}} - E_k}. \tag{3.180}$$

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

To calculate the reflection probability, we first remember that we have multiply shown that the relation

$$\tan\delta = -\frac{B}{A} \tag{3.181}$$

holds, where A and B are the coefficients of the incoming and reflected wave respectively; hence, the reflection coefficient

$$r = B = \sin\delta \tag{3.182}$$

and the reflection probability

$$|r|^2 = 1 - \cos^2\delta = 1 - \frac{1}{\sqrt{1+\tan\delta}}. \tag{3.183}$$

Inserting the corresponding expression (3.180) for δ

$$\tan\delta_{\text{even}} = \frac{m}{\hbar^2}\frac{t^2}{\mathcal{E}_{\text{res}} - E_k}, \tag{3.184}$$

we obtain for the reflection probability having the **Breit-Wigner** form,

$$|r(k)|^2 = \frac{\gamma^2/4}{(E_k - \mathcal{E}_{\text{res}})^2 + \gamma^2/4}, \tag{3.185}$$

where $\gamma = 4\frac{m^2}{\hbar^4}t^4$.

Chapter 4

Second Quantisation

A system of N particles is described by a wavefunction of N position arguments $\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$. 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 quantisation**.[1]

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[2]

$$|\Psi(\mathbf{y}, \mathbf{x})|^2 = |\Psi(\mathbf{x}, \mathbf{y})|^2. \tag{4.1}$$

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

$$\Psi(\mathbf{y}, \mathbf{x}) = e^{i\theta}\Psi(\mathbf{x}, \mathbf{y}). \tag{4.2}$$

What can we say about θ? Take another two positions $\mathbf{x}'$, and $\mathbf{y}'$, then

$$\Psi(\mathbf{y}', \mathbf{x}') = e^{i\theta}\Psi(\mathbf{x}', \mathbf{y}'), \tag{4.3}$$

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

$$\Psi(\mathbf{x}, \mathbf{y}) = e^{2i\theta}\Psi(\mathbf{x}, \mathbf{y}), \tag{4.4}$$

that is $e^{i\theta} = \pm 1$ and the wavefunction for two particles is either *symmetric* or *antisymmetric.*

A more formal approach is to consider the **exchange operator** $\hat{P}_{12}$ that exchanges the two arguments

$$\hat{P}_{12}\Psi(\mathbf{x}, \mathbf{y}) = \Psi(\mathbf{y}, \mathbf{x}), \tag{4.5}$$

[1] The name is very obscure, but will become a bit clearer later.
[2] This is what we *mean* by indistinguishable.

which is evidently a linear operator that furthermore squares to give the identity $\hat{P}_{12}^2 = \mathbb{I}$. The eigenvalues of $\hat{P}_{12}$ 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

$$\hat{H} = -\frac{\hbar^2}{2m_e}\left[\nabla_x^2 + \nabla_y^2\right] + \frac{e^2}{|\mathbf{x} - \mathbf{y}|} \tag{4.6}$$

evidently it doesn't matter whether we apply $\hat{P}_{12}$ before or after $\hat{H}$. Thus $[\hat{H}, \hat{P}_{12}] = 0$ and basic ideas of quantum mechanics tell us that:

1. Eigenstates of the Hamiltonian have definite exchange symmetry;[3]

2. The symmetry of the wavefunction is a constant of the motion.

4.1.1 From Two to Many

What changes when we consider systems of N identical particles? The wavefunction is now a function of the N coordinates $\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$, and we can consider an exchange operator $\hat{P}_{ij}$ that swaps the i^{th} and ^{j}th arguments. The same physical reasoning as before singles out eigenstates of the $\left\{\hat{P}_{ij}\right\}$. Note that $[\hat{P}_{12}, \hat{P}_{23}] \neq 0$, and thus one might worry whether it is *mathematically* possible to have a simultaneous eigenstate of all the $\hat{P}_{ij}$. 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.

Consider operating on a many particle state with the following operator,

$$\begin{aligned}
\hat{P}_{12}\hat{P}_{23}\hat{P}_{12}\left|\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \cdots, \mathbf{r}_N\right\rangle &= \hat{P}_{12}\hat{P}_{23}\left|\Psi(\mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_3, \cdots, \mathbf{r}_N)\right\rangle \\
&= \hat{P}_{12}\left|\Psi(\mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_1, \cdots, \mathbf{r}_N)\right\rangle \\
&= \left|\Psi(\mathbf{r}_3, \mathbf{r}_2, \mathbf{r}_1, \cdots, \mathbf{r}_N)\right\rangle \\
&= \hat{P}_{13}\left|\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \cdots, \mathbf{r}_N)\right\rangle,
\end{aligned} \tag{4.7}$$

thus it clear that

$$\hat{P}_{12}\hat{P}_{23}\hat{P}_{12} = \hat{P}_{13}. \tag{4.8}$$

Following the same approach it is also immediately clear that we can extend this equality to

$$\hat{P}_{12}\hat{P}_{23}\hat{P}_{12} = \hat{P}_{13} = \hat{P}_{23}\hat{P}_{12}\hat{P}_{23}. \tag{4.9}$$

[3] In a real two-electron system overall antisymmetry is guaranteed by the appropriate choice of spin wavefunction

In order to make a statement about the eigenvalues of $\hat{P}_{ij}$ for a simultaneous eigenstate of all $\hat{P}_{ij}$, $|\Psi\rangle$, let us define the eigenvalues as

$$E_{ij} = \langle\Psi|\hat{P}_{ij}|\Psi\rangle \,. \tag{4.10}$$

Thence

$$\begin{aligned} E_{kl} &= \langle\Psi|\hat{P}_{kl}|\Psi\rangle \\ &= \langle\Psi|\hat{P}_{ik}\hat{P}_{il}\hat{P}_{ik}|\Psi\rangle \\ &= \langle\Psi|\hat{P}_{ik}\hat{P}_{jl}\hat{P}_{ij}\hat{P}_{jl}\hat{P}_{ik}|\Psi\rangle \\ &= E_{ik}^2 E_{jl}^2 E_{ij} \\ &= E_{ij}, \end{aligned} \tag{4.11}$$

where we have used that $E_{ij} = \pm 1 \,\forall i, j$. Thus all eigenvalues are equal and in fact equally $+1$ or -1.

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).

If we dealt with *distinguishable* particles, the wavefunction of a pair of particles in states φ_1 and φ_2 would be

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \varphi_1(\mathbf{r}_1)\varphi_2(\mathbf{r}_2). \tag{4.12}$$

Accounting for indistinguishability, we have either[4]

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}[\varphi_1(\mathbf{r}_1)\varphi_2(\mathbf{r}_2) \pm \varphi_2(\mathbf{r}_1)\varphi_1(\mathbf{r}_2)] \tag{4.13}$$

with the upper plus sign for bosons and the lower minus 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.

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

$$P_{12}(\mathbf{r}_1, \mathbf{r}_2) = P_1(\mathbf{r}_1)P_2(\mathbf{r}_2). \tag{4.14}$$

This also follows from taking the square modulus of Eq. (4.12).

The result implied by the wavefunction Eq. (4.13) for a pair of identical bosons or fermions is

Most people find this result rather counterintuitive. It shows that, because probabilities arise from the squares of amplitudes.

[4] The $1/\sqrt{2}$ yields a normalised wavefunction if $\varphi_{1,2}(\mathbf{r})$ are *orthonormal*.

Fig. 4.1: Four possible outcomes after the passage of two bosons through a beam splitter.

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,

$$\frac{1}{\sqrt{2}}(|\text{Left}\rangle \pm |\text{Right}\rangle). \tag{4.15}$$

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

$$\hat{H} = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2 + V(\mathbf{r}_i)\right], \tag{4.16}$$

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 $\{\alpha_i\}$, $\{i = 1, 2, \cdots, N\}$ 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[5]

$$\begin{aligned} |\Psi_{\alpha_1\alpha_2\cdots\alpha_N}\rangle &= \varphi_{\alpha_1}(\mathbf{r}_1)\varphi_{\alpha_2}(\mathbf{r}_2)\cdots\varphi_{\alpha_N}(\mathbf{r}_N) \\ &= |\varphi_{\alpha_1}\rangle\,|\varphi_{\alpha_2}\rangle\cdots|\varphi_{\alpha_N}\rangle\,. \end{aligned} \tag{4.17}$$

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 *symmetrisation* and *antisymmetrisation*

$$\hat{\mathcal{S}} = \frac{1}{N!}\sum_P \hat{P}, \quad \hat{\mathcal{A}} = \frac{1}{N!}\sum_P \operatorname{sgn}(\hat{P})\hat{P}. \tag{4.18}$$

The sums are over all $N!$ permutations of N objects, $\hat{P}$ denotes the corresponding permutation operator, and $\operatorname{sgn}(\hat{P})$ 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. (4.17) as

$$\boxed{\begin{aligned} \left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle &= \sqrt{\frac{N!}{\prod_\alpha N_\alpha!}}\hat{\mathcal{S}}\varphi_{\alpha_1}(\mathbf{r}_1)\varphi_{\alpha_2}(\mathbf{r}_2)\cdots\varphi_{\alpha_N}(\mathbf{r}_N) \\ \left|\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle &= \sqrt{N!}\hat{\mathcal{A}}\varphi_{\alpha_1}(\mathbf{r}_1)\varphi_{\alpha_2}(\mathbf{r}_2)\cdots\varphi_{\alpha_N}(\mathbf{r}_N). \end{aligned}} \tag{4.19}$$

Such states are called **product states**. The normalisation factor[6] 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

[5] We will frequently switch between the wavefunction ($\varphi(\mathbf{r})$) and bra-ket notation ($|\varphi\rangle$). In the latter notation the product wavefunction in Eq. (4.12) is written $|\varphi_1\rangle\,|\varphi_2\rangle$.

[6] The normalisation factors yield normalised wavefunctions if the single particle state $|\varphi_\alpha\rangle$ are orthonormal (as the eigenstates of the single particle Hamiltonian are).

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

$$E = \sum_{i=1}^{N} E_{\alpha_i} = \sum_{\alpha} N_\alpha E_\alpha. \tag{4.20}$$

The easiest way of constructing the totally antisymmetric three-fermion wavefunction is by using the totally antisymmetric property of the Levi-Civita tensor.,

$$|\Psi_3\rangle = N\varepsilon_{ijk} |\varphi_i\rangle |\varphi_j\rangle |\varphi_k\rangle , \tag{4.21}$$

where N is a normalisation factor and $i, j, k \in \{1, 2, 3\}$. Here,

$$N = \frac{1}{\sqrt{\varepsilon_{ijk}\varepsilon_{lmn}\Big(\langle\varphi_i| \langle\varphi_k| \langle\varphi_k|\Big)\Big(|\varphi_l\rangle |\varphi_m\rangle |\varphi_n\rangle\Big)}}. \tag{4.22}$$

For a state with three bosons, two in state φ_1 and one in state φ_2, the totally symmetric wavefunction can generally be constructed by adding all permutations of the single-particle wavefunctions,

$$|\Psi_3\rangle = N \sum_{P_3} \left|\varphi_{P_3(1)}\right\rangle \left|\varphi_{P_3(2)}\right\rangle \left|\varphi_{P_3(3)}\right\rangle , \tag{4.23}$$

where in this case $|\varphi_3\rangle = |\varphi_1\rangle$. Hence we have

$$|\Psi_3\rangle = \frac{1}{\sqrt{3}}(|\varphi_1\rangle |\varphi_1\rangle |\varphi_2\rangle + |\varphi_1\rangle |\varphi_2\rangle |\varphi_1\rangle + |\varphi_2\rangle |\varphi_1\rangle |\varphi_1\rangle). \tag{4.24}$$

Let us also verify that the normalisation factors in Eq. (4.19) are correct. We will make use of the property of the single-particle wavefunctions, $\langle\alpha_i|\alpha_j\rangle = \delta_{i,j}$. Let us first consider the totally antisymmetric N-particle wavefunction,

$$\begin{aligned}
\left\langle \Psi_N^A \middle| \Psi_N^A \right\rangle &= \frac{1}{N!} \sum_{P_N, Q_N} \mathrm{sgn}(P_N)\mathrm{sgn}(Q_N) \left\langle \alpha_{P_N(1)} \middle| \alpha_{Q_N(1)} \right\rangle \left\langle \alpha_{P_N(2)} \middle| \alpha_{Q_N(2)} \right\rangle \cdots \left\langle \alpha_{P_N(N)} \middle| \alpha_{Q_N(N)} \right\rangle \\
&= \frac{1}{N!} \sum_{P_N, Q_N} \mathrm{sgn}(P_N)\mathrm{sgn}(Q_N) \delta_{P_N(1),Q_N(1)} \delta_{P_N(2),Q_N(2)} \cdots \delta_{P_N(N),Q_N(N)} \\
&= \frac{1}{N!} \sum_{P_N} \mathrm{sgn}(P_N)^2 \\
&= \frac{1}{N!} \sum_{P_N} \\
&= 1,
\end{aligned} \tag{4.25}$$

where P, Q are N-body permutations.

