Lecture Notes for Quantum Mechanics II, Spring 2026

Please send questions, comments, or corrections to r.barnett@imperial.ac.uk.

Chapter 1

1D Quantum Mechanics Revisited

This chapter will focus on quantum mechanics in one spatial dimension. We take the approach of treating the canonical position and momentum operators on an equal footing, and work with basis-independent operators when possible. We will find that much follows from the canonical commutation relation $[\hat{x}, \hat{p}] = i\hbar$. We will spend some time considering the Schrödinger equation in momentum space as this is probably unfamiliar.

1.1 A major theme from QM1

In this section we briefly review a major theme of QM1. To start, we write down the time-dependent Schrödinger equation (TDSE)

$$i\hbar\partial_t |\psi(t)\rangle = \hat{\mathcal{H}} |\psi(t)\rangle \tag{1.1}$$

where we recall that $\hbar$ is Planck's constant, t is time, $|\psi(t)\rangle$ is the wave function, and $\hat{\mathcal{H}}$ is the (Hermitian) Hamiltonian operator. In these notes, we will denote operators with hats. This is the central equation in quantum mechanics. In quantum mechanics, observables correspond to Hermitian operators. To evaluate the time-dependent expectation of observable $\hat{A}$, the standard approach is to (1) solve the Schrödinger equation (given some initial wave function) and (2) evaluate $\langle\psi(t)| \hat{A} |\psi(t)\rangle$.

Provided $\hat{\mathcal{H}}$ is time independent, the solution to (1.1) can be written as

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t} |\psi(0)\rangle .$$

In this, $e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}$ is definied by its series expansion. We can check that this solves (1.1) with the correct initial condition. This solution, however, is oftentimes not immediately useful. To find a more explicit expression for the time-dependent wave function, we solve the time-independent Schrödinger equation (TISE):

$$\hat{\mathcal{H}} |\phi_n\rangle = E_n |\phi_n\rangle$$

where we require the eigenstates (also known as eigenkets or stationary states) $|\phi_n\rangle$ to be in the Hilbert space (or suitable generalisation) of the problem of interest to us, and E_n are the eigenenergies. For simplicity, for the present case we are assuming that the spectrum is discrete (eigenenergies are labeled by integer n) and $|\phi_n\rangle$ span the Hilbert space – that is, they are complete. Since $\hat{\mathcal{H}}$ is Hermitian, we can take the eigenstates to be orthonormal:

$$\langle\phi_n|\,\phi_m\rangle = \delta_{nm}$$

where δ_{nm} is the Kronecker delta. Next, we note that a resolution of the identity is given by

$$\mathbb{1} = \sum_n |\phi_n\rangle\,\langle\phi_n|\,.$$

This can be directly checked by using the orthonormality condition to verify that $\mathbb{1}\,|\phi_n\rangle = |\phi_n\rangle$.

The next step is to insert this resolution of the identity into our expression for the time-dependent wave function:

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}\,|\psi(0)\rangle = \sum_n e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}\,|\phi_n\rangle\,\langle\phi_n|\,\psi(0)\rangle = \sum_n e^{-\frac{i}{\hbar}E_n t}\,|\phi_n\rangle\,\langle\phi_n|\,\psi(0)\rangle$$

where we note that $e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}\,|\phi_n\rangle = e^{-\frac{i}{\hbar}E_n t}\,|\phi_n\rangle$.

So, with the solution of the time-independent problem, we may find the general time dependence of the wave function through

$$|\psi(t)\rangle = \sum_n e^{-\frac{i}{\hbar}E_n t}\,|\phi_n\rangle\,\langle\phi_n|\,\psi(0)\rangle. \tag{1.2}$$

We can then evaluate the expectation value of the observable of our choice.

1.2 Position and momentum revisited

1.2.1 Canonical commutation relations

The previous section was fairly general. In the present section we will consider quantum mechanical problems in one spatial dimension, and label the position operator as $\hat{x}$ and the momentum operator as $\hat{p}$. In the following, we will treat these operators on a more-or-less equal footing. These Hermitian operators satisfy the canonical commutation relation:

$$[\hat{x}, \hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar.$$

This relation is of crucial importance in quantum mechanics. Historical note: Dirac exploited an analogy with classical mechanics (the so-called Poisson bracket) to write down expressions like what is above. (Heisenberg had arrive at the $[\hat{x}, \hat{p}]$ relation earlier, though.) This process is now usually referred to a canonical quantisation.

The standard way to go from classical to quantum is to promote the classical momentum and position to operators:

$$x \to \hat{x}, \quad p \to \hat{p}$$

and impose the canonical commutation relation (this is also known as canonical quantisation). The classical energy then becomes the quantum Hamiltonian. We then solve the TDSE and evaluate the expectation value of an observable of our choice (as in the previous section).

1.2.2 Eigenstates of the position and momentum operators

Both position and momentum have continuous (rather than discrete) spectra. There is no reason to restrict the location of a particle to be at discrete 'spots'. The rigorous treatment of an infinite-dimensional vector space spanned by eigenstates exhibiting a continuous spectrum is somewhat involved. We will not pursue such a treatment in the course. Fortunately, relevant results from finite dimensional vector spaces usually carry over to the infinite dimensional case in a very natural way.

Let's first focus on position. We denote the eigenstates of $\hat{x}$ as $|x\rangle$ and the eigenvalues by x:

$$\hat{x}\,|x\rangle = x\,|x\rangle\,.$$

The ket $|x\rangle$ corresponds to a state tightly localised at position x. Since $\hat{x}$ is Hermitian, we have that $\langle x|\,x'\rangle = 0$ when $x \neq x'$. Noting this, we use the following normalisation condition:

$$\langle x|\,x'\rangle = \delta(x - x')$$

where $\delta(x - x')$ is the Dirac delta function.[1] A resolution of the identity is given by

$$\mathbb{1} = \int dx\,|x\rangle\,\langle x|\,.$$

The above expression is integrated over all space. When there is little risk of ambiguity, we will not explicitly write out the limits of integration (using a similar practice below for momentum). It is instructive to compare these results to the analogous discrete ones from the previous section: $\langle \phi_n|\,\phi_m\rangle = \delta_{nm}$ and $\mathbb{1} = \sum_n |\phi_n\rangle\,\langle \phi_n|$. Everything seems to naturally work out. That is, the sum for the discrete case becomes an integral for the continuous case. Additionally, one needs the Dirac (rather than Kronecker) delta to ensure that $\mathbb{1}\,|x\rangle = |x\rangle$.

Everything that we did with $\hat{x}$ in the previous paragraph can also be done with $\hat{p}$. In particular, we have

$$\hat{p}\,|p\rangle = p\,|p\rangle\,,$$

$$\langle p|\,p'\rangle = \delta(p - p'),$$

and

$$\mathbb{1} = \int dp\,|p\rangle\,\langle p|\,.$$

[1] Strictly speaking, the Dirac delta is a *distribution* and not a function. However, the terminology 'Dirac delta function' is widespread. We will usually just call it the 'Dirac delta'.

1.2.3 The position basis

So far, apart from the cannonical commutation relation, position and momentum have been treated separately. How do we compute quantities like $\langle x|\, p\rangle$? To figure this out, we introduce the (spatial) **translation operator**:

$$\hat{\mathcal{T}}(a) = e^{-\frac{i}{\hbar}\hat{p}a}$$

where a is a scalar quantity having units of length. This operator will be discussed more later in our discussion on symmetries. Since $\hat{p}$ is Hermitian, it is readily verified that $\hat{\mathcal{T}}(a)$ is a unitary operator: $\hat{\mathcal{T}}^\dagger(a)\hat{\mathcal{T}}(a) = \hat{\mathcal{T}}(-a)\hat{\mathcal{T}}(a) = \mathbb{1}$. Next, let us consider the quantity

$$\hat{F}(a) \equiv \hat{\mathcal{T}}^\dagger(a)\hat{x}\hat{\mathcal{T}}(a).$$

To find a more explicit expression for $\hat{F}(a)$ we take its derivative with respect to a to find

$$\frac{d}{da}\hat{F}(a) = \frac{i}{\hbar}e^{\frac{i}{\hbar}\hat{p}a}(\hat{p}\hat{x} - \hat{x}\hat{p})e^{-\frac{i}{\hbar}\hat{p}a} = -\frac{i}{\hbar}e^{\frac{i}{\hbar}\hat{p}a}[\hat{x},\hat{p}]e^{-\frac{i}{\hbar}\hat{p}a} = e^{\frac{i}{\hbar}\hat{p}a}e^{-\frac{i}{\hbar}\hat{p}a} = \mathbb{1}$$

where we have used the canonical commutation relation. Next, we solve this (operator) ODE. With the initial condition $\hat{F}(0) = \hat{x}$, we readily find the solution to be

$$\hat{F}(a) = \hat{\mathcal{T}}^\dagger(a)\hat{x}\hat{\mathcal{T}}(a) = \hat{x} + a. \tag{1.3}$$

How does the translation operator act on position eigenstates? Note that, using (1.3) we have that

$$\hat{\mathcal{T}}^\dagger(a)\hat{x}\hat{\mathcal{T}}(a)\,|x\rangle = (\hat{x} + a)\,|x\rangle = (x + a)\,|x\rangle$$

where we remember that $\hat{x}\,|x\rangle = x\,|x\rangle$. Next, multiplying on the left by $\hat{\mathcal{T}}(a)$ we find

$$\hat{x}\hat{\mathcal{T}}(a)\,|x\rangle = (x + a)\hat{\mathcal{T}}(a)\,|x\rangle\,.$$

Therefore, $\hat{\mathcal{T}}(a)\,|x\rangle$ is an eigenstate of the position operator with eigenvalue $x + a$. Evidently $\hat{\mathcal{T}}(a)\,|x\rangle = |x + a\rangle$. Technically, this really only tells us that, since the spectrum of $\hat{x}$ is non-degenerate, $\hat{\mathcal{T}}(a)\,|x\rangle$ is proportional to $|x + a\rangle$. But remember that eigenstates are only defined up to normalisation and phase. Thus, given $|x\rangle$, the identification $|x + a\rangle = \hat{\mathcal{T}}(a)\,|x\rangle$ can be thought of as fixing the phase of $|x + a\rangle$.

In summary, the key relations of the translation operator for the present purpose are:

$$\hat{\mathcal{T}}^\dagger(a)\hat{x}\hat{\mathcal{T}}(a) = \hat{x} + a$$

and

$$\hat{\mathcal{T}}(a)\,|x\rangle = |x + a\rangle\,.$$

Take an arbitrary state $|\psi\rangle$. In the position basis, $\psi(x) \equiv \langle x|\,\psi\rangle$. This is the familiar wave function entering the position-space Schrödinger equation. Similarly, in the momentum basis we have $\tilde{\psi}(p) \equiv \langle p|\,\psi\rangle$.

Next, let's consider the quantity $\langle x|\,\hat{p}\,|\psi\rangle$ where $|\psi\rangle$ is an arbitrary state. Such an expression will tell us how to evaluate momentum in the position basis. To evaluate this, we consider the following for an arbitrary ket $|\psi\rangle$:

$$\psi(x+a) = \langle x+a|\,\psi\rangle = \langle x|\,\hat{\mathcal{T}}^{\dagger}(a)\,|\psi\rangle = \langle x|\left[1 + \frac{i}{\hbar}\hat{p}a + \frac{1}{2}\left(\frac{i}{\hbar}\hat{p}a\right)^2 + \ldots\right]|\psi\rangle\,.$$

Next we Taylor expand $\psi(x+a)$ in a: $\psi(x+a) = \psi(x) + \partial_x\psi(x)a + \ldots$ and match powers of a with the far RHS of the above expression. The zeroth order result gives simply $\psi(x) = \langle x|\,\psi\rangle$. The first order result gives our desired result:

$$\langle x|\,\hat{p}\,|\psi\rangle = -i\hbar\partial_x\psi(x). \tag{1.4}$$

The above can be read as 'momentum in the position basis is $-i\hbar\partial_x$.' Sometimes people simply put $\hat{p} = -i\hbar\partial_x$. However, for the present purposes it is best to not do this, and instead regard $\hat{p}$ as a basis-independent abstract operator. We can also conclude that for positive integer n,

$$\langle x|\,\hat{p}^n\,|\psi\rangle = (-i\hbar\partial_x)^n\psi(x)$$

(see exercises).

Our next aim is to write the Schrödinger equation in the position basis. We consider a single particle in a potential so that

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x}).$$

Multiplying $i\hbar\partial_t\,|\psi(t)\rangle = \hat{\mathcal{H}}\,|\psi(t)\rangle$ on the left by $\langle x|$ we find the familiar expression

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

where $\psi(x,t) = \langle x|\,\psi(t)\rangle$.