Lets now consider the totally symmetric N-particle wavefunction:

$$\begin{aligned}
\left\langle \Psi_N^S \middle| \Psi_N^S \right\rangle &= \frac{1}{N! \prod_\alpha N_\alpha} \sum_{P_N, Q_N} \left\langle \alpha_{P_N(1)} \middle| \alpha_{Q_N(1)} \right\rangle \left\langle \alpha_{P_N(2)} \middle| \alpha_{Q_N(2)} \right\rangle \cdots \left\langle \alpha_{P_N(N)} \middle| \alpha_{Q_N(N)} \right\rangle \\
&= \frac{1}{\prod_\alpha N_\alpha} \sum_{P_N} \left\langle \alpha_{P_N(1)} \middle| \alpha_1 \right\rangle \left\langle \alpha_{P_N(2)} \middle| \alpha_2 \right\rangle \cdots \left\langle \alpha_{P_N(N)} \middle| \alpha_N \right\rangle
\end{aligned} \tag{4.26}$$

Here we assume w.l.o.g. that the $|\alpha_i\rangle$ have been order in groups of identical single-particle states. Then the only permutations leading to non-zero contributions are the ones where the $\langle\alpha_i|$ are ordered in the same groups and only permutations within those groups occur.

$$\begin{aligned}\left\langle \Psi_N^S \middle| \Psi_N^S \right\rangle &= \frac{1}{\prod_\alpha N_\alpha} \prod_\alpha \Bigg(\sum_{P_{N_\alpha}} \left\langle \alpha_{P_{N_{\alpha_1}}(1)} \middle| \alpha_1 \right\rangle \cdots \left\langle \alpha_{P_{N_{\alpha_1}}(N_{\alpha_1})} \middle| \alpha_{N_{\alpha_1}} \right\rangle \cdots \\ &\qquad\qquad \times \left\langle \alpha_{P_{N_{\alpha_M}}(N-N_{\alpha_M})} \middle| \alpha_{N-N_{\alpha_M}} \right\rangle \cdots \left\langle \alpha_{P_{N_{\alpha_1}}(N)} \middle| \alpha_N \right\rangle \Bigg) \\ &= \frac{1}{\prod_\alpha N_\alpha} \prod_\alpha \sum_{P_{N_\alpha}} \\ &= 1, \end{aligned} \tag{4.27}$$

where P, Q are N-body permutations. In line two we have used that $\sum_P \left\langle \alpha_{P(1)} \middle| \alpha_{Q(1)} \right\rangle \left\langle \alpha_{P(2)} \middle| \alpha_{Q(2)} \right\rangle \cdots \left\langle \alpha_{P(N)} \middle| \alpha_{Q(N)} \right\rangle$ is independent of which permutation Q we choose, since all choices of pairing are being evaluated and summed anyway.

A more formal way of putting things is as follows. We first consider the space spanned by states of the form Eq. (4.17). Then we introduce the operators $\hat{\mathcal{S}}$ and $\hat{\mathcal{A}}$, noting that $\hat{\mathcal{S}}^2 = \hat{\mathcal{S}}$ and $\hat{\mathcal{A}}^2 = \hat{\mathcal{A}}$. In other words, there's no point symmetrising or antisymmetrising 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**)

$$\left| \Psi^A_{\alpha_1\alpha_2\cdots\alpha_N} \right\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_1}(\mathbf{r}_1) & \varphi_{\alpha_1}(\mathbf{r}_2) & \cdots & \varphi_{\alpha_1}(\mathbf{r}_N) \\ \varphi_{\alpha_2}(\mathbf{r}_1) & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \varphi_{\alpha_N}(\mathbf{r}_1) & \cdots & \cdots & \varphi_{\alpha_N}(\mathbf{r}_N) \end{vmatrix}. \tag{4.28}$$

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 ($\alpha_i = \alpha_j$).

4.1.1.1 Anyons [*non-examinable*]

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 long undiscovered. The weak point is that nothing requires that the wavefunction of a pair be *single-valued*, as we tacitly assumed in writing Eq. (4.4).

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 $\hat{\mathbf{n}} = (\mathbf{x}-\mathbf{y})/|\mathbf{x}-\mathbf{y}|$, an exchange then corresponds to $\hat{\mathbf{n}} \to -\hat{\mathbf{n}}$ 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.

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.

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.

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

$$\varphi_n(x) = \frac{1}{\sqrt{L}} \exp\left(\frac{2\pi i n x}{L}\right), \quad n = 0, \pm 1, \pm 2, \cdots, \tag{4.29}$$

with energies $E_n = \frac{\hbar^2 n^2}{2mL^2}$. 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 normalisation)

$$\Psi^S(x_1, x_2, \cdots, x_N) = 1. \tag{4.30}$$

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 $n = -(N-1)/2, -(N-3)/2, \cdots, -1, 0, 1, \cdots, (N-1)/2$ (for an even number of particles we have to decide whether to put the last particle at $n = \pm N/2$). Introducing the complex

Fig. 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.

variables $z_i = \exp(2\pi i x_i/L)$, the Slater determinant in Eq. (4.28) becomes

$$\begin{vmatrix} z_1^{-(N-1)/2} & z_2^{-(N-1)/2} & \cdots & z_N^{-(N-1)/2} \\ z_1^{-(N-3)/2} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ z_1^{(N-1)/2} & \cdots & \cdots & z_N^{(N-1)/2} \end{vmatrix}. \tag{4.31}$$

Let's evaluate this complicated looking expression in a simple case. With three particles we have

$$\begin{aligned} \begin{vmatrix} z_1^{-1} & z_2^{-1} & z_3^{-1} \\ 1 & 1 & 1 \\ z_1 & z_2 & z_3 \end{vmatrix} &= \frac{z_1}{z_2} - \frac{z_2}{z_1} + \frac{z_3}{z_1} - \frac{z_1}{z_3} + \frac{z_2}{z_3} - \frac{z_3}{z_2} \\ &= \left(\sqrt{\frac{z_3}{z_1}} - \sqrt{\frac{z_1}{z_3}}\right)\left(\sqrt{\frac{z_1}{z_2}} - \sqrt{\frac{z_2}{z_1}}\right)\left(\sqrt{\frac{z_2}{z_3}} - \sqrt{\frac{z_3}{z_2}}\right) \\ &\propto \sin\left(\frac{\pi[x_1 - x_2]}{L}\right) \sin\left(\frac{\pi[x_3 - x_1]}{L}\right) \sin\left(\frac{\pi[x_2 - x_3]}{L}\right). \end{aligned} \tag{4.32}$$

The vanishing of the wavefunction when $x_i = x_j$ (see Fig. 4.2) is consistent with the Pauli principle. You should check that additionally it is periodic and totally antisymmetric.

To show that this does generalise for any (odd) N, following from Eq. (4.31)

$$\begin{aligned} S &= \begin{vmatrix} z_1^{-(N-1)/2} & z_2^{-(N-1)/2} & \cdots & z_N^{-(N-1)/2} \\ z_1^{-(N-3)/2} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ z_1^{(N-1)/2} & \cdots & \cdots & z_N^{(N-1)/2} \end{vmatrix} \\ &= (z_1 z_2 \cdots z_N)^{-(N-1)/2} \begin{vmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_N \\ \vdots & \vdots & \ddots & \vdots \\ z_1^{N-1} & z_2^{N-1} & \cdots & z_N^{N-1} \end{vmatrix}. \end{aligned} \tag{4.33}$$

We can use the identity for the **Vandermonde** determinant,

$$\begin{vmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_N \\ \vdots & \vdots & \ddots & \vdots \\ z_1^{N-1} & z_2^{N-1} & \cdots & z_N^{N-1} \end{vmatrix} = \prod_{i<j}^{N} (z_i - z_j) \tag{4.34}$$

to then see that

$$
\begin{aligned}
S &= (z_1 z_2 \cdots z_N)^{-(N-1)/2} \prod_{i<j}^{N} (z_i - z_j) \\
&\propto \left(\prod_{i<j}^{N} \frac{(z_i - z_j)}{2 i z_i^{1/2} z_j^{1/2}} \right) \\
&= \prod_{i<j}^{N} \sin\left(\frac{\pi (x_i - x_j)}{L} \right),
\end{aligned}
\tag{4.35}
$$

where the factor of proportionality is a phase-factor. This is antisymmetric, and periodic when *all* $x_i \to x_i + L$.

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 kF. In this case $k_{\mathrm{F}} = (N-1)\pi/L$. The corresponding momentum $p_{\mathrm{F}} = \hbar k_{\mathrm{F}}$ is the **Fermi momentum**; the corresponding energy $E_{\mathrm{F}} = \frac{\hbar^2 k_{\mathrm{F}}^2}{2m}$ the **Fermi energy**, and so on.

4.3 Creation and Annihilation Operators

We have already gleaned the essential idea of second quantisation. 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 quantisation 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.[7] 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. (4.17). A first guess at defining a **creation operator**[8] that puts a particle in state $|\varphi_\alpha\rangle$ would be

$$
\hat{c}_\alpha : |\Psi_{\alpha_1\alpha_2\cdots\alpha_N}\rangle \xrightarrow{?} \sqrt{N+1}\, |\varphi_\alpha\rangle\, \Psi_{\alpha_1\alpha_2\cdots\alpha_N} = \sqrt{N+1} \Psi_{\alpha\alpha_1\alpha_2\cdots\alpha_N} \tag{4.36}
$$

(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 any state can be written as a linear combination of the states $\{|\Psi_{\alpha_1\alpha_2\cdots\alpha_N}\rangle\}$, the action of $\hat{c}_\alpha$ can be extended to any state by linearity. Eq. (4.36) has an obvious shortcoming, however, in that it does not preserve the

[7] 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.

[8] Formally, the space of distinguishable N particle states is $\mathcal{H}_N = \overbrace{\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1}^{n \text{ times}}$. 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**.

symmetry of the wavefunction. This is easily remedied by applying the symmetrisation operator that we introduced in Eq. (4.18) after adding a particle (we discuss the boson case first), so a better definition is

$$\hat{c}_\alpha : \left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle \to \sqrt{N+1}\hat{\mathcal{S}}\left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle, \quad \text{for bosons.} \tag{4.37}$$

Bearing in mind the normalisation factors in Eq. (4.19),

$$\begin{aligned}
\hat{c}_\alpha : \left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle &\to \sqrt{N+1}\hat{\mathcal{S}}\left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle \\
&= \sqrt{N+1}\frac{1}{(N+1)!}\sum_{P_{N+1}} P_{N+1}\left|\varphi_\alpha\right\rangle\left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle \\
&= \sqrt{N+1}\frac{1}{(N+1)!}\sum_{P_{N+1}} P_{N+1}\left|\varphi_\alpha\right\rangle\sqrt{\frac{1}{N!\prod_{\alpha_i}N_{\alpha_i}!}}\sum_{P_N}P_N\left|\varphi_{\alpha_1}\right\rangle\cdots\left|\varphi_{\alpha_N}\right\rangle \\
&= \sqrt{N+1}\frac{1}{(N+1)!}\sum_{P_{N+1}} P_{N+1}\left|\varphi_\alpha\right\rangle\sqrt{\frac{N!}{\prod_{\alpha_i}N_{\alpha_i}!}}\left|\varphi_{\alpha_1}\right\rangle\cdots\left|\varphi_{\alpha_N}\right\rangle \\
&= \sqrt{\frac{1}{(N+1)!\prod_{\alpha_i}N_{\alpha_i}!}}\sum_{P_{N+1}} P_{N+1}\left|\varphi_\alpha\right\rangle\left|\varphi_{\alpha_1}\right\rangle\cdots\left|\varphi_{\alpha_N}\right\rangle \\
&= \frac{\sqrt{N_\alpha+1}}{\sqrt{N_\alpha+1}}\sqrt{\frac{1}{(N+1)!\prod_{\alpha_i\neq\alpha}N_{\alpha_i}!N_\alpha!}}\sum_{P_{N+1}} P_{N+1}\left|\varphi_\alpha\right\rangle\left|\varphi_{\alpha_1}\right\rangle\cdots\left|\varphi_{\alpha_N}\right\rangle \\
&= \sqrt{N_\alpha+1}\left|\Psi^S_{\alpha\alpha_1\cdots\alpha_N}\right\rangle
\end{aligned} \tag{4.38}$$

In line three we have use all permutations P_N are all "included" in P_{N+1}.

If we label totally symmetric states by their occupation numbers, so that $\left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle = |N_0, N_1, \cdots\rangle$, this equation may be written

$$\hat{c}_\alpha\left|N_0, N_1, \cdots, N_\alpha, \cdots\right\rangle \to \sqrt{N_\alpha+1}\left|N_0, N_1, \cdots, N_\alpha+1, \cdots\right\rangle. \tag{4.39}$$

By considering matrix elements $\langle N_0, N_1, \cdots|\hat{c}_\alpha|N_0', N_1', \cdots\rangle$ we can conclude

$$\hat{c}^\dagger_\alpha\left|N_0, N_1, \cdots, N_\alpha, \cdots\right\rangle \to \sqrt{N_\alpha}\left|N_0, N_1, \cdots, N_\alpha-1, \cdots\right\rangle. \tag{4.40}$$

In other words, the conjugate of the creation operator is a **destruction operator**, that removes one particle from a given state. From Eq. (4.39) and Eq. (4.40) come the fundamental relationships

$$\left[\hat{c}^\dagger_\alpha, \hat{c}_\beta\right] = \delta_{\alpha\beta} \tag{4.41}$$

$$\left[\hat{c}_\alpha, \hat{c}_\beta\right] = \left[\hat{c}^\dagger_\alpha, \hat{c}^\dagger_\beta\right] = 0. \tag{4.42}$$

For reasons that will become clear shortly we normally write things in terms of the annihilation operator $\hat{a}_\alpha \equiv \hat{c}^\dagger_\alpha$, in which case the above takes the form

$$\boxed{\begin{aligned}\left[\hat{a}_\alpha, \hat{a}^\dagger_\beta\right] &= \delta_{\alpha\beta} \\ \left[\hat{a}_\alpha, \hat{a}_\beta\right] = \left[\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\right] &= 0.\end{aligned}} \tag{4.43}$$

The same relations describe the ladder operators of a set of independent harmonic oscillators, revealing a deep connection between these two systems. The combination $\hat{N} = \hat{a}^\dagger_\alpha \hat{a}_\alpha$ is called the **number operator** for state α for obvious reasons

$$\hat{N}_\alpha \left| N_0, N_1, \cdots, N_\alpha \right\rangle = N_\alpha \left| N_0, N_1, \cdots, N_\alpha \right\rangle . \tag{4.44}$$

From Eq. (4.43) it follows that

$$\begin{aligned} \left[\hat{a}_\alpha, \hat{N}_\alpha\right] &= \hat{a}_\alpha \\ \left[\hat{a}^\dagger_\alpha, \hat{N}_\alpha\right] &= -\hat{a}^\dagger_\alpha . \end{aligned} \tag{4.45}$$

You can think of the first of these as "count then destroy minus destroy then count", for example.