1.2.4 The momentum basis

One can follow a nearly identical approach as was done in the previous section to find how to write quantities in the momentum basis. In particular, we start with the unitary momentum translation operator

$$\hat{U}(q) = e^{i\hat{x}q/\hbar}.$$

As the treatment strongly mirrors that of the previous section, we will only write down the relevant relations, leaving their confirmation to the reader. The above operator can be found to

translate momentum as it should: $\hat{U}^\dagger(q)\hat{p}\hat{U}(q) = \hat{p} + q$, $\hat{U}(q)\,|p\rangle = |p+q\rangle$. One takes a general state $|\psi\rangle$ written in the momentum basis to be $\tilde{\psi}(p) = \langle p|\,\psi\rangle$. Next one can consider the series expansion of $\tilde{\psi}(p+q)$ in two different ways (see treatment in previous section) to determine that

$$\langle p|\,\hat{x}^n\,|\psi\rangle = (i\hbar\partial_p)^n\tilde{\psi}(p)$$

for positive integer n. That is, the position operator in the momentum basis is $i\hbar\partial_p$. Finally, by acting on the (operator) time-dependent Schrödinger equation on the left with $\langle p|$ gives the Schrödinger equation in the momentum basis

$$i\hbar\partial_t\tilde{\psi}(p,t) = \frac{p^2}{2m}\tilde{\psi}(p,t) + V(i\hbar\partial_p)\tilde{\psi}(p,t)$$

where we have assumed that $V(\hat{x})$ can be expanded as a power series in $\hat{x}$.

1.2.5 The Fourier transform

To complete the story, we need to find an expression for the inner product of the position and momentum eigenkets: $\langle x|\,p\rangle$. This will allow us to directly convert a state in the position basis to one in the momentum basis and vice-versa.

To evaluate this, we first consider the quantity $\langle x|\,\hat{p}\,|p\rangle$. Since $|p\rangle$ is an eigenstate of the momentum operator, we have $\langle x|\,\hat{p}\,|p\rangle = p\,\langle x|\,p\rangle$. On the other hand, because of (1.4) we have that $\langle x|\,\hat{p}\,|p\rangle = -i\hbar\partial_x\,\langle x|\,p\rangle$. We therefore find the following differential equation for $\langle x|\,p\rangle$:

$$p\,\langle x|\,p\rangle = -i\hbar\partial_x\,\langle x|\,p\rangle.$$

We readily solve this to find $\langle x|\,p\rangle = A(p)e^{ixp/\hbar}$ where $A(p)$ is an arbitrary function of p.

Next, let's consider the same expression from the previous paragraph, but with position and momentum swapped: $\langle p|\,\hat{x}\,|x\rangle$. Using that $|x\rangle$ is a position eigenstate as well as our way of writing the position operator in the momentum basis, we arrive at the differential equation:

$$x\,\langle p|\,x\rangle = i\hbar\partial_p\,\langle p|\,x\rangle.$$

This, again, can be readily solved to find $\langle p|\,x\rangle = B(x)e^{-ixp/\hbar}$ where $B(x)$ is an arbitrary function of x. Taking the complex conjugate gives:

$$\langle x|\,p\rangle = B^*(x)e^{ixp/\hbar}.$$

Finally, comparing this expression with the last expression of the previous paragraph we see that both $A(p)$ and $B(x)$ must be constants (no dependence on either x or p). So we have arrived at:

$$\langle x|\,p\rangle = Ae^{ixp/\hbar}.$$

To fix A, we consider the following:

$$\delta(x-x') = \langle x|\,x'\rangle = \int dp\,\langle x|\,p\rangle\,\langle p|\,x'\rangle = \int dp|A|^2e^{i(x-x')p/\hbar}.$$

In the above we have inserted a resolution of the identity operator (in the momentum basis). Introducing the scaled momentum $k = p/\hbar$ (such steps can be avoided when working in units where $\hbar = 1$!), we then have

$$\delta(x - x') = \hbar \int dk |A|^2 e^{i(x-x')k} = |A|^2 2\pi\hbar\delta(x - x')$$

where we have used the following expression for the Dirac delta function:

$$\delta(x) = \frac{1}{2\pi} \int dk e^{ikx}.$$

Choosing A to be purely real and positive (convention) we therefore find

$$\langle x | \, p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ixp/\hbar}.$$

Armed with our expression for $\langle x | \, p \rangle$ we may now convert between position space and momentum space wave functions. Inserting a resolution of the identity in appropriate places we find:

$$\psi(x) = \langle x | \, \psi \rangle = \int dp \, \langle x | \, p \rangle \, \langle p | \, \psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dp e^{ixp/\hbar} \tilde{\psi}(p)$$

$$\tilde{\psi}(p) = \langle p | \, \psi \rangle = \int dx \, \langle p | \, x \rangle \, \langle x | \, \psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-ixp/\hbar} \psi(x).$$

The above is nothing other than the Fourier transform!

1.2.6 The Schrödinger equation in momentum space: examples

The SE in position space is much more common than the SE in momentum space. There are, however, examples where momentum is the more natural basis to use. In the first example, we consider the Hamiltonian corresponding to a particle under a linear potential: $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \gamma\hat{x}$. In the momentum basis, the TISE $\hat{\mathcal{H}} \, |\phi\rangle = E \, |\phi\rangle$ becomes

$$\frac{p^2}{2m}\tilde{\phi}(p) + i\hbar\gamma\partial_p\tilde{\phi}(p) = E\tilde{\phi}(p),$$

a first-order differential equation. We solve this differential equation to find

$$\tilde{\phi}(p) = e^{\frac{-i}{\gamma\hbar}(Ep - p^3/6m)}\tilde{\phi}(0).$$

To find this stationary state in the position basis, we use the Fourier transform. The resulting $\phi(x)$ does not have a simple closed-form expression – it is typically expressed in terms of the so-called Airy function.

As a next example, we consider finding the ground-state energy of the following Hamiltonian

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} - \gamma\delta(\hat{x})$$

where γ is positive. The following potential, as we will see, turns out to have a single bound (localised in position space) state. Let's consider the TISE for the above in momentum space:

$$\frac{p^2}{2m}\tilde{\phi}(p) - \gamma \langle p| \delta(\hat{x}) |\phi\rangle = E\tilde{\phi}(p).$$

To simplify the second term on the LHS of the above, let's insert a resolution of the identity: $\langle p| \delta(\hat{x}) |\phi\rangle = \int dx \langle p| x\rangle \langle x| \delta(\hat{x}) |\phi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\phi(x=0)$. So the TISE becomes:

$$\frac{p^2}{2m}\tilde{\phi}(p) - \frac{\gamma}{\sqrt{2\pi\hbar}}\phi(0) = E\tilde{\phi}(p).$$

Note that the above equation has a term involving the wave function in real space. To be consistent, it must be that (using Fourier transform):

$$\phi(0) = \frac{\gamma}{\sqrt{2\pi\hbar}}\int dp\tilde{\phi}(p) = -\phi(0)\frac{\gamma}{2\pi\hbar}\int dp\frac{1}{E - \frac{p^2}{2m}}.$$

Assuming that $E < 0$ (as is the case for a bound state), evaluating the integral[2] and solving for E gives

$$E = -\frac{m\gamma^2}{2\hbar^2}$$

which is the ground-state energy we are after. The corresponding eigenfunction is $\tilde{\phi}(p) = A/(p^2 + 2m|E|)$ where A is a normalisation constant.

Fourier transforming $\tilde{\phi}(p)$ to position space[3] and normalising gives

$$\phi(x) = \sqrt{\kappa}e^{-\kappa|x|}$$

where $\kappa = m\gamma/\hbar^2$. It is reassuring that this solves the Schrödinger equation in the position basis (note that $\partial_x^2|x| = 2\delta(x)$) with the correct energy.

1.2.7 Generalisation to three dimensions

The arguments in this section can be naturally generalised to three spatial dimensions. The difficult part is done – any added difficulty in going to three dimensions mainly has to do with notation. Below we collect the three-dimensional versions of some main results from this section.

[2]The following integral is useful: $\int_{-\infty}^{\infty}\frac{dp}{p^2+\eta^2} = \frac{\pi}{|\eta|}$ where η is assumed to be real and non-zero. This can be either looked up or directly derived.

[3]It is a little tricky but give it a try. Taking such Fourier transforms though are not directly in the remit of this module and so not examinable.

$$\hat{\mathbf{r}} = \hat{x}\mathbf{i} + \hat{y}\mathbf{j} + \hat{z}\mathbf{k} = \hat{x}_1\mathbf{i} + \hat{x}_2\mathbf{j} + \hat{x}_3\mathbf{k}$$
$$\hat{\mathbf{p}} = \hat{p}_x\mathbf{i} + \hat{p}_y\mathbf{j} + \hat{p}_z\mathbf{k} = \hat{p}_1\mathbf{i} + \hat{p}_2\mathbf{j} + \hat{p}_3\mathbf{k}$$
$$[\hat{x}_i, \hat{x}_j] = 0, \quad [\hat{p}_i, \hat{p}_j] = 0, \quad [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$
$$\hat{\mathbf{r}}\,|\mathbf{r}\rangle = \mathbf{r}\,|\mathbf{r}\rangle$$
$$\hat{\mathbf{p}}\,|\mathbf{p}\rangle = \mathbf{p}\,|\mathbf{p}\rangle$$
$$\langle\mathbf{r}|\,\mathbf{r}'\rangle = \delta^{(3)}(\mathbf{r} - \mathbf{r}') = \delta(x - x')\delta(y - y')\delta(z - z')$$
$$\langle\mathbf{p}|\,\mathbf{p}'\rangle = \delta^{(3)}(\mathbf{p} - \mathbf{p}') = \delta(p_x - p'_x)\delta(p_y - p'_y)\delta(p_z - p'_z)$$
$$\langle\mathbf{r}|\,\hat{\mathbf{p}}\,|\psi\rangle = -i\hbar\nabla_{\mathbf{r}}\,\langle\mathbf{r}|\,\psi\rangle$$
$$\langle\mathbf{p}|\,\hat{\mathbf{r}}\,|\psi\rangle = i\hbar\nabla_{\mathbf{p}}\,\langle\mathbf{p}|\,\psi\rangle$$
$$\langle\mathbf{r}|\,\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{i\mathbf{r}\cdot\mathbf{p}/\hbar}$$

1.3 Exercises

Exercise 1.1 *Consider a particle in the infinite square well potential such that $V = 0$ for $0 \leq x \leq L$ and $V = \infty$ otherwise. Suppose the particle is in the initial state $|\psi(0)\rangle = (|\phi_1\rangle + |\phi_2\rangle)/\sqrt{2}$ where $|\phi_1\rangle$ and $|\phi_2\rangle$ are the ground and first excited states of the Hamiltonian. Find the expectation value of the position operator as a function of time.*

Exercise 1.2 *In section 1.1, the Hamiltonian was assumed to be time independent. For a time-dependent Hamiltonian $\hat{\mathcal{H}}(t)$, an obvious guess for the solution to the TDSE is $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}(t)t}\,|\psi(0)\rangle$. Explain why this is wrong. Can you think of a way to generalise to the time-dependent case?*

Exercise 1.3 *Show that $[\hat{x}^2, \hat{p}^2] = 2i\hbar(\hat{x}\hat{p} + \hat{p}\hat{x})$.*

Exercise 1.4 *For a sufficiently well-behaved function of the position operator $f(\hat{x})$, show that $[\hat{p}, f(\hat{x})] = -i\hbar\partial_{\hat{x}}f(\hat{x})$*

Exercise 1.5 *Consider a to be small. With the series expansion for the translation operator: $\hat{\mathcal{T}}(a) = 1 + \frac{-i}{\hbar}\hat{p}a + \frac{1}{2!}\left(\frac{-i}{\hbar}\hat{p}a\right)^2 + \ldots$ and a similar one for $\hat{\mathcal{T}}^\dagger(a) = \hat{\mathcal{T}}(-a)$, verify that (1.3) is correct up to and including terms of order a^2.*

Exercise 1.6 *Show that $[\hat{x}, \hat{\mathcal{T}}(a)] = a\hat{\mathcal{T}}(a)$.*

Exercise 1.7 *The mathematical integrity of the integral representation of the Dirac delta is questionable (try directly evaluating it!). One may think of the Dirac delta as a limit of distributions. For positive η, define $\delta_\eta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ikx}e^{-\eta|k|}$. Show that $\delta_\eta(x) = \frac{1}{\pi}\frac{\eta}{x^2+\eta^2}$. Observe that $\delta_\eta(x)$ becomes sharply peaked about $x = 0$ as η becomes small. Show that $\int_{-\infty}^{\infty} dx\delta_\eta(x) = 1$. $\delta_\eta(x)$ becomes the Dirac delta when we take η to zero. Boldly taking the $\eta \to 0$ limit before doing the integral gives the integral representation of the Dirac delta.*

Exercise 1.8 *Show that $\langle x|\,\hat{p}^n\,|\psi\rangle = (-i\hbar\partial_x)^n\psi(x)$ for positive integer n. Hint: consider the ket $|\phi\rangle = \hat{p}^{n-1}\,|\psi\rangle$ so that $\langle x|\,\hat{p}^n\,|\psi\rangle = \langle x|\,\hat{p}\,|\phi\rangle$.*

Chapter 2

The Different Pictures of Quantum Mechanics

In this chapter, we will consider the different "pictures" of quantum mechanics. Oftentimes a problem in quantum mechanics is more natural to analyse in one picture than it is in another. The time evolution operator establishes a bridge between the different pictures so we will discuss it first.

2.1 The time-evolution operator

We take the time evolution operator to be the time-dependent operator $\hat{\mathcal{U}}(t)$ that satisfies the evolution equation

$$i\hbar\partial_t\hat{\mathcal{U}}(t) = \hat{\mathcal{H}}(t)\hat{\mathcal{U}}(t)$$

with initial condition $\hat{\mathcal{U}}(0) = \mathbb{1}$. We will later see how this can be used to evolve states. Our first observation is that $\hat{\mathcal{U}}(t)$ is unitary. Why is this? At $t = 0$, $\hat{\mathcal{U}}$ is just the identity operator and so $\hat{\mathcal{U}}^\dagger\hat{\mathcal{U}} = \mathbb{1}$ then. What about later times? We can use the above evolution equation to determine that (remembering $\hat{\mathcal{H}}^\dagger = \hat{\mathcal{H}}$)

$$\partial_t(\hat{\mathcal{U}}^\dagger(t)\hat{\mathcal{U}}(t)) = \frac{i}{\hbar}\left(\hat{\mathcal{U}}^\dagger\hat{\mathcal{H}}\hat{\mathcal{U}} - \hat{\mathcal{U}}^\dagger\hat{\mathcal{H}}\hat{\mathcal{U}}\right) = 0.$$

From this we see that $\hat{\mathcal{U}}^\dagger(t)\hat{\mathcal{U}}(t) = \mathbb{1}$ at the later times and so $\hat{\mathcal{U}}(t)$ remains unitary.

Next, let's multiply the evolution equation by some time-independent state $|\psi(0)\rangle$. We get

$$i\hbar\partial_t\left(\hat{\mathcal{U}}(t)\,|\psi(0)\rangle\right) = \hat{\mathcal{H}}(t)\left(\hat{\mathcal{U}}(t)\,|\psi(0)\rangle\right).$$

This looks like the Schrödinger equation that a state with initial condition $|\psi(0)\rangle$ would satisfy. Since a solution of the time-dependent Schrödinger equation with specified initial state is unique we may identify:

$$|\psi(t)\rangle = \hat{\mathcal{U}}(t)\,|\psi(0)\rangle\,.$$

This is a useful result. To find out what a state does at later times just multiply by $\hat{\mathcal{U}}(t)$ (if we know it!) – no need to solve the Schrödinger equation.

Next we observe that evolution in this way preserves normalisation because of its unitarity. That is,

$$\langle\psi(t)|\,\psi(t)\rangle = \langle\psi(0)|\,\hat{\mathcal{U}}^\dagger(t)\hat{\mathcal{U}}(t)\,|\psi(0)\rangle = \langle\psi(0)|\,\psi(0)\rangle.$$

So if we start with a state normalised to one, we continue to have a state normalised to one.

When $\hat{\mathcal{H}}$ is time-independent, we can directly solve the time-evolution equation with appropriate initial conditions to find

$$\hat{\mathcal{U}}(t) = e^{\frac{-i}{\hbar}\hat{\mathcal{H}}t}.$$

When the Hamiltonian is time dependent, such a result does not generally hold. In the following we will derive a fairly compact expression for the time-evolution operator for this case. Integrating the evolution equation from zero to t gives

$$\hat{\mathcal{U}}(t) = \mathbb{1} - \frac{i}{\hbar}\int_0^t dt'\hat{\mathcal{H}}(t')\hat{\mathcal{U}}(t').$$

We note that $\hat{\mathcal{U}}$ appears in two places in this equation. Inserting the one on the left into the one on the right gives

$$\hat{\mathcal{U}}(t) = \mathbb{1} - \frac{i}{\hbar}\int_0^t dt'\hat{\mathcal{H}}(t') + \left(\frac{-i}{\hbar}\right)^2\int_0^t dt'\int_0^{t'} dt''\hat{\mathcal{H}}(t')\hat{\mathcal{H}}(t'')\hat{\mathcal{U}}(t'').$$

Continuing with this procedure, we can find a series expansion for the evolution operator:

$$\hat{\mathcal{U}}(t) = \mathbb{1} + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \hat{F}_n$$

where

$$\hat{F}_n = \int_0^t dt_1\int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n\hat{\mathcal{H}}(t_1)\ldots\hat{\mathcal{H}}(t_n).$$

This is called the Dyson series.

To make further progress, we introduce the so-called time-ordering operator T_t. This "meta operator" puts quantities evaluated at later times to the left of quantities evaluated at earlier times, disregarding commutation relations in the process. For instance, $T_t(\hat{\mathcal{H}}(t_1)\hat{\mathcal{H}}(t_2))$ is $\hat{\mathcal{H}}(t_1)\hat{\mathcal{H}}(t_2)$ when $t_1 > t_2$ and $\hat{\mathcal{H}}(t_2)\hat{\mathcal{H}}(t_1)$ when $t_2 > t_1$. Next we claim the useful result:

$$\hat{F}_n = \frac{1}{n!}T_t(\hat{F_1}^n).$$

Trying showing this, starting with $n = 2$. Using this result, the series above can be re-summed to give the compact result we are seeking:

$$\hat{\mathcal{U}}(t) = T_t e^{\frac{-i}{\hbar}\int_0^t dt'\hat{\mathcal{H}}(t')}.$$

Note that when $[\hat{\mathcal{H}}(t), \hat{\mathcal{H}}(t')] = 0$ for all t and t', we can drop the time-ordering operator in this expression (why?).

2.2 The Heisenberg picture

Now with $\hat{\mathcal{U}}(t)$ at our disposal we can continue to our discussion of the Heisenberg picture. To motivate this, let's consider the expectation value of some operator $\hat{A}$ (an observable, for instance). To simplify the discussion, we will take $\hat{A}$ to have no intrinsic time dependence (but this case can also be handled). What is the time-dependent expectation value of $\hat{A}$, evaluated with state $|\psi(t)\rangle$ evolving according to the Schrödinger equation? With the information we now have at hand, we can write this in two different ways

$$\langle \hat{A} \rangle(t) = \langle \psi(t) | \, \hat{A} \, | \psi(t) \rangle = \langle \psi(0) | \left[\hat{\mathcal{U}}^\dagger(t) \hat{A} \hat{\mathcal{U}}(t) \right] | \psi(0) \rangle \, .$$

The above suggests two equivalent approaches to evaluating the expectation value:

- The familiar approach of taking the state ket to evolve through $|\psi(t)\rangle = \hat{\mathcal{U}}(t) \, |\psi(0)\rangle$ and keeping the operator to be time independent. This is called the Schrödinger picture.

- Letting the operator evolve through $\hat{A}_{\rm H}(t) \equiv \hat{\mathcal{U}}^\dagger(t) \hat{A} \hat{\mathcal{U}}(t)$ while keeping the state fixed at $|\psi(0)\rangle$. This is called the Heisenberg picture. In the following, we will use subscript H to denote quantities evaluated in the Heisenberg picture.

Physically, we measure observables and not wave functions. Both methods give the same answer for the expectation values of observables, and so provide equally valid descriptions of reality.

We now move on to discuss how we might compute the time dependence of an operator in the Heisenberg picture. Taking the time derivative of $\hat{A}_{\rm H}$ and using the evolution equation for $\hat{\mathcal{U}}$ we find

$$\frac{d}{dt} \hat{A}_{\rm H}(t) = \frac{\partial \hat{\mathcal{U}}^\dagger(t)}{\partial t} \hat{A} \hat{\mathcal{U}}(t) + \hat{\mathcal{U}}^\dagger(t) \hat{A} \frac{\partial \hat{\mathcal{U}}(t)}{\partial t} = \frac{-i}{\hbar} \hat{\mathcal{U}}^\dagger(t) [\hat{A}, \hat{\mathcal{H}}] \hat{\mathcal{U}}(t).$$

We have found the Heisenberg equations of motion

$$i\hbar \frac{d}{dt} \hat{A}_{\rm H}(t) = \hat{\mathcal{U}}^\dagger(t) [\hat{A}, \hat{\mathcal{H}}] \hat{\mathcal{U}}(t) = [\hat{A}_{\rm H}(t), \hat{\mathcal{H}}_{\rm H}(t)]$$

where $\hat{\mathcal{H}}_{\rm H}(t) = \hat{\mathcal{U}}^\dagger(t) \hat{\mathcal{H}} \hat{\mathcal{U}}(t)$. Note that when the Hamiltonian is time-independent (as is often the case), we have $\hat{\mathcal{H}}_{\rm H}(t) = \hat{\mathcal{H}}$ (why?). Also note that we must have the initial condition $\hat{A}_{\rm H}(t = 0) = \hat{A}$ since the time-evolution operator is the identity when $t = 0$.

2.3 Applications of the Heisenberg equations of motion

With the Heisenberg equations of motion at hand, we will discuss a number of applications. Some of these results would be fairly demanding to obtain in the Schrödinger picture.

2.3.1 First examples

Example 1

First we consider the motion of a particle under a Hamiltonian with a linear potential. In particular, we take the motion of the particle to governed by

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \gamma\hat{x}$$

and further take the initial expectation values of position and momentum to be $\langle\hat{x}\rangle(t=0) = \langle\psi(0)|\,\hat{x}\,|\psi(0)\rangle = \bar{x}$ and $\langle\hat{p}\rangle(t=0) = \bar{p}$. What is the value of the expectation value of the position at later times?

This problem would be somewhat involved to work in the Schrödinger picture as the stationary states of the Hamiltonian are Airy functions, c.f. Sec. 1.2.6. However, as we now see, it is very manageable in the Heisenberg picture.

First we need to set up the equations of motion. For position, they are

$$i\hbar\frac{d}{dt}\hat{x}_{\mathrm{H}}(t) = \hat{\mathcal{U}}^\dagger(t)[\hat{x},\hat{\mathcal{H}}]\hat{\mathcal{U}}(t) = \hat{\mathcal{U}}^\dagger(t)i\hbar\hat{p}/m\hat{\mathcal{U}}(t) = i\hbar\hat{p}_{\mathrm{H}}(t)/m.$$

For momentum,

$$i\hbar\frac{d}{dt}\hat{p}_{\mathrm{H}}(t) = \hat{\mathcal{U}}^\dagger(t)[\hat{p},\hat{\mathcal{H}}]\hat{\mathcal{U}}(t) = \hat{\mathcal{U}}^\dagger(t) - i\hbar\gamma\hat{\mathcal{U}}(t) = -i\hbar\gamma.$$

Rearranging the above gives:

$$\begin{aligned} m\frac{d}{dt}\hat{x}_{\mathrm{H}} &= \hat{p}_{\mathrm{H}} \\ \frac{d}{dt}\hat{p}_{\mathrm{H}} &= -\gamma \end{aligned}$$

which are operator versions of the corresponding equations of motion in classical mechanics.[1]

With the correct initial conditions ($\hat{x}_{\mathrm{H}}(t=0) = \hat{x}, \hat{p}_{\mathrm{H}}(t=0) = \hat{p}$), the above equations of motion are readily solved:

$$\begin{aligned} \hat{x}_{\mathrm{H}} &= \hat{x} + \frac{1}{m}\hat{p}t - \frac{\gamma}{2m}t^2 \\ \hat{p}_{\mathrm{H}} &= \hat{p} - \gamma t. \end{aligned}$$

From this, it directly follows that

$$\langle x\rangle(t) = \langle\psi(0)|\,\hat{x}_{\mathrm{H}}\,|\psi(0)\rangle = \bar{x} + \frac{1}{m}\bar{p}t - \frac{\gamma}{2m}t^2.$$

Example 2

[1] This analogy holds for other types of potentials. However, the *expectation values* only obey classical equations of motion when the potential is at most quadratic in $\hat{x}$.