It follows that a normalised state $\left|\Psi^S_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle$ of the many boson system may be written as

$$\left| N_0, N_1, \cdots \right\rangle = \frac{\left(\hat{a}^\dagger_0\right)^{N_0}}{\sqrt{N_0!}} \frac{\left(\hat{a}^\dagger_1\right)^{N_1}}{\sqrt{N_1!}} \cdots \left| 0, 0, \cdots \right\rangle . \tag{4.46}$$

The state with no particles $\left|0, 0, \cdots\right\rangle$ is known as the **vacuum state**. We will often denote it by $\left|\mathrm{VAC}\right\rangle$ for brevity.[9] In terms of a wavefunction, you can think of it as equal to 1, so that Eq. (4.37) works out. Alternatively, you can take the relations in Eq. (4.43) as fundamental, in which case $\left|\mathrm{VAC}\right\rangle$ has the defining proper

$$\hat{a}_\alpha \left|\mathrm{VAC}\right\rangle = 0, \quad \forall \alpha \tag{4.47}$$

Now we move on the slightly trickier matter of fermions. Eq. (4.37) suggests that the creation operator should be defined

$$\hat{c}_\alpha \left|\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle \to \sqrt{N+1}\hat{\mathcal{A}} \left|\varphi_\alpha\right\rangle \left|\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle , \quad \text{for fermions.} \tag{4.48}$$

For the fermion annihilation operators $\hat{a}_\alpha = \hat{c}^\dagger_\alpha$ the result corresponding to Eq. (4.43) is

$$\boxed{\begin{aligned} \left\{\hat{a}_\alpha, \hat{a}^\dagger_\beta\right\} &= \delta_{\alpha\beta} \\ \left\{\hat{a}_\alpha, \hat{a}_\beta\right\} = \left\{\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\right\} &= 0, \end{aligned}} \tag{4.49}$$

where $\left\{\hat{A}, \hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ denotes the **anticommutator**.

To prove this, let us start with the lower two commutation relations which are in fact obvious from the antisymmetry of the fermionic many-body wavefunction,

$$\begin{aligned} \left\{\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\right\} \left|\Psi^A_{\alpha_1\cdots\alpha_N}\right\rangle &= + \left|\Psi_{\alpha_\alpha\alpha_\beta\alpha_1\cdots\alpha_N}\right\rangle + \left|\Psi_{\alpha_\beta\alpha_\alpha\alpha_1\cdots\alpha_N}\right\rangle \\ &= + \left|\Psi_{\alpha_\alpha\alpha_\beta\alpha_1\cdots\alpha_N}\right\rangle - \left|\Psi_{\alpha_\alpha\alpha_\beta\alpha_1\cdots\alpha_N}\right\rangle \\ &= 0, \end{aligned} \tag{4.50}$$

provided the two states are both empty (otherwise the RHS vanishes trivially). The second non-numberconserving anticommutation relation can be treated analogously. Thus:

$$\left\{\hat{a}_\alpha, \hat{a}_\beta\right\} = \left\{\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\right\} = 0. \tag{4.51}$$

[9] $\left|\mathrm{VAC}\right\rangle$ is not to be confused with $\left|0\right\rangle$, which will denote the ground state of our many body system with a fixed number of particle.

Now lets consider tha more complicated case of $\left\{\hat{a}_\alpha, \hat{a}^\dagger_\beta\right\}$.

$$\begin{aligned}\left\{\hat{a}_\alpha, \hat{a}^\dagger_\beta\right\}\left|\Psi^A_{\alpha_1\cdots\alpha_N}\right\rangle &= \hat{a}_\alpha\hat{a}^\dagger_\beta\left|\Psi^A_{\alpha_1\cdots\alpha_N}\right\rangle + \hat{a}^\dagger_\beta\hat{a}_\alpha\left|\Psi^A_{\alpha_1\cdots\alpha_N}\right\rangle \\ &= \prod_{\alpha_i\in\{\alpha_1,\cdots,\alpha_N\}}(1-\delta_{\alpha_i,\beta})\hat{a}_\alpha\left|\Psi^A_{\beta\alpha_1\cdots\alpha_N}\right\rangle \\ &\quad + \sum_{\alpha_j\in\{\alpha_1,\cdots,\alpha_N\}}\delta_{\alpha_j,\alpha}(-1)^{(j-1)}\hat{a}^\dagger_\beta\left|\Psi^A_{\alpha_1\cdots\cancel{\alpha_j}\cdots\alpha_N}\right\rangle \\ &= \sum_{\alpha_j\in\{\beta\alpha_1\cdots\alpha_N\}}\prod_{\alpha_i\in\{\alpha_1\cdots\alpha_N\}}(1-\delta_{\alpha_i,\beta})\delta_{\alpha_j,\alpha}(-1)^j\left|\Psi^A_{\beta\alpha_1\cdots\cancel{\alpha_j}\cdots\alpha_N}\right\rangle \\ &\quad + \sum_{\alpha_j\in\{\alpha_1\cdots\alpha_N\}}\prod_{\alpha_i\in\{\alpha_1\cdots\alpha_N\}}(1-\delta_{\alpha_i,\beta})\delta_{\alpha_j,\alpha}(-1)^{(j-1)}\left|\Psi^A_{\beta\alpha_1\cdots\cancel{\alpha_j}\cdots\alpha_N}\right\rangle \\ &\quad + \sum_{\alpha_j\in\{\alpha_1\cdots\alpha_N\}}\delta_{\alpha_j,\beta}\delta_{\alpha_j,\alpha}(-1)^{(j-1)}\left|\Psi^A_{\beta\alpha_1\cdots\cancel{\alpha_j}\cdots\alpha_N}\right\rangle . \end{aligned} \tag{4.52}$$

Here we have made use of

$$\prod_{\alpha_i\in\{\alpha_1\cdots\cancel{\alpha_j}\cdots\alpha_N\}}(1-\delta_{\alpha_i,\beta}) = \prod_{\alpha_i\in\{\alpha_1\cdots\alpha_N\}}(1-\delta_{\alpha_i,\beta}) + \delta_{\alpha_j,\beta}, \tag{4.53}$$

and thus we get that:

$$\begin{aligned}\left\{\hat{a}_\alpha, \hat{a}^\dagger_\beta\right\}\left|\Psi^A_{\alpha_1\cdots\alpha_N}\right\rangle &= \prod_{\alpha_i\in\{\alpha_1\cdots\alpha_N\}}(1-\delta_{\alpha_i,\beta})\delta_{\alpha,\beta}\left|\Psi^A_{\alpha_1\cdots\alpha_j\cdots\alpha_N}\right\rangle \\ &\quad + \sum_{\alpha_j\in\{\alpha_1\cdots\alpha_N\}}\delta_{\alpha_j,\beta}\delta_{\alpha,\beta}\left|\Psi^A_{\alpha_1\cdots\alpha_j\cdots\alpha_N}\right\rangle \\ &= \delta_{\alpha,\beta}\left|\Psi^A_{\alpha_1\cdots\alpha_N}\right\rangle . \end{aligned} \tag{4.54}$$

Of course, you *could* calculate the commutator, but it proves to be complicated (and uninteresting). The number operators, together with Eq. (4.45) (with commutators!), work as in the boson case. Eq. (4.49) implies that $\left(\hat{a}^\dagger_\alpha\right)^2 = 0$, 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, $(\hat{a}_\alpha)^2 = 0$, meaning that we can't remove two particles from the same state.

The state $\left|\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle$ has the representation[10]

$$|N_0, N_1, \cdots\rangle = \left(\hat{a}^\dagger_0\right)^{N_0}\left(\hat{a}^\dagger_1\right)^{N_1}\cdots|0,0,\cdots\rangle , \tag{4.55}$$

which is the same as Eq. (4.46), since $N_\alpha = 0$ or 1 only are allowed.

Suppose we want to move to a different basis of single particle states $\{|\tilde{\varphi}_\alpha\rangle\}$, corresponding to a unitary transformation

$$|\tilde{\varphi}_\alpha\rangle = \sum_\beta \langle\varphi_\beta|\tilde{\varphi}_\alpha\rangle\,|\varphi_\beta\rangle . \tag{4.56}$$

[10]Note that this equation defines the overall sign of the state $|N_0, N_1, \cdots\rangle$. Two states $\left|\Psi^A_{\alpha_1\alpha_2\cdots\alpha_N}\right\rangle$ and $\left|\Psi^A_{\alpha'_1\alpha'_2\cdots\alpha'_N}\right\rangle$ 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.

From Eqs. (4.39) and (4.48), the one particle states with the wavefunctions $\{\varphi_\alpha(\mathbf{r})\}$ are just $\left\{\hat{a}^\dagger_\alpha \left|\text{VAC}\right\rangle\right\}$. So we see that the above basis transformation gives a new set of creation operators

$$\hat{\tilde{a}}^\dagger_\alpha \equiv \sum_\beta \langle\varphi_\beta|\tilde{\varphi}_\alpha\rangle\, \hat{a}^\dagger_\beta. \tag{4.57}$$

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 complex conjugate of the wavefunction. Denoting the corresponding creation operator (sometimes called **field operator**) as $\hat{\psi}^\dagger(\mathbf{r})$, Eq. (4.57) becomes

$$\hat{\psi}^\dagger(|vbr) \equiv \sum_\beta \varphi^*_\beta(|vbr)\hat{a}^\dagger_\beta. \tag{4.58}$$

Now we can see why we chose to work with the annihilation operator rather than the creation operator. The conjugate of Eq. (4.58) is

$$\hat{\psi}(\mathbf{r}) \equiv \sum_\beta \varphi_\beta(\mathbf{r})\hat{a})\beta, \tag{4.59}$$

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. (4.43) and Eq. (4.49), together with the completeness relation

$$\sum_\alpha \varphi^*_\alpha\varphi_\alpha(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{4.60}$$

We find

$$\hat{\psi}(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}) \mp \hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}') \tag{4.61}$$

$$\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r} \mp \hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r} \mp \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}) = 0, \tag{4.62}$$

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.[11]

As an example, let our original basis be the eigenbasis of the free particle Hamiltonian $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m}$ with periodic boundary conditions

$$|\mathbf{k}\rangle = \frac{\exp(i\mathbf{k}\cdot\mathbf{r})}{\sqrt{V}}, \quad \mathbf{k} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right), \quad n_{x,y,z} \in \mathbb{Z}, \tag{4.64}$$

with $V = L_xL_yL_z$. 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

$$\hat{\psi}^\dagger(\mathbf{r}) \equiv \frac{1}{\sqrt{V}}\sum_\mathbf{k} \exp(-i\mathbf{k}\cdot\mathbf{r})\hat{a}^\dagger_\mathbf{k}, \tag{4.65}$$

[11] A compact way of writing creation and annihilation operators without choosing a basis at the outset is to associate an a $\hat{a}_{|\alpha\rangle}$ and a $\hat{a}^\dagger_{|\alpha\rangle}$ with any single particle state $|\alpha\rangle$ and declare the (anti-)commutation relations

$$\hat{a}_{|\alpha\rangle}\hat{a}^\dagger_{|\beta\rangle} \mp \hat{a}^\dagger_{|\beta\rangle}\hat{a}_{|\alpha\rangle} = \langle\alpha|\beta\rangle\,. \tag{4.63}$$

For an orthonormal basis the RHS is $\delta_{\alpha\beta}$.

and similarly

$$\hat{\psi}(\mathbf{r}) \equiv \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{r})\hat{a}_{\mathbf{k}}. \tag{4.66}$$

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!

4.3.1 Bogoliubov Transformation

Consider the Hamiltonian

$$\hat{H} = \varepsilon\left(\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b}\right) + \Delta\left(\hat{a}^\dagger\hat{b}^\dagger + ba\right). \tag{4.67}$$

This Hamiltonian is slightly unusual, as it doesn't conserve the number of particles.

Let's first consider the case of bosons. Then all operators commute except

$$\left[\hat{a}, \hat{a}^\dagger\right] = \left[\hat{b}, \hat{b}^\dagger\right] = 1. \tag{4.68}$$

Define new operators

$$\hat{\alpha} = \hat{a}\cosh\kappa - \hat{b}^\dagger \sinh\kappa \tag{4.69}$$

$$\hat{\beta} = \hat{b}\cosh\kappa - \hat{a}^\dagger \sinh\kappa \tag{4.70}$$

for some κ to be determined.

Let us consider the commutation relations that $\hat{\alpha}$, $\hat{\alpha}^\dagger$, and $\hat{\beta}$, $\hat{\beta}^\dagger$ satisfy. $[\hat{\alpha}, \hat{\alpha}]$, $\left[\hat{\alpha}^\dagger, \hat{\alpha}^\dagger\right]$, $\left[\hat{\beta}, \hat{\beta}\right]$ and $\left[\hat{\beta}^\dagger, \hat{\beta}^\dagger\right]$ are trivially zero.

$$\begin{aligned}\left[\hat{\alpha}, \hat{\alpha}^\dagger\right] &= \left[c\hat{a} - s\hat{b}^\dagger, c\hat{a}^\dagger - s\hat{b}\right] \\ &= c^2\left[\hat{a}, \hat{a}^\dagger\right] + s^2\left[\hat{b}^\dagger, \hat{b}\right] - sc\left[\hat{a}, \hat{b}\right] - sc\left[\hat{b}^\dagger, \hat{a}^\dagger\right] \\ &= c^2 - s^2 \\ &= 1,\end{aligned} \tag{4.71}$$

where we have set $c \equiv \cosh\kappa$ and $s \equiv \sinh\kappa$. Similarly

$$\begin{aligned}\left[\hat{\beta}, \hat{\beta}^\dagger\right] &= \left[c\hat{b} - s\hat{a}^\dagger, c\hat{b}^\dagger - s\hat{a}\right] \\ &= c^2\left[\hat{b}, \hat{b}^\dagger\right] + s^2\left[\hat{a}^\dagger, \hat{a}\right] - sc\left[\hat{b}, \hat{a}\right] - sc\left[\hat{a}^\dagger, \hat{b}^\dagger\right] \\ &= c^2 - s^2 \\ &= 1.\end{aligned} \tag{4.72}$$

And so the same relations are satisfied.