The Heisenberg equations of motion are not confined to the position and momentum operators. As a next example, we consider the evolution of the ladder operators, also known as creation and destruction operators, familiar from the solution of the harmonic oscillator. In the following, we will also take the initial state to be a so-called coherent state. Basic information on coherent states is in Appendix 2.A.

Let's see how the ladder operators evolve in the Heisenberg picture under the harmonic oscillator Hamiltonian $\hat{\mathcal{H}} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2)$. The Heisenberg equation of motion for the ladder operator is:

$$i\hbar\frac{d}{dt}\hat{a}_{\mathrm{H}}(t) = \hat{\mathcal{U}}^\dagger(t)[\hat{a}, \hat{\mathcal{H}}]\hat{\mathcal{U}}(t).$$

To evaluate the piece sandwiched between the evolution operators, we need to figure out $[\hat{a}, \hat{a}^\dagger\hat{a}]$. To calculate this, we can use the identity $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$ (verify this) to find $[\hat{a}, \hat{a}^\dagger\hat{a}] = \hat{a}$. With this, the equation of motion becomes

$$i\hbar\frac{d}{dt}\hat{a}_{\mathrm{H}}(t) = \hbar\omega\hat{\mathcal{U}}^\dagger(t)\hat{a}\hat{\mathcal{U}}(t) = \hbar\omega\hat{a}_{\mathrm{H}}(t).$$

With the initial condition $\hat{a}_{\mathrm{H}}(0) = \hat{a}$ we can immediately solve to find

$$\hat{a}_{\mathrm{H}}(t) = e^{-i\omega t}\hat{a}.$$

What can we use this for? Suppose that initially at $t = 0$, our state is a coherent state $|z\rangle$ such that $\hat{a}\,|z\rangle = z\,|z\rangle$. To find the expectation value of $\hat{a}$ at later times we just need to take the expectation value of $\hat{a}_{\mathrm{H}}(t)$ with this initial state. We find

$$\langle\hat{a}\rangle(t) = \langle\psi(t)|\,\hat{a}\,|\psi(t)\rangle = ze^{-i\omega t}. \tag{2.1}$$

With little additional work, we can find the time-dependent expectation value of the position operator $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$ to be

$$\langle\hat{x}\rangle(t) = \langle\psi(t)|\,\hat{x}\,|\psi(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}(ze^{-i\omega t} + z^*e^{i\omega t}).$$

2.3.2 Many-particle collapse and revival

This example is slightly more involved than the two pervious ones. Instead of the harmonic oscillator Hamiltonian, let's take

$$\hat{\mathcal{H}} = \frac{g}{2}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} = \frac{g}{2}\hat{n}(\hat{n} - 1) \tag{2.2}$$

where $\hat{n} = \hat{a}^\dagger\hat{a}$ and g is a positive constant having units of energy. This example is considerably more involved than the previous one. Do not worry if the manipulations are difficult on your first or second pass, especially if you are learning coherent states in parallel. This example actually brings us up to some influential research from the current era.

The discussed in the following foreshadows our later treatment of second quantisation. It is meant to give a plausible physical interpretation of this example. When $\hat{a}$ is the ladder operator from the harmonic oscillator, the above Hamiltonian does not seem so physical. That is, it would involve terms like $\hat{p}^4$ and $\hat{x}\hat{p}^3$. In the language of second quantisation, the ladder operators take on a new meaning. In second quantisation, the operator $\hat{a}^\dagger$ is interpreted as an operator that adds one particle. To understand physically the present example we contrast the two physical interpretations in this table:

	Harmonic Oscillator	Second Quantisation
$\|n\rangle$	nth eigenstate of harmonic oscillator	State with exactly n particles
$\hat{a}$	Lowering operator that takes a harmonic oscillator eigenstate one rung down the ladder	Destruction operator that destroys a particle
$\hat{a}^\dagger$	Raising operator that takes a harmonic oscillator eigenstate one rung up the ladder	Creation operator that creates one particle
$\hat{n}$	Quantum number operator	Particle number operator

Now back to the Hamiltonian. This Hamiltonian can be thought of as describing pairwise interactions between particles. The interaction between each pair of particles costs an energy g. Since we can form $\binom{n}{2} = n(n-1)/2$ pairs from n particles, the Hamiltonian has its current form.

We now compute the Heisenberg equations of motion for the destruction operators. We find

$$i\hbar\frac{d}{dt}\hat{a}_H(t) = \hat{\mathcal{U}}^\dagger(t)[\hat{a}, \hat{\mathcal{H}}]\hat{\mathcal{U}}(t) = g\hat{\mathcal{U}}^\dagger(t)\hat{n}\hat{a}\hat{\mathcal{U}}(t) = g\hat{n}_H(t)\hat{a}_H(t)$$

(see exercise 2.4). Next we note that $\hat{n}_H(t)$ is time-independent since $\hat{n}$ commutes with the Hamiltonian:

$$i\hbar\frac{d}{dt}\hat{n}_H(t) = \hat{\mathcal{U}}^\dagger(t)[\hat{n}, \hat{H}]\hat{\mathcal{U}}(t) = 0.$$

Therefore, $\hat{n}_H(t) = \hat{n}$. Using this, we can solve the equation of motion for $\hat{a}_H(t)$ to find:

$$\hat{a}_H(t) = e^{-\frac{i}{\hbar}g\hat{n}t}\hat{a}.$$

Next let's use this to evaluate the time dependence of the expectation value of $\hat{a}$ starting from an initial coherent state, like we did in the previous example. That is, we want to compute

$$\langle\hat{a}\rangle(t) = \langle z|\,\hat{a}_H(t)\,|z\rangle\,.$$

Let's first look at $\hat{a}_H(t)\,|z\rangle$. Working on this expression gives

$$\begin{aligned}\hat{a}_H(t)\,|z\rangle &= e^{-\frac{i}{\hbar}g\hat{n}t}\hat{a}\,|z\rangle = ze^{-\frac{i}{\hbar}g\hat{n}t}\,|z\rangle = ze^{-|z|^2/2}e^{-\frac{i}{\hbar}g\hat{n}t}e^{z\hat{a}^\dagger}\,|0\rangle \\ &= ze^{-|z|^2/2}e^{ze^{-\frac{i}{\hbar}g\hat{n}t}\hat{a}^\dagger e^{\frac{i}{\hbar}g\hat{n}t}}e^{\frac{-i}{\hbar}g\hat{n}t}\,|0\rangle = ze^{-|z|^2/2}e^{ze^{-\frac{i}{\hbar}g\hat{n}t}\hat{a}^\dagger e^{\frac{i}{\hbar}g\hat{n}t}}\,|0\rangle\,.\end{aligned}$$

In our previous example, we saw that $e^{i\omega\hat{n}t}\hat{a}e^{-i\omega\hat{n}t} = \hat{a}e^{-i\omega t}$. We can borrow this result for the present calculation (identifying ω with $-g/\hbar$) to find

$$\hat{a}_H(t)\,|z\rangle = ze^{-|z|^2/2}e^{ze^{-\frac{i}{\hbar}gt}\hat{a}^\dagger}\,|0\rangle = z\left|ze^{-\frac{i}{\hbar}gt}\right\rangle.$$

So this result can be expressed in terms of a coherent state with a time-dependent phase. Finally, using the expression for the overlap between two coherent states from the Appendix we have

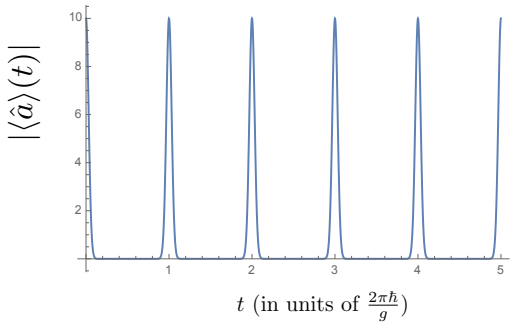
$$\langle\hat{a}\rangle(t) = ze^{|z|^2(e^{-\frac{i}{\hbar}gt}-1)}.$$

Taking the modulus of this expression gives the nice compact result:

$$|\langle\hat{a}\rangle(t)| = |z|e^{-2|z|^2\sin^2\left(\frac{gt}{2\hbar}\right)}.$$

This expression is plotted in the figure below for $|z| = 10$. It supports the following narrative: Interactions cause the initial simple coherent state to collapse to a complex incoherent many-particle state. However, the simple coherent state is periodically revived at later times corresponding to integer multiples of $\frac{2\pi\hbar}{g}$.

The collapse-revival phenomenon was observed with matter waves in [Greiner *et al*, Nature 419, 51 (2002)]. The theoretical modelling in that paper is actually very close to what we did in this example.



2.3.3 Balancing a pencil on its tip

In this example we consider a particle moving under the potential

$$V(\hat{x}) = -\frac{1}{2}m\omega^2\hat{x}^2.$$

This is the familiar potential for the harmonic oscillator with a sign change. To make connection with the classical world, we take m and ω to have 'everyday' values, on the order of grams and inverse seconds. We ask: is it possible to balance a particle at $x = 0$, at the 'top of the hill'? Note that this example is not *quite* what is described in the section title – because for a pencil we'd need to talk about moments of intertia and angular momentum – but it is the same idea.

In classical mechanics, this is possible in principle. That is, a perfectly admissible solution to the classical equations of motion is $x = p = 0$ for all times. In quantum mechanics, does such a solution exist? If not, perhaps we can optimise our initial state so that the particle stays near the top for a long time, longer than the timescale of any experiments we do. This solution would count for all practical purposes.[2]

Denoting the initial state by $|\psi_i\rangle$ we require $\langle\psi_i|\,\hat{x}\,|\psi_i\rangle = \langle\psi_i|\,\hat{p}\,|\psi_i\rangle = 0$. That is, the mean position and momentum of the particle are both initially zero. We further make the technical assumption that $\psi_i(x) = \langle x|\,\psi_i\rangle$ can be taken to be real.[3] To go further with this problem we use the Heisenberg equations of motion:

$$\begin{aligned} m\frac{d}{dt}\hat{x}_{\mathrm{H}}(t) &= \hat{p}_{\mathrm{H}}(t) \\ \frac{d}{dt}\hat{p}_{\mathrm{H}}(t) &= m\omega^2\hat{x}_{\mathrm{H}}(t). \end{aligned}$$

With the initial conditions $\hat{x}_{\mathrm{H}}(0) = \hat{x}$, $\hat{p}_{\mathrm{H}}(0) = \hat{p}$, we can solve to find

$$\begin{aligned} \hat{x}_{\mathrm{H}}(t) &= \hat{x}\cosh(\omega t) + \frac{1}{m\omega}\hat{p}\sinh(\omega t) \\ \hat{p}_{\mathrm{H}}(t) &= \hat{p}\cosh(\omega t) + m\omega\hat{x}\sinh(\omega t). \end{aligned}$$

With this, we can immediately find the time-dependent expectation value of the position operator:

$$\langle\hat{x}\rangle(t) = \langle\psi_i|\,\hat{x}_{\mathrm{H}}\,|\psi_i\rangle = \langle\psi_i|\,\hat{x}\,|\psi_i\rangle\cosh(\omega t) + \frac{1}{m\omega}\langle\psi_i|\,\hat{p}\,|\psi_i\rangle\sinh(\omega t) = 0.$$

Have we found the desired solution? We must remember that, unlike Newtonian physics, quantum mechanics is probabilistic. We can do two different experiments under identical conditions and get two different outcomes. The above just says that the average (that is average over many experiments with identical initial conditions) value of position measured at any time t will be zero. This does not rule out the possibility of the particle going to the left in some experiments while going to the right in others.

It is therefore useful to look at the variance of the position measurements. Since $\langle\hat{x}\rangle = 0$ at all times, we have $\sigma_x^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2 = \langle\hat{x}^2\rangle$. Using again the solution of the Heisenberg equations of motion we find this to be

$$\begin{aligned} \sigma_x^2(t) &= \langle\psi_i|\,\hat{x}_{\mathrm{H}}^2\,|\psi_i\rangle \\ &= \langle\psi_i|\,\hat{x}^2\,|\psi_i\rangle\cosh^2(\omega t) + \frac{1}{m^2\omega^2}\langle\psi_i|\,\hat{p}^2\,|\psi_i\rangle\sinh^2(\omega t) + \frac{1}{m\omega}\langle\psi_i|\,\hat{x}\hat{p}+\hat{p}\hat{x}\,|\psi_i\rangle\sinh(\omega t)\cosh(\omega t) \\ &= \bar{\sigma}_x^2\cosh^2(\omega t) + \frac{1}{m^2\omega^2}\bar{\sigma}_p^2\sinh^2(\omega t) \end{aligned}$$

[2] That is, if you manage to balance a pencil on its tip in a way such that that it takes 10 years to fall over, we can count this as successfully balancing the pencil.

[3] A main reason for this assumption is that it will simplify the following analysis. Similar results will hold for more general $\psi_i(x)$. Secondly, this is a physically sensible assumption. For instance, suppose we prepare the system as the ground state of another Hamiltonian $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V_i(\hat{x})$. Here $V_i(\hat{x})$ could, say, correspond to the potential created by the tweezers you are using to situate the particle. The position-space eigenstates of this Hamiltonian can be taken to be real. That is, if $\phi(x)$ is an eigenstate with energy E then so is $\phi(x) + \phi^*(x)$.

where $\bar{\sigma}_x^2$ and $\bar{\sigma}_p^2$ are the initial x and p variances (at $t = 0$). The last term in the longest line above vanishes since we take $\psi_i(x)$ to be real.[4] Classically, we can think of $\bar{\sigma}_x^2$ and $\bar{\sigma}_p^2$ as accounting for initial errors in how we prepare the system. For instance, sometimes a breeze might nudge the particle in one direction or another and this factors into $\bar{\sigma}_p^2$. Such errors are amplified over time. As we refine our experiment more and more, there is no fundamental limit on how small we can make $\bar{\sigma}_x^2$ and $\bar{\sigma}_p^2$ classically. Quantum mechanically, however, these are constrained by the Heisenberg uncertainty principle:

$$\bar{\sigma}_x^2 \bar{\sigma}_p^2 \geq \frac{\hbar^2}{4}.$$

Giving up hope of making $\sigma_x^2(t)$ identically zero for all times, let's resort to optimising. For fixed time t, we find the $\bar{\sigma}_x^2$ and $\bar{\sigma}_p^2$ (constrained by the uncertainty principle) that minimise σ_x^2. Taking minimum uncertainty states so that $\bar{\sigma}_x^2 \bar{\sigma}_p^2 = \hbar^2/4$, substituting $\bar{\sigma}_p^2 = \hbar^2/4\bar{\sigma}_x^2$ into $\sigma_x^2(t)$, and minimising over $\bar{\sigma}_x^2$, we find the optimal value

$$\left[\sigma_x^2(t)\right]_{\text{opt}} = \ell^2 \sinh(2\omega t)$$

where $\ell = \sqrt{\frac{\hbar}{2m\omega}}$ is a length scale. $[\sigma_x^2(t)]_{\text{opt}}$ can be thought of as a lower bound of $\sigma_x^2(t)$ which is saturated provided certain initial conditions are taken.

Now let's look at some numbers. Using everyday values $m = 10\text{g}$, $\omega = 1\text{Hz}$, we find $\ell \sim 2 \times 10^{-16}\text{m}$, not an everyday length scale (about half the diameter of a proton). The prospect of balancing the particle for a long time seems promising until we realise ℓ^2 multiplies something with exponential time dependence. We see that $\sqrt{[\sigma_x^2(t)]_{\text{opt}}}$ will, alas, reach an everyday length value for an everyday value of t (half a minute or so).

Usually for idealised problems on macroscopic scales, like those from a classical mechanics text book, we do not expect quantum mechanics to play a major role.[5] The present example is an exception to this rule.

2.4 The interaction picture

Lastly we will discuss the interaction picture, which is sometimes referred to as the Dirac picture. This will be used later when we discuss time-dependent perturbation theory. The interaction picture is, in a sense, a hybrid of the Schrödinger and Heisenberg pictures. Suppose that our Hamiltonian can naturally be written as the sum of two parts:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{V}.$$

[4] Since we take $\psi_i(x)$ to be real, we have (integrating by parts)

$$\langle\psi_i|\,\hat{x}\hat{p}\,|\psi_i\rangle = \int dx \psi_i(x) x(-i\hbar\partial_x)\psi_i(x) = -\int dx \psi_i(x)(-i\hbar\partial_x)(x\psi_i(x)) = -\langle\psi_i|\,\hat{p}\hat{x}\,|\psi_i\rangle\,.$$

[5] Of course quantum mechanics can have a lot to say about whether such idealisations are appropriate.

We define the time evolution operator $\hat{\mathcal{U}}(t)$ for $\hat{\mathcal{H}}$ in the usual way. Additionally, we consider an operator $\hat{\mathcal{U}}_0(t)$ that describes the time evolution in the absence of $\hat{V}$. This is defined through the differential equation

$$i\hbar\partial_t\hat{\mathcal{U}}_0(t) = \hat{\mathcal{H}}_0\hat{\mathcal{U}}_0(t)$$

with initial condition $\hat{\mathcal{U}}_0(0) = \mathbb{1}$.

Paralleling our earlier discussion of the Heisenberg picture, consider the time-dependent expectation value of some operator $\hat{A}$:

$$\langle A\rangle = \langle\psi(t)|\,\hat{A}\,|\psi(t)\rangle = \langle\psi(0)|\,\hat{\mathcal{U}}^\dagger\hat{A}\hat{\mathcal{U}}\,|\psi(0)\rangle\,.$$

Now insert the identity operator $\mathbb{1} = \hat{\mathcal{U}}_0(t)\hat{\mathcal{U}}_0^\dagger(t)$ as follows

$$\langle A\rangle = \langle\psi(0)|\,\hat{\mathcal{U}}^\dagger\hat{\mathcal{U}}_0\hat{\mathcal{U}}_0^\dagger\hat{A}\hat{\mathcal{U}}_0\hat{\mathcal{U}}_0^\dagger\hat{\mathcal{U}}\,|\psi(0)\rangle\,.$$

Defining $\hat{\mathcal{U}}_I(t) = \hat{\mathcal{U}}_0^\dagger(t)\hat{\mathcal{U}}(t)$, $\hat{A}_I(t) = \hat{\mathcal{U}}_0^\dagger(t)\hat{A}\hat{\mathcal{U}}_0(t)$, and $|\psi_I(t)\rangle = \hat{\mathcal{U}}_I(t)\,|\psi(0)\rangle$, the expectation value becomes

$$\langle A\rangle = \langle\psi_I(t)|\,\hat{A}_I(t)\,|\psi_I(t)\rangle\,.$$

In the interaction picture, both operators and states evolve. In particular, operators evolve as $\hat{A}_I(t) = \hat{\mathcal{U}}_0^\dagger(t)\hat{A}\hat{\mathcal{U}}_0(t)$ while states evolve as $|\psi_I(t)\rangle = \hat{\mathcal{U}}_I(t)\,|\psi(0)\rangle$. As verified above, one obtains the same result for expectation values as one does in the Schrödinger or Heisenberg pictures.

Our next aim is to obtain a time evolution equation for $\hat{\mathcal{U}}_I(t)$. This is straightforward but involves a few steps:

$$\begin{aligned}i\hbar\partial_t\hat{\mathcal{U}}_I(t) &= \hat{\mathcal{U}}_0^\dagger(t)(-\hat{\mathcal{H}}_0)\hat{\mathcal{U}}(t) + \hat{\mathcal{U}}_0^\dagger(t)(\hat{\mathcal{H}})\hat{\mathcal{U}}(t) = \hat{\mathcal{U}}_0^\dagger(t)(\hat{\mathcal{H}} - \hat{\mathcal{H}}_0)\hat{\mathcal{U}}(t) = \hat{\mathcal{U}}_0^\dagger(t)\hat{V}\hat{\mathcal{U}}(t)\\ &= \hat{\mathcal{U}}_0^\dagger(t)\hat{V}\hat{\mathcal{U}}_0(t)\hat{\mathcal{U}}_0^\dagger(t)\hat{\mathcal{U}}(t) = \hat{V}_I(t)\hat{\mathcal{U}}_I(t).\end{aligned}$$

So our desired time-evolution equation is

$$i\hbar\partial_t\hat{\mathcal{U}}_I(t) = \hat{V}_I(t)\hat{\mathcal{U}}_I(t).$$

2.5 Exercises

Exercise 2.1 *Take a two-dimensional Hilbert space spanned by orthonormal basis $\{|R\rangle\,, |L\rangle\}$. Consider the Hamiltonian*

$$\hat{\mathcal{H}} = -w(|L\rangle\langle R| + |R\rangle\langle L|)$$

where w is a real constant. Find the time-evolution operator corresponding to this Hamiltonian in two ways: (1) by finding an eigenbasis for $\hat{\mathcal{H}}$ (it is okay to write the evolution operator in this eigenbasis) and (2) by directly expanding $\hat{\mathcal{U}}(t) = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}$ and re-summing to obtain a final expression with only two terms.

Physically such a Hamiltonian could describe tunnelling between two potential wells – $|R\rangle$ and $|L\rangle$ describe states states localised in the right and left wells respectively.

Exercise 2.2 *Suppose that we allow w from the previous problem to have time dependence: $w \to w(t)$. Let $w(t) = e^{-\alpha t} w_0$ where $\alpha, w_0 > 0$. What is the time evolution operator for this case? Suppose we start with a particle in the right well. What is the probability that it will be in the right well at time $t = +\infty$? Such time dependence corresponds to raising the potential barrier as a function of time so that tunnelling becomes more and more suppressed as time goes on. Consider your answer for limiting cases (e.g. taking α to be large and positive). Does your result make sense?*

Exercise 2.3 *Verify equation (2.1) with a calculation exclusively in the Schrödinger picture.*

Exercise 2.4 *Show that $[\hat{a}, \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a}] = 2\hat{n}\hat{a}$.*

Exercise 2.5 *Show that the solution of the Heisenberg equations of motion governed by the free-particle Hamiltonian $\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2$ are given by $\hat{x}_{\mathrm{H}}(t) = \hat{x} + \frac{\hat{p}}{m}t$ and $\hat{p}_{\mathrm{H}}(t) = \hat{p}$. Consider an initial (un-normalised) state $\psi_i(x) = e^{ikx} e^{-\frac{x^2}{4\bar{\sigma}_x^2}}$ where k is real and $\bar{\sigma}_x$ is real and positive. Use the Heisenberg equations of motion to compute the expectation value of the position operator and variance in position as a function of time.*

Exercise 2.6 *Consider the Hamiltonian*

$$\hat{\mathcal{H}} = (\varepsilon + g)\hat{a}^\dagger \hat{a} + \frac{g}{2}(\hat{a}\hat{a} + \hat{a}^\dagger \hat{a}^\dagger)$$

where $\hat{a}$ is the typical ladder operator where $[\hat{a}, \hat{a}^\dagger] = 1$ and ε and g are positive. Compute and solve the Heisenberg equations of motion for $\hat{a}_{\mathrm{H}}$. At time $t = 0$, the system starts in the initial state $|0\rangle$ where $|0\rangle$ is the vacuum state: $\hat{a}\,|0\rangle = 0$ (or lowest-energy state of the Harmonic oscillator). Compute the time-dependent expectation value of the number operator $\hat{a}^\dagger \hat{a}$ at later times.