Now, let us consider finding a value of κ to be chosen so that, when written in terms of $\hat{\alpha}$ and $\hat{\beta}$, there are no "anomalous" terms in $\hat{H}$ (i.e. no terms $\hat{\alpha}\hat{\beta}$ or $\hat{\alpha}^\dagger\hat{\beta}^\dagger$. In this way we will find the eigenvalues of the Hamiltonian.

In terms $\hat{\alpha}$ and $\hat{\beta}$, the Hamiltonian becomes

$$\begin{aligned}
\hat{H} &= \varepsilon\Big[\Big(c\hat{\alpha}^\dagger + s\hat{\beta}\Big)\Big(c\hat{\alpha} + s\hat{\beta}^\dagger\Big) + \Big(s\hat{\alpha} + c\hat{\beta}^\dagger\Big)\Big(s\hat{\alpha}^\dagger + c\hat{\beta}\Big)\Big] \\
&\quad + \Delta\Big[\Big(c\hat{\alpha}^\dagger + s\hat{\beta}\Big)\Big(s\hat{\alpha} + c\hat{\beta}^\dagger\Big) + \Big(s\hat{\alpha}^\dagger + c\hat{\beta}\Big)\Big(c\hat{\alpha} + s\hat{\beta}^\dagger\Big)\Big] \\
&= \hat{\alpha}^\dagger\hat{\alpha}\Big(\varepsilon c^2 + 2\Delta sc\Big) + \hat{\alpha}\hat{\alpha}^\dagger\Big(\varepsilon s^2\Big) + \hat{\alpha}^\dagger\hat{\beta}^\dagger\Big(\varepsilon sc + \Delta\Big(c^2 + s^2\Big)\Big) + \hat{\beta}^\dagger\hat{\alpha}^\dagger(\varepsilon sc) \\
&\quad + \hat{\beta}\hat{\alpha}\Big(\varepsilon sc + \Delta\Big(c^2 + s^2\Big)\Big) + \hat{\alpha}\hat{\beta}(\varepsilon sc) + \hat{\beta}\hat{\beta}^\dagger\Big(\varepsilon s^2 + 2\Delta sc\Big) + \hat{\beta}^\dagger\hat{\beta}\Big(\varepsilon c^2\Big).
\end{aligned} \tag{4.73}$$

For the irregular terms to vanish we hence require

$$\begin{aligned}
0 &= 2\varepsilon sc + \Delta\Big(c^2 + s^2\Big) \\
&= \varepsilon \sinh 2\kappa + \Delta \cosh 2\kappa,
\end{aligned} \tag{4.74}$$

and thus

$$\tanh 2\kappa = -\frac{\Delta}{\varepsilon}. \tag{4.75}$$

Now repeat to the problem for fermions. The first thing we will need to figure out is what kind of transformation preserves the anticommutation relations. If we choose a transformation

$$\hat{\alpha} = u\hat{a} + v\hat{b}^\dagger \tag{4.76}$$

$$\hat{\beta}^\dagger = -v\hat{a} + u\hat{b}^\dagger, \tag{4.77}$$

we find anticommutation relations for $\hat{\alpha}$ and $\hat{\beta}$ like e.g.:

$$\begin{aligned}
\Big\{\hat{\alpha}, \hat{\alpha}^\dagger\Big\} &= \Big\{u\hat{a} + v\hat{b}^\dagger, u\hat{a}^\dagger + v\hat{b}\Big\} \\
&= u^2\Big\{\hat{a}, \hat{a}^\dagger\Big\} + s^2\Big\{\hat{b}, \hat{b}\Big\} + uv\Big\{\hat{a}, \hat{b}\Big\} + uv\Big\{\hat{b}^\dagger, \hat{a}^\dagger\Big\} \\
&= u^2 + v^2.
\end{aligned} \tag{4.78}$$

Hence we find that we require

$$u^2 + v^2 = 1. \tag{4.79}$$

This lets us identify $u = \cos\kappa$ and $v = \sin\kappa$. An expansion of the Hamiltonian in the new basis

$$\begin{aligned}
\hat{H} &= \varepsilon\Big[\Big(c\hat{\alpha}^\dagger - s\hat{\beta}\Big)\Big(c\hat{\alpha} - s\hat{\beta}^\dagger\Big) + \Big(s\hat{\alpha} + c\hat{\beta}^\dagger\Big)\Big(s\hat{\alpha}^\dagger + c\hat{\beta}\Big)\Big] \\
&\quad + \Delta\Big[\Big(c\hat{\alpha}^\dagger - s\hat{\beta}\Big)\Big(s\hat{\alpha} + c\hat{\beta}^\dagger\Big) + \Big(s\hat{\alpha}^\dagger + c\hat{\beta}\Big)\Big(c\hat{\alpha} - s\hat{\beta}^\dagger\Big)\Big] \\
&= \hat{\alpha}^\dagger\hat{\alpha}\Big(\varepsilon c^2 + 2\Delta sc\Big) + \hat{\alpha}\hat{\alpha}^\dagger\Big(\varepsilon s^2\Big) + \hat{\alpha}^\dagger\hat{\beta}^\dagger\Big(-\varepsilon sc + \Delta\Big(c^2 - s^2\Big)\Big) + \hat{\beta}^\dagger\hat{\alpha}^\dagger(\varepsilon sc) \\
&\quad + \hat{\beta}\hat{\alpha}\Big(-\varepsilon sc + \Delta\Big(c^2 - s^2\Big)\Big) + \hat{\alpha}\hat{\beta}(\varepsilon sc) + \hat{\beta}\hat{\beta}^\dagger\Big(\varepsilon s^2 - 2\Delta sc\Big) + \hat{\beta}^\dagger\hat{\beta}\Big(\varepsilon c^2\Big).
\end{aligned} \tag{4.80}$$

leads to the requirement that

$$\begin{aligned}
0 &= 2\varepsilon sc - \Delta\Big(c^2 - s^2\Big) \\
&= \varepsilon \sin 2\kappa - \Delta \cos 2\kappa,
\end{aligned} \tag{4.81}$$

and thus

$$\tan 2\kappa = \frac{\Delta}{\varepsilon}. \tag{4.82}$$

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

$$
\begin{aligned}
\hat{\alpha} &= \hat{U}\hat{\alpha}\hat{U}^\dagger \\
\hat{\beta} &= \hat{U}\hat{b}\hat{U}^\dagger, \quad \hat{U}^\dagger = \hat{U}^{-1}.
\end{aligned} \tag{4.83}
$$

Let us first evaluate a few commutation relations.

$$
\begin{aligned}
\left[\hat{a}, \hat{U}\right]_\mp &= \exp\left(-\kappa\hat{b}\hat{a}\right)\left[\hat{a}, \hat{a}^\dagger\right]_\mp \frac{\partial}{\partial \hat{a}^\dagger} \exp\left(\kappa\hat{a}^\dagger\hat{b}^\dagger\right) \\
&= \exp\left(-\kappa\hat{b}\hat{a}\right)\kappa\hat{b}^\dagger \exp\left(\kappa\hat{a}^\dagger\hat{b}^\dagger\right) \\
&= \hat{U}\kappa\hat{b}^\dagger.
\end{aligned} \tag{4.84}
$$

In the first line we have used that the operators come in pairs and thus e.g. $\left[\hat{a}, \exp\left(-\kappa\hat{b}\hat{a}\right)\right]_\mp = 0$.

$$
\begin{aligned}
\therefore \hat{\alpha} &= \hat{U}\hat{a}\hat{U}^\dagger \\
&= \pm\left[\hat{a}, \hat{U}\right]_\mp \hat{U}^\dagger \pm \hat{a} \\
\hat{a} &= \pm\hat{\alpha} + \kappa\hat{\beta}^\dagger,
\end{aligned} \tag{4.85}
$$

where the $\pm$ correspond to the bosonic and fermionic cases, respectively. Similarly

$$
\begin{aligned}
\hat{a}^\dagger &= \pm\hat{\alpha}^\dagger + \kappa^\dagger\hat{\beta}, \\
\hat{b} &= \kappa\hat{\alpha}^\dagger \pm \hat{\beta}, \\
\hat{b}^\dagger &= \kappa^\dagger\hat{\alpha} \pm \hat{\beta}^\dagger.
\end{aligned} \tag{4.86}
$$

Now let us rewrite the Hamiltonian in terms of $\hat{\alpha}$ and $\hat{\beta}$ (assuming that k is real):

$$
\begin{aligned}
\hat{H} = \varepsilon&\left[\hat{\alpha}^\dagger\hat{\alpha} \mp \kappa\left(\hat{\alpha}^\dagger\hat{\beta}^\dagger + \hat{\beta}\hat{\alpha}\right) + \kappa^2\hat{\beta}\hat{\beta}^\dagger + \hat{\beta}^\dagger\hat{\beta} \pm \kappa\left(\hat{\beta}^\dagger\hat{\alpha}^\dagger + \hat{\alpha}\hat{\beta}\right) + \kappa^2\hat{\alpha}\hat{\alpha}^\dagger\right] \\
&+ \Delta\left[\pm\kappa\left(\hat{\alpha}^\dagger\hat{\alpha} - \hat{\beta}\hat{\beta}^\dagger\right) - \hat{\alpha}^\dagger\hat{\beta}^\dagger + \kappa^2\hat{\beta}\hat{\alpha} \pm \kappa\left(\hat{\alpha}\hat{\alpha}^\dagger - \hat{\beta}^\dagger\hat{\beta}\right) - \hat{\beta}\hat{\alpha} + \kappa^2\hat{\alpha}^\dagger\hat{\beta}^\dagger\right] \\
= \varepsilon&\left[\hat{\alpha}^\dagger\hat{\alpha}2\kappa\left(\hat{\alpha}^\dagger\hat{\beta}^\dagger + \hat{\beta}\hat{\alpha}\right) + \kappa^2\hat{\beta}\hat{\beta}^\dagger + \hat{\beta}^\dagger\hat{\beta} + \kappa^2\hat{\alpha}\hat{\alpha}^\dagger\right] \\
&+ \Delta\left[\pm\kappa\left(\hat{\alpha}^\dagger\hat{\alpha} - \hat{\beta}\hat{\beta}^\dagger\right) - \hat{\alpha}^\dagger\hat{\beta}^\dagger + \kappa^2\hat{\beta}\hat{\alpha} \pm \kappa\left(\hat{\alpha}\hat{\alpha}^\dagger - \hat{\beta}^\dagger\hat{\beta}\right) - \hat{\beta}\hat{\alpha} + \kappa^2\hat{\alpha}^\dagger\hat{\beta}^\dagger\right]
\end{aligned} \tag{4.87}
$$

Hence we can eliminate the non-number conserving terms provided

$$
0 = \left(1 - \kappa^2\right)\Delta \pm 2\kappa\varepsilon, \tag{4.88}
$$

which we can easily arrange.

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.

4.4.1 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[12]. 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 non-interacting particles in Eq. (4.16). In general, the action of an operator $\hat{\mathrm{A}}$ on the single particle states may written in terms of the matrix element $\langle\varphi_\alpha|\hat{\mathrm{A}}|\varphi_\beta\rangle$,

$$\hat{\mathrm{A}} = \sum_\alpha |\varphi_\alpha\rangle \langle\varphi_\alpha|\hat{\mathrm{A}}|\varphi_\beta\rangle\,. \tag{4.89}$$

In words, the action of $\hat{\mathrm{A}}$ is to take the particle from state $|\varphi_\beta\rangle$ to a superposition of states with amplitudes given by the matrix elements $A_{\alpha\beta} \equiv \langle\varphi_\alpha|\hat{\mathrm{A}}|\varphi_\beta\rangle$. Now it's not hard to see that this action can be replicated on the one particle states $\hat{a}^\dagger_\alpha |\mathrm{VAC}\rangle$ with

$$\hat{A} \equiv \sum_{\alpha,\beta} \hat{a}^\dagger_\alpha \hat{a}_\beta \tag{4.90}$$

(for the moment we'll use an upright case for the non-second quantised operator to make the distinction clear, but later we'll drop this). To see this, first note that Eq. (4.45) can be generalised to

$$\begin{aligned}\left[\hat{a}_\alpha, \hat{a}^\dagger_\beta \hat{a}_\gamma\right] &= \delta_{\alpha\beta}\hat{a}_\gamma \\ \left[\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta \hat{a}_\gamma\right] &= -\delta_{\alpha\gamma}\hat{a}^\dagger_\beta.\end{aligned} \tag{4.91}$$

Using the second of these relations, together with the fact that $\hat{A}\,|\mathrm{Vac}\rangle = 0$

$$\begin{aligned}\hat{A}\hat{a}^\dagger_\beta\,|\mathrm{VAC}\rangle &= \left(\left[\hat{A}, \hat{a}^\dagger_\beta\right] + \hat{a}^\dagger_\beta \hat{A}\right)|\mathrm{VAC}\rangle \\ &= \sum_\alpha A_{\alpha\beta}\hat{a}^\dagger_\alpha\,|\mathrm{VAC}\rangle\,,\end{aligned} \tag{4.92}$$

which is precisely Eq. (4.89).

As an example, let us consider

Notice that $\hat{A}$ *looks* formally like the expectation value of $\hat{\mathrm{A}}$ in a single particle state $\sum_\alpha \hat{a}\,|\varphi_\alpha\rangle$. The difference, of course, is that the $\hat{a}_\alpha$ 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 $\hat{H}$ has a second quantised representation formally identical to the expectation value of its single particle counterpart* $\hat{\mathrm{A}}$.

[12] More formally, each term acts on one factor in the product $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1$ of single particle Hilbert spaces.

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. (4.16). According to the above prescription, this should have the second quantised form

$$\hat{H} \equiv \sum_{\alpha,\beta} \langle\varphi_\alpha|\hat{\mathrm{H}}|\varphi_\beta\rangle\, \hat{a}^\dagger_\alpha \hat{a}_\beta, \tag{4.93}$$

where $\hat{\mathrm{H}}$ is the single particle Hamiltonian $\hat{\mathrm{H}} = -\frac{\hbar^2}{2m}\nabla_i^2 + V(\mathbf{r}_i)$. This takes on a very simple form if the basis $\{|\varphi_\alpha\rangle\}$ is just the eigenbasis of this Hamiltonian, in which case $\langle\varphi_\alpha|\hat{\mathrm{H}}|\varphi_\beta\rangle = E_\alpha\delta_{\alpha\beta}$ and

$$\hat{H} \equiv \sum_\alpha E_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha = \sum_\alpha E_\alpha \hat{N}_\alpha. \tag{4.94}$$

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. (4.20).

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

$$\begin{aligned}\hat{H} &= \int d\mathbf{r}\left[-\frac{\hbar^2}{2m}\hat{\psi}^\dagger(\mathbf{r})\nabla^2\hat{\psi}(\mathbf{r} + V(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\right] \\ &= \int d\mathbf{r}\left[\frac{\hbar^2}{2m}\boldsymbol{\nabla}\hat{\psi}^\dagger(\mathbf{r})\cdot\boldsymbol{\nabla}\hat{\psi}(\mathbf{r}) + V(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\right],\end{aligned} \tag{4.95}$$

where in the second line we have integrated by parts, assuming that boundary terms at infinity vanish. The equality of (4.95) and (4.94) may be seen by using Eq. (4.59).

The Heisenberg equation of motion corresponding to Eq. (4.95) is

$$\begin{aligned}i\hbar\partial_t\hat{\psi}(\mathbf{r},t) &= -\left[\hat{H},\hat{\psi}(\mathbf{r},t)\right] \\ &= -\frac{\hbar^2}{2m}\nabla^2\hat{\psi}(\mathbf{r},t) + \hat{V}(\mathbf{r})\hat{\psi}(\mathbf{r},t),\end{aligned} \tag{4.96}$$

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

$$\hat{\rho}(\mathbf{x}) \equiv \delta(\mathbf{x}-\mathbf{r}). \tag{4.97}$$

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 quantised form of the operator is then

$$\hat{\rho}(\mathbf{x}) \equiv \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x}). \tag{4.98}$$

As a check, integrating over position should give the total number of particles

$$\hat{N} = \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x}) = \sum_\alpha \hat{a}^\dagger_\alpha\hat{a}_\alpha = \sum_\alpha \hat{\mathrm{N}}_\alpha, \tag{4.99}$$

as it does! Another useful thing to know is the expectation value of the density on a basis state $|N_0, N_1, \cdots\rangle$

$$\langle N_0, N_1, \cdots|\hat{\rho}(\mathbf{r})|N_0, N_1, \cdots\rangle = \sum_\alpha N_\alpha |\varphi_\alpha(\mathbf{x})|^2, \tag{4.100}$$

which is most easily proved by substituting the representation (4.59). This seems like a very reasonable generalisation 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 quantised form

$$\hat{\mathbf{J}}(\mathbf{r}) = -i\frac{\hbar}{2m}\Big[\hat{\psi}^\dagger(\mathbf{r})\Big(\boldsymbol{\nabla}\hat{\psi}(\mathbf{r})\Big) - \Big(\boldsymbol{\nabla}\hat{\psi}(\mathbf{r})\Big)\hat{\psi}(\mathbf{r})\Big]. \tag{4.101}$$

Often we consider the Fourier components of the density or current

$$\boxed{\begin{aligned} \hat{\rho}_{\mathbf{q}} &\equiv \int \mathrm{d}\mathbf{r}\, \hat{\rho}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} = \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}-\mathbf{q}/2}\hat{a}_{\mathbf{k}+\mathbf{q}/2} && (4.102)\\ \hat{\mathbf{J}}_{\mathbf{q}} &\equiv \int \mathrm{d}\mathbf{r}\, \hat{\mathbf{J}}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} = \sum_{\mathbf{k}} \frac{\mathbf{k}}{m}\hat{a}^\dagger_{\mathbf{k}-\mathbf{q}/2}\hat{a}_{\mathbf{k}+\mathbf{q}/2}. && (4.103)\end{aligned}}$$

The $\mathbf{q} = \mathbf{0}$ modes are just the total particle number and $\frac{1}{m}$ times the total momentum, respectively.

The operator for the density of spin of a system of spin-1/2 fermions is

$$\hat{\mathbf{S}}(\mathbf{r}) = \frac{1}{2}\sum_{s,s'} \hat{\psi}^\dagger_s(\mathbf{r})\hat{\boldsymbol{\sigma}}_{ss'}\hat{\psi}_{s'}(\mathbf{r}), \tag{4.104}$$

where $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ are the Pauli matrices and $\hat{\psi}^\dagger(\mathbf{r})$, $\hat{\psi}(\mathbf{r})$ satisfy

$$\Big\{\hat{\psi}_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big\} = \delta_{s,s'}\delta(\mathbf{r} - \mathbf{r}'). \tag{4.105}$$

Now to consider the commutation relations $\Big[\hat{S}_i(\mathbf{r}), \hat{S}_j(\mathbf{r}')\Big]$,

$$\begin{aligned}
\Big[\hat{S}_i(\mathbf{r}), \hat{S}_j(\mathbf{r}')\Big] &= \frac{1}{4}\sum_{s,s',t,t'} \Big[\hat{\psi}^\dagger(\mathbf{r})\hat{\sigma}_{i s,s'}\hat{\psi}_{s'}(\mathbf{r}),\, \hat{\psi}^\dagger_t(\mathbf{r}')\hat{\sigma}_{j t,t'}\hat{\psi}_{t'}(\mathbf{r}')\Big]\\
&= \frac{1}{4}\sum_{s,s',t,t'} \hat{\sigma}_{i s,s'}\hat{\sigma}_{j t,t'}\Big[\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}_{s'}(\mathbf{r}),\, \hat{\psi}^\dagger_t(\mathbf{r}')\hat{\psi}_{t'}(\mathbf{r}')\Big]\\
&= \frac{1}{4}\sum_{s,s',t,t'} \hat{\sigma}_{i s,s'}\hat{\sigma}_{j t,t'}\Big(\hat{\psi}^\dagger_s(\mathbf{r})\Big\{\Big[\hat{\psi}_{s'}(\mathbf{r}), \hat{\psi}^\dagger_t(\mathbf{r}')\Big]\hat{\psi}_{t'}(\mathbf{r}') + \hat{\psi}^\dagger_t\Big[\hat{\psi}_{s'}(\mathbf{r}), \hat{\psi}_{t'}(\mathbf{r})\Big]\Big\}\\
&\quad + \Big\{\Big[\hat{\psi}^\dagger_s(\mathbf{r}), \hat{\psi}^\dagger_t(\mathbf{r}')\Big]\hat{\psi}_{t'}(\mathbf{r}') + \hat{\psi}^\dagger_t(\mathbf{r}')\Big[\hat{\psi}^\dagger_s(\mathbf{r}), \hat{\psi}_{t'}(\mathbf{r}')\Big]\Big\}\hat{\psi}_{s'}(\mathbf{r})\Big).
\end{aligned} \tag{4.106}$$

Now we make use of

$$\Big[\hat{\psi}^\dagger_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big] = \Big\{\hat{\psi}^\dagger_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big\} - 2\hat{\psi}^\dagger_{s'}(\mathbf{r}')\hat{\psi}^\dagger_s(\mathbf{r}) \tag{4.107}$$

and note that all the terms not containing anticommutators conveniently cancel out. We also make use of the anticommutation relation

$$\Big\{\hat{\psi}_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big\} = \delta_{s,s'}\delta(\mathbf{r}-\mathbf{r}') \tag{4.108}$$

$$\Big\{\hat{\psi}_s(\mathbf{r}), \hat{\psi}_{s'}(\mathbf{r}')\Big\} = \Big\{\hat{\psi}^\dagger_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big\} = 0 \tag{4.109}$$

and thus get to

$$\begin{aligned}
\Big[\hat{S}_i(\mathbf{r}), \hat{S}_j(\mathbf{r}')\Big] &= \frac{1}{4}\sum_{s,s',t,t'} \hat{\sigma}_{i s,s'}\hat{\sigma}_{j t,t'}\delta(\mathbf{r}-\mathbf{r}')\Big(\delta_{s',t}\hat{\psi}^\dagger_s(\mathbf{r})\hat{\psi}_{t'}(\mathbf{r}') - \delta_{s,t'}\hat{\psi}^\dagger_t(\mathbf{r}')\hat{\psi}_{s'}(\mathbf{r})\Big)\\
&= \frac{1}{4}\sum_{s,s',t'} \delta(\mathbf{r}-\mathbf{r}')\Big(\hat{\sigma}_{i s,s'}\hat{\sigma}_{j s',t'}\hat{\psi}^\dagger_s(\mathbf{r})\hat{\psi}_{t'}(\mathbf{r}) - \hat{\sigma}_{i s,s'}\hat{\sigma}_{j t',s'}\hat{\psi}^\dagger_{t'}(\mathbf{r})\hat{\psi}_s(\mathbf{r})\Big)\\
&= \frac{1}{4}\delta(\mathbf{r}-\mathbf{r}')\sum_{s,s',t'} \hat{\psi}^\dagger_s(\mathbf{r})\hat{\psi}_{t'}(\mathbf{r})\Big(\hat{\sigma}_{i s,s'}\hat{\sigma}_{j s',t'} - \hat{\sigma}_{j s,s'}\hat{\sigma}_{i s',t'}\Big)\\
&= \frac{1}{4}\delta(\mathbf{r}-\mathbf{r}')\sum_{s,s',t'} \hat{\psi}^\dagger_s(\mathbf{r})\hat{\psi}_{t'}(\mathbf{r})[\hat{\sigma}_i, \hat{\sigma}_j]_{s,t'}\\
&= \frac{1}{2}\varepsilon_{ijk}\delta(\mathbf{r}-\mathbf{r}')\sum_{s,s',t'} \hat{\psi}^\dagger_s\hat{\sigma}_{k s,t'}\hat{\psi}_{t'}(\mathbf{r})\\
&= i\varepsilon_{ijk}\delta(\mathbf{r}-\mathbf{r}')\hat{S}_k(\mathbf{r})
\end{aligned} \tag{4.110}$$

This is what we were expecting in the first place.

For the Hamiltonian

$$\hat{H} = \frac{\hbar^2}{2m}\sum_s \int \mathrm{d}^3\mathbf{r}\, \boldsymbol{\nabla}\hat{\psi}^\dagger_s \boldsymbol{\nabla}\hat{\psi}_s, \tag{4.111}$$

find the form of the Heisenberg equation of motion

$$\partial_t \hat{\mathbf{S}}(\mathbf{r},t) = i\Big[\hat{H}, \hat{\mathbf{S}}(\mathbf{r},t)\Big]/\hbar. \tag{4.112}$$

We can first expand the commutator

$$\begin{aligned}
\Big[\int \mathrm{d}^3\mathbf{r}\, \boldsymbol{\nabla}\hat{\psi}^\dagger_s(\mathbf{r})\boldsymbol{\nabla}\hat{\psi}_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\hat{\psi}_{s''}(\mathbf{r})\Big] = \int \mathrm{d}^3 \Big\{&\boldsymbol{\nabla}\hat{\psi}^\dagger_s(\mathbf{r})\Big[\boldsymbol{\nabla}\hat{\psi}_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big]\hat{\psi}_{s''}(\mathbf{r}')\\
&+ \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big[\boldsymbol{\nabla}\hat{\psi}^\dagger_s(\mathbf{r}), \hat{\psi}_{s''}(\mathbf{r}')\Big]\boldsymbol{\nabla}\hat{\psi}_s(\mathbf{r})\Big\}.
\end{aligned} \tag{4.113}$$

Upon integration by parts with vanishing boundary terms,

$$\begin{aligned}
\Big[\int \mathrm{d}^3\mathbf{r}\, \boldsymbol{\nabla}\hat{\psi}^\dagger_s(\mathbf{r})\boldsymbol{\nabla}\hat{\psi}_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\hat{\psi}_{s''}(\mathbf{r})\Big] &= -\int \mathrm{d}^3\,\mathrm{d}\mathbf{r}\,\Big\{\nabla^2\hat{\psi}^\dagger_s(\mathbf{r})\Big[\hat{\psi}_s(\mathbf{r}), \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big]\hat{\psi}_{s''}(\mathbf{r}')\\
&\qquad + \hat{\psi}^\dagger_{s'}(\mathbf{r}')\Big[\hat{\psi}^\dagger_s, \hat{\psi}_{s''}(\mathbf{r}')\Big]\nabla^2\hat{\psi}_s(\mathbf{r})\Big\}\\
&= -\int \mathrm{d}^3\,\mathrm{d}\mathbf{r}\,\Big\{\delta_{s,s'}\delta(\mathbf{r}-\mathbf{r}')\nabla^2\hat{\psi}^\dagger_s(\mathbf{r})\hat{\psi}_{s''}(\mathbf{r}')\\
&\qquad + \delta_{s,s''}\delta(\mathbf{r}-\mathbf{r}')\hat{\psi}^\dagger_{s'}(\mathbf{r}')\nabla^2\hat{\psi}_s(\mathbf{r})\Big\}\\
&= -\delta_{s,s'}\nabla^2_{\mathbf{r}'}\hat{\psi}^\dagger_s(\mathbf{r}')\hat{\psi}_{s''}(\mathbf{r}') + \delta_{s,s''}\hat{\psi}^\dagger_{s'}(\mathbf{r}')\nabla^2_{\mathbf{r}'}\hat{\psi}(\mathbf{r}').
\end{aligned} \tag{4.114}$$

Throughout ∇^2 only operates on $\mathbf{r}$, whilst in the last line $\nabla^2_{\mathbf{r}'}$ operates on $\mathbf{r}'$. Using the above findings we see that:

$$\begin{aligned}\partial_t \hat{S}_j(\mathbf{r}) &= -\frac{i\hbar}{4m}\sum_{s',s''}\hat{\sigma}_{j\,s',s''}\nabla^2\Big(\hat{\psi}^\dagger_{s'}(\mathbf{r})\hat{\psi}_{s''}(\mathbf{r})\Big)\\ &= -\frac{i\hbar}{2m}\nabla^2\hat{S}_j(\mathbf{r}).\end{aligned} \tag{4.115}$$

This clearly reminds us of the free particle Schrödinger equation.