Exercise 2.7 *Consider the Hermitian operators $\hat{\gamma}$ and $\hat{\xi}$ that satisfy the following relations: $\hat{\gamma}^2 = \hat{\xi}^2 = 1$ and $\hat{\gamma}\hat{\xi} = -\hat{\xi}\hat{\gamma}$. From these we form the Hamiltonian*

$$\hat{\mathcal{H}} = iw\hat{\gamma}\hat{\xi}$$

where w is a positive constant with units of energy. Such operators correspond to Majorana Fermions *which are being pursued as potential hardware for quantum computers. Determine the Heisenberg equations of motion for the operators $\hat{\gamma}$ and $\hat{\xi}$. Solve these equations to determine $\hat{\gamma}_H(t)$ and $\hat{\xi}_H(t)$. Suppose at time $t = 0$ we have $\langle\psi(0)|\,\hat{\gamma}\,|\psi(0)\rangle = \cos(\alpha)$ and $\langle\psi(0)|\,\hat{\xi}\,|\psi(0)\rangle = \sin(\alpha)$ where α is a real number. What will be the expectation value of $\hat{\gamma}$ and $\hat{\xi}$ at later times?*

2.A Appendix: Coherent States

In this Appendix, we will describe coherent states. A coherent state is taken to be the eigenstate of the ladder operator $\hat{a}$ (from, for example, the solution of the harmonic oscillator) with eigenvalue $z \in \mathbb{C}$:

$$\hat{a}\,|z\rangle = z\,|z\rangle\,. \tag{2.3}$$

In the following, we are going to work out what $|z\rangle$ is in the basis of harmonic oscillator eigenstates. Denote the harmonic oscillator eigenstates by $|n\rangle$ where n is a non-negative integer. Recall the useful definitions and relations from the solution of the harmonic oscillator:

$$\begin{aligned}
[\hat{a}, \hat{a}^\dagger] &= 1 \\
\hat{n} &= \hat{a}^\dagger \hat{a} \\
\hat{n}\,|n\rangle &= n\,|n\rangle \\
\hat{a}\,|n\rangle &= \sqrt{n}\,|n-1\rangle \quad \text{for } n > 0 \\
\hat{a}\,|0\rangle &= 0 \\
\hat{a}^\dagger\,|n\rangle &= \sqrt{n+1}\,|n+1\rangle\,.
\end{aligned}$$

Using this, we can write equation (2.3) in the basis of the eigenstates of the harmonic oscillator $\langle n|\,\hat{a}\,|z\rangle = z\,\langle n|\,z\rangle$ as

$$\sqrt{n+1}\,\langle n+1|\,z\rangle = z\,\langle n|\,z\rangle.$$

Let $\langle n=0|\,z\rangle = \alpha$. Then through the above relation we find (check)

$$\langle n|\,z\rangle = \frac{z^n}{\sqrt{n!}}\alpha.$$

Inserting a resolution of the identity, we can now express $|z\rangle$ in the $|n\rangle$ basis as

$$|z\rangle = \sum_{n=0}^{\infty} |n\rangle\,\langle n|\,z\rangle = \sum_{n=0}^{\infty} \alpha \frac{z^n}{\sqrt{n!}}\,|n\rangle\,.$$

To fix α, we normalize $|z\rangle$:

$$1 = \langle z|\,z\rangle = |\alpha|^2 \sum_{n=0}^{\infty} \frac{|z|^{2n}}{n!} = |\alpha|^2 e^{|z|^2}.$$

Picking α to be positive and real we have $\alpha = e^{-|z|^2/2}$. So we have arrived at the expression

$$|z\rangle = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}\,|n\rangle\,. \tag{2.4}$$

Using $|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\,|0\rangle$ (from the solution of the harmonic oscillator) gives the alternative expression of the coherent state

$$|z\rangle = e^{-|z|^2/2} e^{z\hat{a}^\dagger}\,|0\rangle\,.$$

Finally, using equation (2.4) we may compute the overlap of two coherent states to be

$$\langle z_1|\,z_2\rangle = e^{-(|z_1|^2+|z_2|^2)/2} e^{z_1^* z_2}.$$

Chapter 3

Symmetries and Transformations in Quantum Mechanics

In this chapter we will learn how we can use symmetries and general transformations to help solve problems in quantum mechanics. We start by considering a transformation that maps a Hilbert space onto itself. We take the transformation to act on states as $|\alpha\rangle \to |\alpha'\rangle$ for any $|\alpha\rangle$ in the Hilbert space. Informally, we say that this transformation 'takes us to the primed frame'. We further impose the constraint: $|\langle\alpha|\beta\rangle| = |\langle\alpha'|\beta'\rangle|$. We take this constraint from physical considerations. That is, we do not want the mapping to change the probabilities of experimental outcomes. A theorem due to Wigner[1] says that there are only two possible types of transformations that satisfy this constraint: (1) unitary and (2) antiunitary. Since we are already familiar with unitary transformations, we will start with this case.

A separate but related topic we will cover in this chapter involves unitary transformations that do not correspond to a symmetry but can be used to transform the Hamiltonian into a simpler form. For instance, sometimes unitary transformations can be used to remove the intrinsic time dependence of a Hamiltonian.

3.1 Unitary transformations

3.1.1 General considerations

We take the transformation to be achieved by a unitary operator $\hat{U}$. That is, $|\alpha'\rangle = \hat{U}|\alpha\rangle$ for all states $|\alpha\rangle$ in the Hilbert space. We can also allow $\hat{U}$ to depend on parameters like time (in this case, we have a family of transformations). Let's see how the Schrödinger equation transforms. Inserting $|\psi\rangle = \hat{U}^\dagger|\psi'\rangle$ into $\hat{\mathcal{H}}|\psi\rangle = i\hbar\partial_t|\psi\rangle$ and rearranging we find

$$\hat{\mathcal{H}}'|\psi'\rangle = i\hbar\partial_t|\psi'\rangle\,.$$

[1] E. P. Wigner, Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren, Springer (1931).

where

$$\hat{\mathcal{H}}' = \hat{U}\hat{\mathcal{H}}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger.$$

A direct calculation verifies that $\hat{\mathcal{H}}'^\dagger = \hat{\mathcal{H}}'$, i.e. $\hat{\mathcal{H}}'$ is Hermitian as we would hope. For special situations when $\hat{\mathcal{H}} = \hat{\mathcal{H}}'$, we say that $\hat{U}$ corresponds to a symmetry of $\hat{\mathcal{H}}$. For this case, if $|\psi\rangle$ satisfies the TDSE, then so will $\hat{U}|\psi\rangle$. On the other hand, such transformations can still be useful when $\hat{\mathcal{H}} \neq \hat{\mathcal{H}}'$. For instance, we might be able to find a unitary transformation that brings $\hat{\mathcal{H}}$ to a simpler form. For the case of time-independent unitary symmetry ($\partial_t\hat{U} = 0$) we have $\hat{\mathcal{H}} = \hat{U}\hat{\mathcal{H}}\hat{U}^\dagger$ which can be rewritten as $[\hat{U}, \hat{\mathcal{H}}] = 0$. For this case, $\hat{U}$ and $\hat{\mathcal{H}}$ will share a complete set of eigenstates – that is, they are simultaneously diagonalisable.

3.1.2 Continuous unitary symmetries

In the following we consider time-independent transformations so that $\hat{\mathcal{H}}' = \hat{U}\hat{\mathcal{H}}\hat{U}^\dagger$. A good strategy for solving the time-independent Schrödinger equation is to find Hermitian operators that commute with the Hamiltonian and simultaneously diagonalise. How is this connected to these ideas concerning unitary transformations? Let $\hat{A}$ be a Hermitian operator. From this, we introduce the family of unitary operators

$$\hat{U}(\xi) = e^{-i\hat{A}\xi}$$

where ξ is restricted to real values. We say that $\hat{A}$ is the generator of the transformation given by $\hat{U}(\xi)$. The following statements are equivalent:

- $[\hat{A}, \hat{\mathcal{H}}] = 0$
- $\hat{U}(\xi)\hat{\mathcal{H}}\hat{U}^\dagger(\xi) = \hat{\mathcal{H}}$ for all real ξ.

If $[\hat{A}, \hat{\mathcal{H}}] = 0$, we say that $\hat{A}$ is the generator of a continuous symmetry of $\hat{\mathcal{H}}$.

Some examples are due.

Continuous translational symmetry

Consider a Hamiltonian describing a particle in one dimension under a potential: $\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + V(\hat{x})$. Suppose that $[\hat{p}, \hat{\mathcal{H}}] = 0$. The preceding equation is just an algebraic relation – what does this mean geometrically? To answer this question, let's consider the equivalent condition $\hat{U}(\xi)\hat{\mathcal{H}}\hat{U}^\dagger(\xi) = \hat{\mathcal{H}}$. In particular, we ask how $\hat{\mathcal{H}}$ changes under this unitary transformation. For convenience we define

$$\hat{U}(\xi) = e^{-i\hat{p}\xi/\hbar}$$

so that ξ has units of length. We recognise this as just the translation operator first encountered in Chapter 1. We find $\hat{\mathcal{H}}' = \frac{1}{2m}\hat{p}^2 + V(\hat{x} - \xi)$. For the Hamiltonian to be invariant under this

transformation, we need $V(\hat{x}-\xi)=V(\hat{x})$ for all ξ. This can only happen when the potential is constant (no $\hat{x}$ dependence): $V(\hat{x})=V_0$. In summary, the condition $[\hat{p},\hat{\mathcal{H}}]=0$ tells us that $\hat{\mathcal{H}}$ has continuous translational symmetry.

Continuous rotational symmetry

Next consider the Hamiltonian describing a particle moving in two dimensions under an external potential: $\hat{\mathcal{H}}=\frac{1}{2m}(\hat{p}_x^2+\hat{p}_y^2)+V(\hat{x},\hat{y})$. Further suppose that $[\hat{L}_z,\hat{\mathcal{H}}]=0$ where $L_z=\hat{x}\hat{p}_y-\hat{y}\hat{p}_x$ is the angular momentum operator. What does this mean?

To answer this, we need to find out how the position and momentum operators transform under $\hat{U}(\xi)=e^{-i\hat{L}_z\xi/\hbar}$. These were worked out (mostly) during lecture and were found to be

$$\begin{pmatrix}\hat{x}'\\ \hat{y}'\end{pmatrix}=\begin{pmatrix}\cos(\xi) & \sin(\xi)\\ -\sin(\xi) & \cos(\xi)\end{pmatrix}\begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix}$$

and

$$\begin{pmatrix}\hat{p}_x'\\ \hat{p}_y'\end{pmatrix}=\begin{pmatrix}\cos(\xi) & \sin(\xi)\\ -\sin(\xi) & \cos(\xi)\end{pmatrix}\begin{pmatrix}\hat{p}_x\\ \hat{p}_y\end{pmatrix}.$$

The unitary transformation rotates both the position and momentum operators (in the same way). Thus, the condition $[\hat{L}_z,\hat{\mathcal{H}}]=0$ tells us that the Hamiltonian is rotationally invariant.

Examples of quantities invariant under continuous rotation are $\hat{x}^2+\hat{y}^2$ and $\hat{p}_x^2+\hat{p}_y^2$ (think about this geometrically). Hamiltonians of the form $\hat{\mathcal{H}}=\frac{1}{2m}(\hat{p}_x^2+\hat{p}_y^2)+V(\hat{x}^2+\hat{y}^2)$ therefore commute with $\hat{L}_z$. This can be exploited to greatly simplify the computation of the eigenspectrum of $\hat{\mathcal{H}}$.

3.1.3 Discrete unitary symmetries

Discrete symmetries are symmetries that do not depend on a continuous parameter. A circle has continuous rotational symmetry while a square has discrete rotational symmetry (corresponding to integer multiples of $\pi/2$ rotations).

Parity symmetry

From Quantum I (or elsewhere) you have likely encountered parity symmetry. We summarise here the important properties of the parity operator $\hat{S}$:

$$\begin{aligned}\hat{S}&=\hat{S}^\dagger=\hat{S}^{-1}\\ \hat{S}\hat{x}\hat{S}&=-\hat{x}\\ \hat{S}\hat{p}\hat{S}&=-\hat{p}\\ \hat{S}\,|x\rangle&=|-x\rangle\\ \hat{S}\,|p\rangle&=|-p\rangle\,.\end{aligned}$$

A Hamiltonian with parity symmetry satisfies $[\hat{\mathcal{H}},\hat{S}]=0$. Its eigenfunctions can be taken to be either even or odd functions of x.

Bloch's theorem

Our next example is likely less familiar. Take again our favourite Hamiltonian $\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + V(\hat{x})$ and suppose that the potential has the following property: $V(\hat{x}+a) = V(\hat{x})$. An example of such a potential is $V(\hat{x}) = \gamma\cos(\frac{2\pi}{a}x)$. While such a Hamiltonian does not necessarily commute with $\hat{p}$, it satisfies $[\hat{U}(a), \hat{\mathcal{H}}] = 0$ where $\hat{U}(a) = e^{-i\hat{p}a/\hbar}$ (check). Therefore $\hat{U}(a)$ and $\hat{\mathcal{H}}$ can be simultaneously diagonalised.

Let's start with the translation operator and solve

$$\hat{U}(a)\left|\phi_\lambda\right\rangle = \lambda\left|\phi_\lambda\right\rangle.$$

Note that since $\hat{U}(a)$ is not Hermitian, λ does not need to be real. The eigenvalues of unitary operators, however, have their own requirements. To see this, we multiply the preceding equation with its adjoint to find

$$\left\langle\phi_\lambda\right|\hat{U}^\dagger(a)\hat{U}(a)\left|\phi_\lambda\right\rangle = \left\langle\phi_\lambda\right|\left.\phi_\lambda\right\rangle = |\lambda|^2\left\langle\phi_\lambda\right|\left.\phi_\lambda\right\rangle$$

and so $|\lambda| = 1$. To make the fact that $|\lambda| = 1$ apparent we write $\lambda = e^{-ika}$ for some real k (having units of 1/length). We also relabel $|\phi_\lambda\rangle$ as $|\phi_k\rangle$. So we have

$$\hat{U}(a)\left|\phi_k\right\rangle = e^{-ika}\left|\phi_k\right\rangle.$$

We have not done much yet. We have just recognised the condition on eigenvalues of unitary operators and relabelled.