4.4.2 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**

$$g(\mathbf{r},\mathbf{r}') \equiv \left\langle \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}')\right\rangle. \tag{4.116}$$

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 $\Psi(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N)$ we have

$$g(\mathbf{r},\mathbf{r}') = N\int \mathrm{d}\mathbf{r}_2\cdots\mathrm{d}\mathbf{r}_N\,\Psi^*(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N)\Psi(\mathbf{r}',\mathbf{r}_2,\cdots,\mathbf{r}_N). \tag{4.117}$$

In other words, $g(\mathbf{r},\mathbf{r}')$ arises from the N particle pure state density matrix $\rho = |\Psi\rangle\langle\Psi|$ by "tracing out" $N-1$ particle coordinates.

A slight generalisation of the above calculation for the density gives for the state $|N_0,N_1,\cdots\rangle$

$$g(\mathbf{r},\mathbf{r}') = \sum_\alpha N_\alpha\varphi^*_\alpha(\mathbf{r})\varphi_\alpha(\mathbf{r}'). \tag{4.118}$$

Let's evaluate this for the ground state of non-interacting Fermi gas. Recall that in this case $N_{\mathbf{k}} = 1$ for $|\mathbf{k}| < k_{\mathrm{F}}$, and 0 otherwise. Thus we have

$$\begin{aligned}g(\mathbf{r},\mathbf{r}') = \frac{1}{V}\sum_{|\mathbf{k}|<k_{\mathrm{F}}} e^{\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} &= \int_{|\mathbf{k}|<k_{\mathrm{F}}}\frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}e^{\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}\\ &= \frac{k_{\mathrm{F}}^3}{2\pi^2}\left[\frac{\sin(k_{\mathrm{F}}|\mathbf{r}'-\mathbf{r}|)}{(k_{\mathrm{F}}|\mathbf{r}'-\mathbf{r}|)^3} - \frac{\cos(k_{\mathrm{F}}|\mathbf{r}'-\mathbf{r}|)}{(k_{\mathrm{F}}|\mathbf{r}'-\mathbf{r}|)^2}\right].\end{aligned} \tag{4.119}$$

Note that $g(\mathbf{r},\mathbf{r}) = \frac{k_{\mathrm{F}3}}{6\pi^2} = n$, 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 $|\mathbf{r}-\mathbf{r}'| \to \infty$.

Fig. 4.3: Single particle density matrix for the Fermi gas.

4.4.3 Correlation functions

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

$$\hat{C}_\rho(\mathbf{r},\mathbf{r}') \equiv \langle : \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}') : \rangle . \tag{4.120}$$

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

$$\hat{a}_\alpha \hat{a}^\dagger_\beta = \delta_{\alpha\beta} \pm \hat{a}^\dagger_\beta \hat{a}_\alpha \quad \text{while} \quad : \hat{a}_\alpha \hat{a}^\dagger_\beta := \pm \hat{a}^\dagger_\beta \hat{a}_\alpha, \tag{4.121}$$

with the upper sign for bosons, and the lower for fermions.

In the present case you can easily convince yourself that

$$\langle \hat{\rho}(\mathbf{r}\hat{\rho}(\mathbf{r}')\rangle = \langle : \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}') : \rangle + \delta(\mathbf{r}-\mathbf{r}') \langle \hat{\rho}(\mathbf{r}) \rangle . \tag{4.122}$$

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

$$N_i = \int_{\text{cube } i} \mathrm{d}\mathbf{r}\, \hat{\rho}(\mathbf{r}). \tag{4.123}$$

Since N_i is only 0 or 1 by assumption, the probability of cube i being occupied is

$$P(\text{cube } i \text{ occupied}) = \langle N_i \rangle , \tag{4.124}$$

that is, the mean occupancy. Likewise the probability of having cubes i and j occupied is

$$P(i \text{ and } j \text{ occupied}) = \langle N_i N_j \rangle \int_{\text{cube } i} \mathrm{d}\mathbf{r} \int_{\text{cube } j} \mathrm{d}\mathbf{r}' \langle \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}') \rangle . \tag{4.125}$$

This tells us that $\langle \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')\rangle$ 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 $i = j$

$$\langle N_i N_j \rangle = \left\langle N_i^2 \right\rangle = \langle N_i \rangle , \tag{4.126}$$

which shows that $\langle \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')\rangle$ always has an additional contribution $\delta(\mathbf{r}-\mathbf{r}')\langle \hat{\rho}(\mathbf{r})\rangle$, determined by the mean density. Eq. (4.122) 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 $\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}')$ to the original state, call it $|\Psi\rangle$. This has the effect of picking out that part of the wavefunction where two particles are localised at these positions. The probability (density) of finding two particles at these locations is then the squared modulus of the resulting state, that is

$$\left| \hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}') |\Psi\rangle \right|^2 = \left\langle \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}') \right\rangle , \tag{4.127}$$

which is just the normal ordered form $\langle : \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}') : \rangle$?

With the physical meaning of $\hat{C}_\rho(\mathbf{r},\mathbf{r}')$ established, let's proceed to the calculation. As in the derivation of Eq. (4.100), we substitute the representation (4.59) to give

$$\langle \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')\rangle = \sum_{\alpha,\beta,\gamma,\delta} \varphi_\alpha^*(\mathbf{r})\varphi_\beta(\mathbf{r})\varphi_\gamma^*(\mathbf{r}')\varphi_\delta(\mathbf{r}') \left\langle \hat{a}_\alpha^\dagger \hat{a}_\beta \hat{a}_\gamma^\dagger \hat{a}_\delta \right\rangle \tag{4.128}$$

If we are considering the expectation in a state of the form $|N_0, N_1, \cdots\rangle$, 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

$$\alpha = \beta,\ \gamma = \delta, \text{ or} \tag{4.129}$$
$$\alpha = \delta,\ \beta = \gamma, \tag{4.130}$$

which give rise to two groups of terms. The first contains the average $\left\langle \hat{a}_\alpha^\dagger \hat{a}_\alpha \hat{a}_\gamma^\dagger \hat{a}_\gamma \right\rangle = N_\alpha N_\gamma$, while the second involves

$$\left\langle \hat{a}_\alpha^\dagger \hat{a}_\gamma \hat{a}_\gamma^\dagger \hat{a}_\alpha \right\rangle = N_\alpha(1 \pm N_\gamma). \tag{4.131}$$

Here we have used

$$\hat{a}^\dagger \hat{a}_\alpha = N_\alpha \tag{4.132}$$
$$\hat{a}_\gamma \hat{a}_\gamma^\dagger = 1 \pm \hat{a}_\gamma^\dagger \hat{a}_\gamma = 1 \pm N_\gamma. \tag{4.133}$$

Overall we have[13]

$$\begin{aligned}\langle \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')\rangle = &\sum_{\alpha,\gamma} \varphi_\alpha^*(\mathbf{r})\varphi_\alpha(\mathbf{r})\varphi_\gamma^*(\mathbf{r}')\varphi_\gamma(\mathbf{r}')N_\alpha N_\gamma \\ &+ \sum_{\alpha,\gamma} \varphi_\alpha^*(\mathbf{r})\varphi_\gamma(\mathbf{r})\varphi_\gamma^*(\mathbf{r}')\varphi_\alpha(\mathbf{r}')N_\alpha(1 \pm N_\gamma).\end{aligned} \tag{4.134}$$

This illustrates a general result, known as **Wick's theorem**, that expectation values in a state $|N_0, N_1, \cdots\rangle$ can be computed by pairing the indices of creation and annihilation operators in all possible ways and using Eq. (4.133).

Using the completeness relation Eq. (4.60) the above result can be written

$$\langle \hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')\rangle = \delta(\mathbf{r}-\mathbf{r}')\langle \hat{\rho}(\mathbf{r})\rangle + \langle \hat{\rho}(\mathbf{r})\rangle \langle \hat{\rho}(\mathbf{r}')\rangle \pm g(\mathbf{r},\mathbf{r}')g(\mathbf{r}',\mathbf{r}). \tag{4.135}$$

or

$$\boxed{\hat{C}_\rho(\mathbf{r},\mathbf{r}') = \langle \hat{\rho}(\mathbf{r})\rangle \langle \hat{\rho}(\mathbf{r}')\rangle \pm g(\mathbf{r},\mathbf{r}')g(\mathbf{r}',\mathbf{r}).} \tag{4.136}$$

For the fermion case, we see that the correlation function vanishes as the separation $|\mathbf{r}-\mathbf{r}'| \to 0$, because $g(\mathbf{r},\mathbf{r})$ (See Fig. 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.

[13] 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 normalised plane waves if you are not sure).

Fig. 4.4: Density correlation function for the Fermi gas.

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.

Note when we have a Bose condensate $g(\mathbf{r},\mathbf{r}')$ tends to a finite value as $|\mathbf{r}-\mathbf{r}'| \to \infty$.

4.4.4 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

$$\hat{H}_{\text{int}} = \sum_{i<j}^{N} U(\mathbf{r}_i - \mathbf{r}_j). \tag{4.137}$$

Here $U(\mathbf{r}_i - \mathbf{r}_j)$ 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 quantised representation: $\rho(\mathbf{x}) = \sum_i^N \delta(\mathbf{x}-\mathbf{r}_i)$, we see that

$$\hat{H}_{\text{int}} \stackrel{?}{=} \frac{1}{2} \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}'\, \hat{\rho}(\mathbf{r}) U(\mathbf{r}-\mathbf{r}') \hat{\rho}(\mathbf{r}') \tag{4.138}$$

almost replicates Eq. (4.137). 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 $1/2$ ensures that we only sum over each pair once. The problem with Eq. (4.138), however, is that it includes the terms with $i = j$ that are excluded from Eq. (4.137), that is, it allows a particle to interact with itself! From **??** you will recall that it is precisely these terms that are responsible for generating the δ-function contribution to Eq. (4.135). Here, as before, the remedy is to normal order the operators

$$\hat{H}_{\text{int}} = \frac{1}{2} \int \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}'\, : \hat{\rho}(\mathbf{r}) U(\mathbf{r}-\mathbf{r}') \hat{\rho}(\mathbf{r}') : \; = \frac{1}{2} \int \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}'\, \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') U(\mathbf{r}-\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}).$$

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 quantisation for bosons, saw the existence of the above simple prescription in quantum mechanics as a particular benefit. We have taken the more usual modern approach (in non-relativistic physics) of assuming interactions between pairs only at the outset.

Using Eq. (4.136) we can immediately write down the expectation value of $\hat{H}_{\text{int}}$ in a state $|N_0, N_1, \cdots\rangle$

$$\left\langle \hat{H}_{\text{int}} \right\rangle = \frac{1}{2} \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}'\, \langle \hat{\rho}(\mathbf{r}) \rangle\, U(\mathbf{r}-\mathbf{r}')\, \langle \hat{\rho}(\mathbf{r}') \rangle \pm \frac{1}{2} \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}') g(\mathbf{r},\mathbf{r}') g(\mathbf{r}',\mathbf{r}). \tag{4.139}$$

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 quantised Hamiltonian, including an external potential and pairwise interactions

$$\boxed{\begin{aligned}\hat{H} = &\int d\mathbf{r}\left[\frac{\hbar^2}{2m}\boldsymbol{\nabla}\hat{\psi}^\dagger(\mathbf{r})\cdot\boldsymbol{\nabla}\hat{\psi} + \hat{V}(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\right] \\ &+ \frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})U(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}).\end{aligned}} \tag{4.140}$$

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 non-interacting 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

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) = \prod_i^N \varphi_0(\mathbf{r}_i), \tag{4.141}$$

which we can write in second quantised notation as

$$|\Psi\rangle = \frac{1}{\sqrt{N!}}\left(\hat{a}_0^\dagger\right)^N |\mathrm{VAC}\rangle\,, \tag{4.142}$$

where $\hat{a}_0^\dagger$ 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. 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 single well and adiabatically splitting in two. We can write such a state as

$$\left|\bar{N}_L, \bar{N}_R\right\rangle_\theta \equiv \frac{1}{\sqrt{N!}}\left[\sqrt{\frac{\bar{N}_L}{N}}e^{-i\theta/2}\hat{a}_L^\dagger + \sqrt{\frac{\bar{N}_R}{N}}e^{i\theta/2}\hat{a}_R^\dagger\right]^N |\mathrm{VAC}\rangle\,, \tag{4.143}$$

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. (4.143) with the wavefunctions $\varphi_{L,R}$ evolving freely. We compute the subsequent expectation value of the density using the second quantised representation

$$\hat{\rho}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}), \quad \hat{\psi}(\mathbf{r}) = \varphi_L(\mathbf{r})\hat{a}_L + \varphi_R(\mathbf{r})\hat{a}_R + \cdots\,, \tag{4.144}$$

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

$$\langle\hat{\rho}(\mathbf{r},t)\rangle_\theta = \bar{N}_L|\varphi_L(\mathbf{r},t)|^2 + \bar{N}_R|\varphi_R(\mathbf{r},t)|^2 + \underbrace{2\sqrt{\bar{N}_L\bar{N}_R}\,\mathrm{Re}\Big\{e^{i\theta}\varphi_L^*(\mathbf{r},t)\varphi_R(\mathbf{r},t)\Big\}}_{\equiv\rho_{\mathrm{int}}(\mathbf{r},t)}. \quad (4.145)$$

If the clouds begin to overlap, the last term in Eq. (4.145) 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 $d \gg R_0$

$$\varphi_{L,R}(\mathbf{r},t) = \frac{1}{(\pi R_t^2)^{3/4}}\exp\left(-\frac{(\mathbf{r}\pm\mathbf{d}/2)^2(1-i\hbar t/mR_0^2)}{2R_t^2}\right), \quad (4.146)$$

with

$$R_t^2 = R_0^2 + \left(\frac{\hbar t}{mR_0}\right)^2. \quad (4.147)$$

Eq. (4.146) 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.(4.146) gives

$$|\varphi_{L,R}(\mathbf{r},t\to\infty)|^2 \propto \exp\left[-\left(\frac{mR_0[\mathbf{r}\pm\mathbf{d}/2]}{\hbar t}\right)^2\right], \quad (4.148)$$

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 $n(\mathbf{p})\equiv\hat{a}_{\mathbf{p}}^\dagger\hat{a}_{\mathbf{p}}$ before expansion.