Next, write this equation in the position basis to find

$$\phi_k(x-a) = e^{-ika}\phi_k(x).$$

Define $u_k(x) = e^{-ikx}\phi_k(x)$. From the above equation, we see that $u_k(x-a) = u_k(x)$. This is true for arbitrary x and so $u_k(x+a) = u_k(x)$. In other words, $u_k(x)$ is periodic!

In summary, eigenstates of Hamiltonians with discrete translational symmetry can be written as

$$\phi_k(x) = e^{ikx}u_k(x)$$

where $u_k(x)$ has the same periodicity as the Hamiltonian. This is the celebrated Bloch's theorem. It is routinely used in the field of solid state physics to understand the properties of electrons in solids.

3.1.4 Time-dependent unitary transformations

The unitary operators we have considered in the previous few sections were time independent. We now move on to the case of time-dependent unitary transformations. The discussion here will be somewhat brief – such transformations are probably best understood by working through problems.

The so-called Galilean transformation can be achieved with the unitary operator

$$\hat{U}(t) = e^{-i\hat{p}vt/\hbar} e^{i\hat{x}mv/\hbar} e^{i\frac{1}{2}mv^2 t/\hbar}.$$

With this operator, one can work out that

$$\hat{x}' = \hat{U}(t)\hat{x}\hat{U}^\dagger(t) = \hat{x} - vt$$

and

$$\hat{p}' = \hat{U}(t)\hat{p}\hat{U}^\dagger(t) = \hat{p} - mv.$$

This is the operator analog of the Galilean transformation from classical mechanics. It describes how position and momentum coordinates change when you transform to a 'boosted' frame. In relativity this transformation is replaced by the Lorentz transformation. The Galilean transformation is appropriate for this module though because we are only considering non-relativistic scenarios. The free particle Hamiltonian $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m}$ is invariant under the Galilean transformation as one might expect. That is, for this Hamiltonian, $\hat{\mathcal{H}} = \hat{U}\hat{\mathcal{H}}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger$. As a result, given a solution of the time-dependent Schrödinger equation $|\psi\rangle$, you can find that another one is $\hat{U}^\dagger|\psi\rangle$.

Such transformations can be very useful for solving time-dependent problems. For instance, suppose that we have a time-dependent Hamiltonian of the form

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x} - vt).$$

A strategy for solving this would be to boost to the moving frame (using $\hat{U}$ above with the opposite sign of v). The resulting Hamiltonian will then be time-independent. One can then solve for, say, a stationary state of $\mathcal{H}'$ and transform back to obtain a time-dependent solution of the original Schrödinger equation.

Time-dependent unitary transformations also are very useful for problems where it is helpful to transform to a 'non-intertial' or accelerating reference frame. You can use such techniques to solve the quantum version of the forced Harmonic oscillator. An exercise at the end of this chapter focuses on the case of uniform acceleration.

3.2 Relation between symmetry and degeneracy

One often associates symmetries with degeneracies. This can be systematically handled with the machinery of group representation theory. In the following, we will illustrate the main idea without getting bogged down in the formalism. The setup: Suppose we managed to find two operators $\hat{A}$ and $\hat{B}$ that both commute with a Hamiltonian $\hat{\mathcal{H}}$ of interest to us but not with each other: $[\hat{A}, \hat{B}] = \hat{C} \neq 0$.

Now let us consider an eigenstate $|\phi\rangle$ of $\hat{\mathcal{H}}$ with eigenvalue E: $\hat{\mathcal{H}}|\phi\rangle = E|\phi\rangle$. This state will either be non-degenerate or it will be degenerate.[2] Let's consider the case of it being non-degenerate. In this case, $|\phi\rangle$ will also be an eigenstate of both $\hat{A}$ and $\hat{B}$ because of the following

[2]To be precise, we say that an eigenenergy E is n-fold degenerate (where $n > 1$) if there are exactly n linearly independent eigenstates with eigenenergy E. We will also say an eigenstate $|\phi\rangle$ is degenerate if there exists another eigenstate, linearly independent of $|\phi\rangle$, but with the same eigenenergy as $|\phi\rangle$.

reason: Since $\hat{A}$ commutes with $\hat{\mathcal{H}}$, $\hat{A}\,|\phi\rangle$ will be an eigenstate of $\hat{\mathcal{H}}$ with eigenvalue E (check). So now we have two eigenstates of $\hat{\mathcal{H}}$ with eigenvalue E, namely $\hat{A}\,|\phi\rangle$ and $|\phi\rangle$. Since E is taken to be non-degenerate, its corresponding eigenstate is unique (up to amplitude and phase). Therefore it must be that $\hat{A}\,|\phi\rangle = a\,|\phi\rangle$ for some scalar a. The same reasoning tells us that $\hat{B}\,|\phi\rangle = b\,|\phi\rangle$. From this we have

$$\hat{C}\,|\phi\rangle = [\hat{A}, \hat{B}]\,|\phi\rangle = (ab - ba)\,|\phi\rangle = 0.$$

We have learned the following about an eigenstate $|\phi\rangle$ of $\hat{\mathcal{H}}$. If $|\phi\rangle$ is a non-degenerate eigenstate of $\hat{\mathcal{H}}$ then $\hat{C}\,|\phi\rangle = 0$. To put this another way: if $|\phi\rangle$ is an eigenstate of $\hat{\mathcal{H}}$ and $\hat{C}\,|\phi\rangle \neq 0$ (that is $|\phi\rangle$ is not in the null space of $\hat{\mathcal{H}}$) then $|\phi\rangle$ is degenerate. For the case when $\hat{C}$ is invertible or 'full rank', all eigenvalues of $\hat{\mathcal{H}}$ will be at least doubly degenerate.

From the above, we can learn a lot about degeneracies in the spectrum of a Hamiltonian if we can find two operators that commute with the Hamiltonian but not with each other. Such a procedure is very useful for Hamiltonians that we do not know how to diagonalise.

Below we apply this procedure to a rather simple problem. While using such symmetry arguments for analysing this simple problem could be viewed as 'overkill', it is interesting to see how this all works out.

Example

Consider a free particle confined to move along a circle of circumference L. The Hamiltonian for this system is $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m}$ and we further have the constraint that $\phi(x) = \phi(x + L)$ for all states in the Hilbert space. The eigenstates and eigenenergies of this system (in the position basis) are

$$\phi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}$$
$$E_n = \frac{\hbar^2 k_n^2}{2m}$$

where $k_n = \frac{2\pi}{L} n$ (n is an integer). The k-values are restricted in this way due to the periodicity requirement.

This Hamiltonian has both parity and (continuous) translational symmetry: $[\hat{p}, \hat{\mathcal{H}}] = [\hat{S}, \hat{\mathcal{H}}] = 0$. If $[\hat{S}, \hat{p}] \neq 0$ we are in luck. A calculation shows $[\hat{S}, \hat{p}] = 2\hat{S}\hat{p}$. This operator is nearly, but not quite, invertible. It has a single null vector which is which is the state with $k_n = 0$. So if an eigenstate does not have $k_n = 0$ (or $n = 0$) it will be degenerate. Comparing to the above we see that, indeed, all states are (doubly) degenerate ($E_n = E_{-n},\ \phi_n \neq \phi_{-n}$) except when $n = 0$.

It is useful to contrast this result with the particle in an infinite square well potential. The spectrum of the latter problem has no degeneracies. While a parity symmetry for the square well exists (shift the box say so that it is centred at $x = 0$) it does not have translational invariance.

3.3 Antiunitary transformations and time-reversal symmetry

Think about watching a video involving simple kinematic motion. Now suppose we run the video backwards. How are the kinematic quantities affected? This is how we think about the operation of time reversal. In particular, under time reversal we require that

$$\hat{x} \to \hat{x'} = \hat{T}\hat{x}\hat{T}^{-1} = \hat{x}$$
$$\hat{p} \to \hat{p}' = \hat{T}\hat{p}\hat{T}^{-1} = -\hat{p}.$$

where $\hat{T}$ is the time-reversal operator which is to be determined. We additionally require the spin operator to transform under time reversal as

$$\hat{\mathbf{S}} \to -\hat{\mathbf{S}}.$$

Since we have not properly covered spin yet, you can think of the above by making the analogy with angular momentum. For instance, think about watching a video of a spinning plate and then watching the video backwards – its angular momentum changes sign. If a Hamiltonian is unchanged by the above operations, then we say it is time-reversal invariant.

Next we search for an operator that carries out the above transformation. It does not take long to convince ourselves that a unitary transformation will not work. That is, taking $\hat{T} = \hat{U}$ where $\hat{U}^\dagger\hat{U} = \mathbb{1}$ we have $[\hat{x}', \hat{p}'] = \hat{U}[\hat{x}, \hat{p}]\hat{U}^\dagger = i\hbar$. But we also have $[\hat{x}', \hat{p}'] = [\hat{x}, -\hat{p}] = -i\hbar$. We therefore, due to Wigner's theorem, resort to an antiunitary transformation.

3.3.1 General properties of antiunitary transformations

An antiunitary transformation is a mapping $|\alpha\rangle \to \hat{T}|\alpha\rangle = |\alpha'\rangle$, $|\beta\rangle \to \hat{T}|\beta\rangle = |\beta'\rangle$ of a Hilbert space onto itself for which $\langle\alpha|\,\beta\rangle = \langle\beta'|\,\alpha'\rangle$ for all states $|\alpha\rangle$ and $|\beta\rangle$ in the Hilbert space. From this it can be deduced that

$$\hat{T}(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^*\hat{T}|\alpha\rangle + c_2^*\hat{T}|\beta\rangle$$

where c_1 and c_2 are scalars (check). This is the requirement for antilinear operators and so antiunitary operators are also antilinear operators. As Dirac's bra-ket notation was invented to handle linear operators, we have to exercise some caution when incorporating antilinear operators. In particular, we will understand $\hat{T}$ as always acting on kets to its right and we will not attempt to define $\hat{T}^\dagger$. We also derived in lecture the following useful relation

$$\langle\alpha'|\,\hat{A}'\,|\beta'\rangle = \langle\beta|\,\hat{A}^\dagger\,|\alpha\rangle$$

where $\hat{A}$ is an operator and $\hat{A}' = \hat{T}A\hat{T}^{-1}$.

3.3.2 Time reversal for a spinless particle

As a first pass at developing a time-reversal operator let us try $\hat{T} = \hat{K}$ where we require $\hat{K}$ to be antilinear and also $\hat{K}\,|x\rangle = |x\rangle$ for all position eigenkets $|x\rangle$. We will have to augment later when we incorporate spin. Is $\hat{K}$ an antiunitary operator? Let's take two states in the Hilbert space $|\alpha\rangle$ and $|\beta\rangle$. To find out how $\hat{K}$ acts on these we expand in the position basis:

$$\begin{aligned}|\alpha'\rangle =&\hat{K}\,|\alpha\rangle = \hat{K}\int dx\,\langle x|\,\alpha\rangle\,|x\rangle = \hat{K}\int dx\alpha(x)\,|x\rangle \\ &= \int dx\alpha^*(x)\,|x\rangle\end{aligned}$$

due to antilinearity. Similarly,

$$|\beta'\rangle = \int dx\beta^*(x)\,|x\rangle\,.$$

Therefore,

$$\langle\beta'|\,\alpha'\rangle = \int dx\beta(x)\alpha^*(x) = \langle\alpha|\,\beta\rangle$$

and so this is an antiunitary transformation. Next we observe that $\hat{K}^2 = \mathbb{1}$. This can be verified by applying $\hat{K}$ to the expression for $|\alpha'\rangle$ above. We find $\hat{K}^2\,|\alpha\rangle = |\alpha\rangle$. Since $|\alpha\rangle$ is arbitrary, $\hat{K}^2 = \mathbb{1}$ or $\hat{K}^{-1} = \hat{K}$.

Next let's see what this operation does to momentum kets. Expanding in the position basis,

$$\hat{K}\,|p\rangle = \hat{K}\int dx\,\langle x|\,p\rangle\,|x\rangle = \int dx\,\langle x|\,p\rangle^*\,|x\rangle = \int dx\,\langle x|\,-p\rangle\,|x\rangle = |-p\rangle$$

and so $\hat{K}\,|p\rangle = |-p\rangle$.