The final term of Eq. (4.145) is the

$$\rho_{\mathrm{int}}(\mathbf{r},t) = A(\mathbf{r},t)\cos\left(\theta + \frac{\hbar\mathbf{r}\cdot\mathbf{d}}{mR_0^2R_t^2}t\right) \quad (4.149)$$

$$A(\mathbf{r},t) = \frac{2\sqrt{\bar{N}_L\bar{N}_R}}{\pi^{3/2}R_t^2}\exp\left(-\frac{\mathbf{r}^2+\mathbf{d}^2/4}{R_t^2}\right). \quad (4.150)$$

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[14]

$$|N_L,N_R\rangle_F \equiv \frac{1}{\sqrt{N_L!N_R!}}\left(\hat{a}_L^\dagger\right)^{N_L}\left(\hat{a}_R^\dagger\right)_{N_R}|\mathrm{VAC}\rangle\,. \quad (4.151)$$

[14]The F is for Fock, as product states are sometimes known as **Fock states**.

Computing the density in the same way yields

$$\langle \hat{\rho}(\mathbf{r},t)\rangle_F = N_L|\varphi_L(\mathbf{r},t)|^2 + N_R|\varphi_R(\mathbf{r},t)|^2, \tag{4.152}$$

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 $\hat{\rho}(\mathbf{r})$ but rather the measured value of some observable(s) $\hat{\rho}(\mathbf{r})$. 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.

Fig. 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.

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 $n(\mathbf{p}) \equiv \hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}}$, 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 4.6, 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

$$\prod_i \hat{a}^\dagger_i \left|\mathrm{VAC}\right\rangle, \tag{4.153}$$

where $\hat{a}^\dagger_i$ creates a particle localised at site $\mathbf{r}_i$ in the lattice, with (let's say) Gaussian wavefunction

$$\varphi_i(\mathbf{r}) = \frac{1}{(\pi R^2)^{3/4}}\exp\left(-\frac{(\mathbf{r}-\mathbf{r}_i)^2}{2R^2}\right) \tag{4.154}$$

Fig. 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.

Chapter **5**

Density Matrices

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

$$|\hat{\mathbf{n}}\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} \end{pmatrix}. \tag{5.1}$$

This state has the property that it is an eigenstate of $\hat{\mathbf{n}} \cdot \hat{\mathbf{S}}$ with eigenvalue $+\hbar/2$, where

$$\hat{\mathbf{n}} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}. \tag{5.2}$$

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 $\hat{\mathbf{n}}$ 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 $P(\hat{\mathbf{n}})$. The expectation value of any observable $\hat{\mathcal{O}}$ can then be written as the integral over the unit sphere

$$\overline{\left\langle \hat{\mathcal{O}} \right\rangle} = \int d\Omega_{\hat{\mathbf{n}}}\, P(\hat{\mathbf{n}})\, \langle \hat{\mathbf{n}}|\hat{\mathcal{O}}|\hat{\mathbf{n}}\rangle\,. \tag{5.3}$$

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

$$\hat{\rho}_P \equiv \int d\Omega_{\hat{\mathbf{n}}}\, P(\hat{\mathbf{n}})\, |\hat{\mathbf{n}}\rangle\, \langle\hat{\mathbf{n}}|\,. \tag{5.4}$$

Then we have

$$\overline{\left\langle \hat{\mathcal{O}} \right\rangle} = \mathrm{tr}\left[\hat{\rho}_P \hat{\mathcal{O}}\right], \tag{5.5}$$

where tr denotes the trace. The operator $\hat{\rho}_P$ is called the density matrix. One immediate benefit of phrasing things in terms of $\hat{\rho}_P$ is that it makes it clear that $P(\hat{\mathbf{n}})$ contains a great deal of redundancy. $\hat{\rho}_P$ is a 2×2 Hermitian matrix

$$\hat{\rho}_P^\dagger = \hat{\rho}_P, \tag{5.6}$$

and therefore depends on only 4 real parameters, rather than a continuous function. In fact, there is are two more conditions. By taking $\hat{\mathcal{O}} = \mathbb{I}$ in Eq. (5.5)

$$\mathrm{tr}\ \hat{\rho}_P = 1. \tag{5.7}$$

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

$$\langle \Psi | \hat{\rho}_P | \Psi \rangle \geq 0 \tag{5.8}$$

for all $|\Psi\rangle$. We say that $\hat{\rho}_P$ is **positive semi definite**.

At this point let's dispense with $P(\hat{\mathbf{n}})$ altogether, and define a density matrix to be any operator satisfying the three conditions Eqs. (5.6-5.8). The expectation value of any observable is given by Eq. (5.5).

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.

As an example, let us consider the general form of a spin 1/2 density matrix. One approach would be to start from the density matrix for a given basis $\{|n\rangle\}$,

$$\rho_{nm} = \langle n | \hat{\rho} | m \rangle\,. \tag{5.9}$$

A completely general complex 2×2 matrix can be written as

$$\hat{\rho} = c_0 \mathbb{I} + c_1 \hat{\sigma}_x + c_2 \hat{\sigma}_y + c_3 \hat{\sigma}_z, \tag{5.10}$$

where $\hat{\sigma}_i$ are the Pauli (spin) matrices. Requiring that tr $\hat{\rho} = 1$ (for a pure state) implies that $c_0 = \frac{1}{2}$. Setting $\hat{\mathbf{n}} \equiv \frac{\mathbf{c}}{c}$, where $c = (c_1, c_2, c_3)$ and $r = |\mathbf{c}|$ we get

$$\hat{\rho} = \frac{1}{2}\mathbb{I} + \frac{r}{2}\hat{\mathbf{n}} \cdot \hat{\boldsymbol{\sigma}}. \tag{5.11}$$

For a physical state, the eigenvalues of $\hat{\rho}$ must be less than or equal to 1 thence $r \leq 1$. Thus, the space of spin 1/2 density matrices is identified with the unit ball (**Bloch sphere**).

Another approach would be starting from the density operator Eq. (5.4)

$$\hat{\rho}_P = \int \mathrm{d}\Omega_{\hat{\mathbf{n}}'}\, P(\hat{\mathbf{n}}')\, |\hat{\mathbf{n}}'\rangle \langle \hat{\mathbf{n}}'| \tag{5.12}$$

and seeing that a projection onto the two-state basis $|\uparrow\rangle$, $|\downarrow\rangle$ with

$$|\hat{\mathbf{n}}\rangle = \cos(\theta/2) e^{-i\phi/2} |\uparrow\rangle + \sin(\theta/2) e^{i\phi/2} |\downarrow\rangle \tag{5.13}$$

leads to

$$\hat{\rho} = \int \mathrm{d}\Omega_{\hat{\mathbf{n}}'}\, P(\hat{\mathbf{n}}')\frac{1}{2}(\mathbb{I} + \hat{\mathbf{n}}' \cdot \hat{\boldsymbol{\sigma}}). \tag{5.14}$$

Using $\int \mathrm{d}\Omega_{\hat{\mathbf{n}}'}\, P(\hat{\mathbf{n}}') = 1$ and setting

$$\int \mathrm{d}\Omega_{\hat{\mathbf{n}}'}\, P(\hat{\mathbf{n}}')\hat{\mathbf{n}}' \equiv r\hat{\mathbf{n}} \tag{5.15}$$

gives us the required result. Again it remains to show that $r \leq 1$. Let us for simplicity consider a case where only discrete spin orientations $\hat{\mathbf{n}}'_i$ occur with non-zero probabilities P_i. Then $\int \mathrm{d}\Omega_{\hat{\mathbf{n}}'}\, P(\hat{\mathbf{n}}')\hat{\mathbf{n}}' \to \sum_i P_i \hat{\mathbf{n}}'_i$ and with $\left|\hat{\mathbf{n}}'_i + \hat{\mathbf{n}}'_j\right| \leq |\hat{\mathbf{n}}'_i| + \left|\hat{\mathbf{n}}'_j\right|$ we see that

$$r = \left|\sum_i P_i \hat{\mathbf{n}}'_i\right| \leq \sum_i P_i |\hat{\mathbf{n}}'_i| = 1. \tag{5.16}$$

Since $\hat{\rho}$ is Hermitian, it has a representation in terms of its eigenvalues and (orthogonal) eigenstates

$$\hat{\rho} = \sum_\alpha P_\alpha \left|\varphi_\alpha\right\rangle \left\langle\varphi_\alpha\right|. \tag{5.17}$$

The conditions Eqs. (5.7) and (5.8) imply

$$\sum_\alpha P_\alpha = 1 \quad \text{and} \quad P_\alpha \geq 0. \tag{5.18}$$

Thus, although the definition provided by Eqs. (5.6-5.8) 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

Chapter 6

Lie Groups [*non-examinable*]

Chapter 7

Relativistic Quantum Physics [*non-examinable*]

Bibliography

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Appendix **A**

Appendix: Operator Algebra

A.1 General Operator Algebra

Some properties of the **commutator** $[A, B] = AB - BA$ of operators[1] A and B

$$\begin{aligned} &[A, BC] = [A, B]C + B[A, C], && \text{Leibniz rule} \\ &[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0, && \text{Jacobi identity} \end{aligned} \tag{A.1}$$

The following formula is frequently useful[2]

$$\begin{aligned} e^A B e^{-A} &= B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \cdots \\ &\equiv e^{[A, \cdot]} B \end{aligned} \tag{A.2}$$

[1]In AQP operators wore hats: we'll omit them unless there is a danger of ambiguity.
[2]It sometimes goes by the name *Hadamard lemma*.

Appendix B

Appendix:

B.1 Finding the Green's Function

We promised a more methodical derivation of the Green's function Eq. (3.63). Starting from the defining equation Eq. (3.62)

$$\left[E_k + \frac{\hbar^2}{2m}\nabla^2\right] G_k(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \tag{B.1}$$

we find that the Fourier transform

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

satisfies

$$\left[k^2 - \mathbf{q}^2\right]\tilde{G}_k(\mathbf{q}) = \frac{2m}{\hbar^2}. \tag{B.3}$$

The Green's function is then given by the integral

$$\begin{aligned} G_k(\mathbf{r},\mathbf{r}') &= \frac{2m}{\hbar^2}\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{\exp(i\mathbf{q}\cdot[\mathbf{r}-\mathbf{r}'])}{k^2-\mathbf{q}^2} \\ &= \frac{m}{\pi^2\hbar^2}\int_0^\infty \frac{\sin(q[\mathbf{r}-\mathbf{r}'])}{k^2-q^2} q\, dq \\ &= \frac{m}{2\pi^2 i\hbar^2|\mathbf{r}-\mathbf{r}'|}\int_{-\infty}^{\infty}\frac{\exp(iq|\mathbf{r}-\mathbf{r}'|)}{k^2-q^2}q\, dq\,, \end{aligned} \tag{B.4}$$

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.[1] The residues at these poles are

$$\mp\frac{1}{2}\exp(\pm ik|\mathbf{r}-\mathbf{r}'|) \quad \text{at} \quad q = \pm k. \tag{B.5}$$

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

$$G_k^+(\mathbf{r},\mathbf{r}') = \frac{m}{2\pi i\hbar^2|\mathbf{r}-\mathbf{r}'|}\int_{-\infty}^{\infty}\frac{\exp(iq|\mathbf{r}-\mathbf{r}'|)}{k^2-q^2+i\varepsilon}q\, dq \tag{B.6}$$

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

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. (3.63).

From the definition of the Green's function, it follows in equation (B.3) that we know the 1D Green's function in k space is,

$$\tilde{G}_k(q) = \frac{2m}{\hbar^2}\frac{1}{k^2 - q^2}. \tag{B.7}$$

We find the 1D $G_k(r, r')$ by the Fourier transform,

$$G_k(r, r') = \frac{2m}{\hbar^2}\int \frac{\mathrm{d}}{2\pi}\frac{\exp(iq(r - r'))}{k^2 - q^2}. \tag{B.8}$$

From Jordan's Lemma we know that if $(r - r') > 0$ we need to close the contour in the lower part of the plane in order for the contribution of the contour as $R \to \infty$ to vanish. Adding an $i\varepsilon$ in the denominator just as in equation (B.6)makes it clear that it is the pole at $-k$ that contributes as an residue; thus, we obtain

$$G_k(r, r') = \frac{2m}{\hbar^2}i\frac{\exp(ik(r - r'))}{-2k} = -\frac{im}{\hbar^2 k}\exp(ik(r - r')). \tag{B.9}$$

On the other hand, if $(r - r') < 00$, we need to close in the upper half (involving the pole at k) which gives

$$G_k(r, r') = -\frac{2m}{\hbar^2}i\frac{\exp(-ik(r - r'))}{2k} = -\frac{im}{\hbar^2 k}\exp(-ik(r - r')), \tag{B.10}$$

where the minus sign comes from the fact that we now integrate the other way round as for $(r - r') > 0$. Thus, we get

$$G_k(r, r') = -\frac{im}{\hbar^2 k}\exp(ik|r - r'|). \tag{B.11}$$

B.1.1 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

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{H}\right]K(\mathbf{r}, t|\mathbf{r}', t') = i\hbar\delta(\mathbf{r} - \mathbf{r}')\delta(t - t') \tag{B.12}$$

$$K(\mathbf{r}, t|\mathbf{r}', t') = 0 \quad \text{for} \quad t < t'. \tag{B.13}$$

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

$$K(\mathbf{r}, t|\mathbf{r}', t') = \int_{-\infty}^{\infty} K_\omega(\mathbf{r}|\mathbf{r}')\exp(-i\omega[t - t'])\frac{\mathrm{d}\omega}{2\pi}. \tag{B.14}$$

Eq. (B.12) tells us that $K_\omega(\mathbf{r}|\mathbf{r}')$ satisfies

$$\left[\hbar\omega - \hat{H}\right]K_\omega(\mathbf{r}|\mathbf{r}') = i\hbar\delta(\mathbf{r} - \mathbf{r}'). \tag{B.15}$$

Comparison of Eq. (B.15) and Eq. (3.62) suggests that for $\hat{H}_0 \equiv -\frac{\hbar^2}{2m}\nabla^2$

$$K_\omega(\mathbf{r}|\mathbf{r}') \stackrel{?}{=} i\hbar G_k(\mathbf{r},\mathbf{r}'), \tag{B.16}$$

with $\frac{\hbar^2 k^2}{2m} = \hbar\omega$. But what about Eq. (B.13)? For $t < t'$ we can, by Jordan's lemma, close the contour of integration in Eq. (B.14) in the upper half plane. If the integrand is analytic in this region, the integral vanishes, as required. From Eq. (B.6), we can see that the "$+i\varepsilon$" 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

$$K_\omega(\mathbf{r}|\mathbf{r}') = i\hbar G_k^+(\mathbf{r},\mathbf{r}'). \tag{B.17}$$

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.

B.2 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:

$$\boxed{|\Psi_k\rangle = |\mathbf{k}_\mathrm{i}\rangle + \hat{G}_k^+\hat{V}\,|\Psi_k\rangle\,,} \tag{B.18}$$

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

$$\hat{G}_k^+ = (E_k - \hat{H}_0 + i\varepsilon)^{-1}. \tag{B.19}$$

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

$$\langle\mathbf{k}_\mathrm{f}|\,\overbrace{\hat{G}_k^+\hat{V}\cdots\hat{G}_k^+\hat{V}}^{n\text{ times}}\,|\mathbf{k}_\mathrm{i}\rangle\,. \tag{B.20}$$

Translating the formula Eq. (3.70) for the scattering amplitude gives[2]

$$f(\mathbf{k}_\mathrm{f},\mathbf{k}_\mathrm{i}) = -\frac{\sqrt{2\pi}m}{\hbar^2}\,\langle\mathbf{k}_\mathrm{f}|\hat{V}|\Psi_k\rangle\,. \tag{B.21}$$

It's convenient to define a **transition operator** $\hat{T}$ by

$$\hat{T}\,|\mathbf{k}_\mathrm{i}\rangle = \hat{V}\,|\Psi_k\rangle\,. \tag{B.22}$$

From Eq. (B.18), we see that $\hat{T}$ obeys the operator equation

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_k^+\hat{T}. \tag{B.23}$$

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

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

$$f(\mathbf{k}_\mathrm{f}, \mathbf{k}_\mathrm{i}) = -\frac{4\pi^2 m}{\hbar^2} \langle \mathbf{k}_\mathrm{f}|\hat{T}|\mathbf{k}_\mathrm{i}\rangle . \tag{B.24}$$

As an illustration of this formalism, consider the following computation[3]

$$\begin{aligned}\langle \Psi_k|\hat{V}|\Psi_k\rangle &= \langle \Psi_k|\hat{T}|\mathbf{k}_\mathrm{i}\rangle \\ &= \langle \Psi_k|\hat{V}|\mathbf{k}_\mathrm{i}\rangle + \langle \Psi_k|\hat{V}\hat{G}_k^+\hat{T}|\mathbf{k}_\mathrm{i}\rangle \\ &= \langle \mathbf{k}_\mathrm{i}|\hat{T}^\dagger|\mathbf{k}_\mathrm{i}\rangle\ \langle \mathbf{k}_\mathrm{i}|\hat{T}^\dagger\hat{G}_k^+\hat{T}|\mathbf{k}_\mathrm{i}\rangle .\end{aligned} \tag{B.25}$$

The left hand side is manifestly real, thus $\mathrm{Im}\Big\{ \langle \Psi_k|\hat{V}|\Psi_k\rangle \Big\} = 0$ and thence

$$-\,\mathrm{Im}\Big\{ \langle \mathbf{k}_\mathrm{i}|\hat{T}^\dagger|\mathbf{k}_\mathrm{i}\rangle \Big\} = \mathrm{Im}\Big\{ \langle \mathbf{k}_\mathrm{i}|\hat{T}^\dagger\hat{G}_k^+\hat{T}|\mathbf{k}_\mathrm{i}\rangle \Big\} \tag{B.26}$$

On the left hand side, the $\hat{T}$-matrix is evaluated on shell. We can rewrite this in terms of the scattering amplitude f according to equation (B.24):

$$\frac{4\pi^2 m}{\hbar} \langle \mathbf{k}_\mathrm{i}|\hat{T}^\dagger|\mathbf{k}_\mathrm{i}\rangle = -f(\mathbf{k}_\mathrm{i}, \mathbf{k}_\mathrm{i}) = f(\theta = 0, \phi = 0), \tag{B.27}$$

since θ measures the angle between $\mathbf{k}_\mathrm{f}$ and $\mathbf{k}_\mathrm{i}$).

On the right hand side we use the identity

$$\frac{1}{x + i\varepsilon} = \mathcal{P}\frac{1}{x} - i\pi\delta(x), \tag{B.28}$$

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

$$\mathrm{Im}\left\{ \frac{1}{E_k - \hat{H}_0 + i\varepsilon} \right\} = -i\pi\delta(E_k - \hat{H}_0). \tag{B.29}$$

We can the insert another identity, $\mathbb{I} = \int \mathrm{d}\mathbf{k}'\, |\mathbf{k}'\rangle \langle \mathbf{k}'|$, between $\hat{G}_k^+$ and $\hat{T}$ in order to evaluate $\hat{H}_0$ in the denominator:

$$\begin{aligned}\mathrm{Im}\Big\{ \langle \mathbf{k}_\mathrm{i}|\hat{T}^\dagger\hat{G}_k^+\hat{T}|\mathbf{k}_\mathrm{i}\rangle \Big\} &= \int \mathrm{d}\mathbf{k}'\, \mathrm{Im}\Big\{ \langle \mathbf{k}_\mathrm{i}|\hat{T}\hat{G}_k^+|\mathbf{k}'\rangle\ \langle \mathbf{k}'|\hat{T}|\mathbf{k}_\mathrm{i}\rangle \Big\} \\ &= -\pi \int \mathrm{d}\mathbf{k}'\ \langle \mathbf{k}_\mathrm{i}|\hat{T}^\dagger\delta(E_{\mathbf{k}_\mathrm{i}} - E_{\mathbf{k}'})|\mathbf{k}'\rangle\ \langle \mathbf{k}'|\hat{T}|\mathbf{k}_\mathrm{i}\rangle \\ &= -\pi \int k'^2\, \mathrm{d}k'\, \mathrm{d}\Omega\, \frac{1}{\hbar^2 k'/m}\ \langle \mathbf{k}_\mathrm{i}|\hat{T}^\dagger\delta(\mathbf{k}_\mathrm{i} - \mathbf{k}')|\mathbf{k}'\rangle\ \langle \mathbf{k}'|\hat{T}|\mathbf{k}_\mathrm{i}\rangle \\ &= -\pi \int \mathrm{d}\Omega\, \frac{mk_i}{\hbar^2}\Big| \langle \mathbf{k}_\mathrm{i}|\hat{T}|\mathbf{k}_\mathrm{i}\rangle\Big|^2,\end{aligned} \tag{B.30}$$

where we define $\mathrm{d}\Omega = \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi$ and have obtained the factor $\frac{1}{\hbar^2 k'/m}$ from changing the variables inside the delta function from E to $\mathbf{k}'$. We notice that the definition of the total scattering cross section is just

$$\sigma_\mathrm{tot} = \int \mathrm{d}\Omega\, f(\theta, \phi) = \int \mathrm{d}\Omega \left(\frac{4\pi^2 m}{\hbar^2}\right)^2 \Big| \langle \mathbf{k}_\mathrm{i}|\hat{T}|\mathbf{k}_\mathrm{i}\rangle\Big|^2 \tag{B.31}$$

[3]Note that $\hat{T}$ is not Hermitian by virtue of the "$+i\varepsilon$" in the Green's function.

Multiplying equation (B.26) by $\left(\frac{4\pi^2 m}{\hbar^2}\right)^2$, we obtain

$$\frac{4\pi^2 m}{\hbar^2}\,\mathrm{Im}\{f(\theta=0)\} = \frac{m\pi k}{\hbar^2}\sigma_{\mathrm{tot}}, \tag{B.32}$$

thus yielding (yet another) proof of the optical theorem,

$$\sigma_{\mathrm{tot}} = \frac{4\pi}{k}\,\mathrm{Im}\{f(\theta=0)\}. \tag{B.33}$$

B.3 The Quantum Point Contact

Fig. B.1: Schematic view of a quantum point contact.

The quantum point contact (see Fig. B.1 and previous Fig. 3.2) 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,

$$\left[-\frac{\hbar^2}{2m}\partial_x^2 + \mathcal{E}_n(x)\right]\Psi(x) = E_k\Psi(x), \tag{B.34}$$

where

$$\mathcal{E}_n(x) = \frac{\hbar^2}{2m}\frac{\pi^2 n^2}{d(x)^2} \tag{B.35}$$

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

$$\boxed{d(x) \sim d_0 + \frac{x^2}{R},} \tag{B.36}$$

where R is the radius of curvature of the edge of the waveguide. In this region Eq. (B.34) takes the form

$$\left[-\partial_x^2 - \frac{1}{2}k_n x^2\right]\Psi(x) = \left(k^2 - \frac{\pi^2 n^2}{d_0^2}\right)\Psi(x), \tag{B.37}$$

where

$$k_n = \frac{4\pi^2 n^2}{d_0^3 R}. \tag{B.38}$$

Eq. (B.37) 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 Section 2.5)

$$\Psi_{\mathrm{WKB}}(x) = \frac{A}{\sqrt{p(x)}}\exp\left(\frac{i}{\hbar}\int^x p(x')\,\mathrm{d}x'\right) + \frac{B}{\sqrt{p(x)}}\exp\left(-\frac{i}{\hbar}\int^x p(x')\,\mathrm{d}x'\right). \tag{B.39}$$

Now recall the trick we used to solve the Landau–Zener problem in Subsection 1.3.1. 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. (1.82).

The only difference is that the exponential factor analogous to Eq. (1.86) 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. (3.10))

$$\frac{R}{T} = \exp\left(-z_n \pi^2 \sqrt{\frac{2R}{d_0}}\right), \quad z_n = \frac{kd_0}{\pi} - n, \tag{B.40}$$

where in the exponent we have made the simplification $k^2 - \pi^2 n^2/d_0^2 \sim \frac{2\pi n}{d_0}(k - \pi n/d_0)$ for $k \sim \pi n/d_0$.

To verify this we first need to take

$$p(x) = \sqrt{\frac{k_n}{2}x^2 + \frac{\pi^2}{d_0^2}\left(k^2\frac{d_0^2}{\pi^2} - n^2\right)}, \tag{B.41}$$

where we shall denote $\frac{\pi^2}{d_0^2}(k^2 - n^2)$ by b. Following on from equation (1.85), we evaluate

$$2\int_0^{i\sqrt{2b/k_n}} \sqrt{\frac{k_n}{2}x^2 + b} = \frac{i\pi}{2} b \sqrt{\frac{2}{k_n}} \tag{B.42}$$

$$\implies \quad \frac{i\pi}{2}\frac{\pi^2}{d_0^2}\left(k^2\frac{d_0^2}{\pi^2} - n^2\right) \times \frac{d_0}{\pi n}\sqrt{\frac{d_0 R}{2}} = \frac{i\pi^2}{2}\frac{1}{n}\left(k^2\frac{d_0^2}{\pi^2} - n^2\right)\sqrt{\frac{R}{2d_0}}. \tag{B.43}$$

Writing

$$k^2\frac{d_0^2}{\pi^2} - n^2 = 2n\left(k\frac{d_0}{\pi} - n\right) = 2nz, \tag{B.44}$$

we get

$$\frac{R}{T} = \exp\left(-\frac{\pi^2}{\hbar} z \sqrt{\frac{R}{2d_0}}\right) \tag{B.45}$$

Using unitarity $T + R = 1$ we can therefore find the reflection coefficient *exactly*

$$R = \frac{1}{1 + \exp\left(z_n \pi^2 \sqrt{\frac{2R}{d_0}}\right)}. \tag{B.46}$$

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).