Finally, let's figure out how the position and momentum operators transform. Acting with $\hat{x}' = \hat{K}\hat{x}\hat{K}^{-1}$ on an arbitrary ket we have

$$\begin{aligned}\hat{x}'\,|\alpha\rangle = \hat{K}\hat{x}\hat{K}\,|\alpha\rangle = \hat{K}\hat{x}\hat{K}\int dx\alpha(x)\,|x\rangle = \hat{K}\hat{x}\int dx\alpha^*(x)\,|x\rangle \\ = \hat{K}\int dx\alpha^*(x)x\,|x\rangle = \int dx\alpha(x)x\,|x\rangle = \hat{x}\int dx\alpha(x)\,|x\rangle = \hat{x}\,|\alpha\rangle\,.\end{aligned}$$

Therefore $\hat{x}' = \hat{x}$ as we had hoped. Similarly (denoting $\langle p|\,\alpha\rangle = \tilde{\alpha}(p)$),

$$\begin{aligned}\hat{p}'\,|\alpha\rangle = \hat{K}\hat{p}\hat{K}\,|\alpha\rangle = \hat{K}\hat{p}\hat{K}\int dp\tilde{\alpha}(p)\,|p\rangle = \hat{K}\hat{p}\int dp\tilde{\alpha}^*(p)\,|-p\rangle \\ = -\hat{K}\int dp\tilde{\alpha}^*(p)p\,|-p\rangle = -\int dp\tilde{\alpha}(p)p\,|p\rangle = -\hat{p}\int dp\tilde{\alpha}(p)\,|p\rangle = -\hat{p}\,|\alpha\rangle\end{aligned}$$

and so $\hat{p}' = -\hat{p}$. Therefore, $\hat{K}$ fits the bill for a time-reversal operator for a particle without spin and for this case we put $\hat{T} = \hat{K}$.

3.3.3 Time reversal: generalisations

Let's now go back to our discussions of a general anti-unitary operator $\hat{T}$. Suppose that $\{|\phi_n\rangle\}$ forms an orthonormal basis for the Hilbert space under consideration. As usual, we denote the transformed states to be $|\phi'_n\rangle = \hat{T}|\phi_n\rangle$. Then this transformed basis of states also forms an orthonormal basis. This follows directly from the fact that the transformation is antiunitary: $\langle\phi'_n|\,\phi'_m\rangle = \langle\phi_m|\,\phi_n\rangle = \delta_{nm}$.

We can expand this transformed basis of states in terms of the original states as

$$|\phi'_n\rangle = \sum_m U_{mn}\,|\phi_m\rangle\,.$$

The orthogonality of the transformed states implies that U_{mn} are the entries of a unitary matrix. We can also write this in operator form as $|\phi'_n\rangle = \hat{U}\,|\phi_n\rangle$ where $\hat{U} = \sum_{nm}|\phi_n\rangle\langle\phi_m|\,U_{nm}$.

Next, let's consider how a general state α in the Hilbert space transforms. Denoting $\alpha_n = \langle\phi_n|\,\alpha\rangle$ we have

$$\hat{T}\,|\alpha\rangle = \hat{T}\sum_n \alpha_n\,|\phi_n\rangle = \sum_n \alpha_n^*\,|\phi'_n\rangle\,.$$

The same can be achieved if we write $\hat{T} = \hat{U}\hat{K}$ where $\hat{K}$ is an antilinear operator that leaves the original basis unchanged: $\hat{K}\,|\phi_n\rangle = |\phi_n\rangle$. We have thus found the most general form for the anti-unitary operator:

$$\hat{T} = \hat{U}\hat{K}.$$

We note also that $\hat{T}^{-1} = \hat{K}\hat{U}^\dagger$.

Next let's consider how an arbitrary operator $\hat{A}$ transforms under $\hat{T}$. We have

$$\hat{T}\hat{A}\hat{T}^{-1} = \hat{U}\hat{K}\hat{A}\hat{K}\hat{U}^\dagger.$$

Since we need to be extra careful with antiunitary operators, let's consider the piece $\hat{K}\hat{A}\hat{K}$ by itself. First let's write $\hat{A} = \sum_{nm} A_{nm}\,|\phi_n\rangle\langle\phi_m|$ where $A_{nm} = \langle\phi_n|\,\hat{A}\,|\phi_m\rangle$. Acting with an arbitrary preferred basis state, we have

$$\begin{aligned}\hat{K}\hat{A}\hat{K}\,|\phi_m\rangle = \hat{K}\hat{A}\,|\phi_m\rangle &= \hat{K}\sum_n A_{nm}\,|\phi_n\rangle \\ &= \sum_n A_{nm}^*\,|\phi_n\rangle\,.\end{aligned}$$

Introducing $\hat{A}^* = \sum_{nm} A_{nm}^*\,|\phi_n\rangle\langle\phi_m|$ we can check that $\hat{K}\hat{A}\hat{K}\,|\phi_m\rangle = \hat{A}^*\,|\phi_m\rangle$ and so $\hat{K}\hat{A}\hat{K} = \hat{A}^*$.

One must be very careful with such expressions since the act of complex conjugation depends on the basis being used. The above should read "the complex conjugate of $\hat{A}$ in the $\{|\phi_n\rangle\}$ basis." Using another basis, and taking the complex conjugate as above will generally lead to a different

result. In contrast, the adjoint operation is basis independent. With this caveat noted, the time-reversed expression for the operator $\hat{A}$ is:

$$\hat{T}\hat{A}\hat{T}^{-1} = \hat{U}\hat{A}^*\hat{U}^\dagger.$$

The above extension is required when generalising the notion of time-reversal to treat spin. Additionally, one can find the time-reversal operator for more complex systems, like collections of particles with both spatial and spin degrees of freedom, in the same manner. It turns out that either $\hat{T}^2 = \mathbb{1}$ or $\hat{T}^2 = -\mathbb{1}$. In particular $\hat{T}^2 = -\mathbb{1}$ for 'half-integer spin' systems while $\hat{T}^2 = \mathbb{1}$ for 'integer spin' systems. This has important consequences.

3.3.4 Consequences of time-reversal symmetry

In this last section, we state some consequences of time-reversal symmetry. In all cases, we take the relevant Hamiltonian time independent and to be time-reversal invariant $\hat{T}\hat{\mathcal{H}}\hat{T}^{-1} = \hat{\mathcal{H}}$. The following consequences were shown in lecture.

Consequence 1. Suppose that $|\psi(t)\rangle$ is a solution of the TDSE. Then $\hat{T}\,|\psi(-t)\rangle$ is also a solution.

Consequence 2. A non-degenerate eigenstate $|\phi\rangle$ of $\hat{\mathcal{H}}$ can be taken to be invariant under time reversal: $|\phi\rangle = \hat{T}\,|\phi\rangle$.

Consequence 3 (Kramer's theorem). Suppose that $\hat{T}^2 = -\mathbb{1}$. Then there are no non-degenerate eigenstates of $\hat{\mathcal{H}}$.

3.4 Exercises

Exercise 3.1 *Consider a general Hermitian quantity which is quadratic in the position operators in two spatial dimensions: $\hat{A} = \sum_{ij} Q_{ij}\hat{x}_i\hat{x}_j$. Show that we can take the 2×2 matrix Q to be real and symmetric without loss of generality. Suppose that $[\hat{A}, \hat{L}_z] = 0$. What conditions does this impose on Q?*

Exercise 3.2 *From $\hat{\mathcal{H}}'$ defined early in this Chapter, show that $\hat{\mathcal{H}} = \hat{U}^\dagger\hat{\mathcal{H}}'\hat{U} - i\hbar\hat{U}^\dagger\partial_t\hat{U}$.*

Exercise 3.3 *(more difficult) Consider the Hamiltonian $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x} - \frac{1}{2}\alpha t^2)$ where α is a positive constant. Find a time-dependent unitary transformation that makes this Hamiltonian time-independent. Write the transformed Hamiltonian as $\hat{\mathcal{H}}' = \frac{\hat{p}^2}{2m} + V_{\text{eff}}(\hat{x})$ where V_{eff} is to be determined.*

Exercise 3.4 *Consider a two-dimensional Hilbert space spanned orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle\}$. In this basis, suppose we have three (spin) operators $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ that take on the following matrix forms*

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \text{ and } \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

in this basis (where $(S_x)_{nm} = \langle\phi_n|\,\hat{S}_x\,|\phi_m\rangle$, etc). Find a unitary operator $\hat{U}$ such that the spin operators change sign under time reversal where $\hat{T} = \hat{U}\hat{K}$ and $\hat{K}\,|\phi_n\rangle = |\phi_n\rangle$.

Exercise 3.5 *Using the result from the previous exercise, find the most general Hamiltonian in this two-dimensional Hilbert space that is invariant under time reversal.*

Exercise 3.6 *(more difficult) Suppose we have a time-reversal invariant $\hat{\mathcal{H}}$ and that $\hat{T}^2 = -\mathbb{1}$. By Kramer's theorem, we know that $\hat{\mathcal{H}}$ will have no non-degenerate states. In this exercise we prove a more general result. Show that $\hat{\mathcal{H}}$ can only have even degeneracies (that is it cannot have an n-fold degeneracy for odd n).*

Chapter 4

Spin and Elements of Quantum Technologies

In the first part of this chapter we will review orbital angular momentum and introduce spin. We will learn that the formalism used to describe a spin-half system is all that is needed to describe a qubit, which is the fundamental building block of a quantum computer. In the final part of the chapter we will expand our discussion to quantum technologies.

4.1 Spin and angular momentum

4.1.1 Algebraic theory of orbital angular momentum

To start we will review the key properties of orbital angular momentum. It is assumed that the reader has worked with angular momentum in quantum mechanics before. For reference, each of the recommended books for this module cover angular momentum. The orbital angular momentum operator is defined as $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$. Its components can be shown to satisfy the following algebra:

$$[\hat{L}_a, \hat{L}_b] = \sum_c i\hbar \varepsilon_{abc} \hat{L}_c \tag{4.1}$$

where ε_{abc} is the Levi-Civita symbol.[1]

The algebra (4.1) can be used to learn a lot about the spectrum of the commuting observables

[1]The Levi-Civita symbol ε_{abc} takes on the values of -1,1, or 0. In particular if abc is an even permutation of xyz it is 1. If it is an odd permutation of xyz it is -1. Otherwise $\varepsilon_{abc} = 0$. It is worthwhile learning how to incorporate ε_{abc} as it is a big space saver, and can also help simplify computations. The summation in (4.1) $\sum_c$ is understood to be over $c = x, y, z$. Sometimes the following notation is used: $\hat{L}_1 = \hat{L}_x$, $\hat{L}_2 = \hat{L}_y$, $\hat{L}_3 = \hat{L}_z$. In this case the summation is over $c = 1, 2, 3$.

$\hat{L}^2$ and $\hat{L}_z$. Denoting the eigenstates as $|\ell, m\rangle$ in Quantum 1 it was found that

$$\begin{aligned}
\hat{L}^2 |\ell, m\rangle &= \hbar^2 \ell(\ell+1) |\ell, m\rangle \\
\hat{L}_z |\ell, m\rangle &= \hbar m |\ell, m\rangle \\
\hat{L}_+ |\ell, m\rangle &= \hbar\sqrt{\ell(\ell+1) - m(m+1)}\, |\ell, m+1\rangle \\
\hat{L}_- |\ell, m\rangle &= \hbar\sqrt{\ell(\ell+1) - m(m-1)}\, |\ell, m-1\rangle
\end{aligned}$$

where $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$. It was found that ℓ must take on non-negative integer or non-negative half-integer values, and m must take values from $-\ell$ to ℓ in integer steps. It should be emphasised that these relations follow purely from (4.1). In particular, the fact that $\hat{\mathbf{L}}$ can be written in terms of position and momentum operators was not used.

4.1.2 Orbital angular momentum states in real space: spherical harmonics

We next move on to consider position space expressions for the eigenstates of the previous subsection. In the following we will use spherical coordinates where $x = r\sin(\theta)\cos(\varphi)$, $y = r\sin(\theta)\sin(\varphi)$, $z = r\cos(\theta)$. In going to the position basis one makes the substitutions $\hat{p}_a \to -i\hbar\frac{\partial}{\partial_{x_a}}$ and $\hat{x}_a \to x_a$. Making this substitution, and converting to spherical coordinates, one finds through a rather onerous but otherwise straightforward calculation that

$$\hat{L}^2 \to -\hbar^2 \left(\frac{1}{\sin(\theta)} \partial_\theta (\sin(\theta)\partial_\theta) + \frac{1}{\sin^2(\theta)} \partial_\varphi^2 \right) \tag{4.2}$$

$$\hat{L}_z \to -i\hbar\partial_\varphi. \tag{4.3}$$

The coordinate r does not make an appearance in the above. Accordingly, we introduce the position ket $|\theta, \varphi\rangle$ which can thought of as denoting a localised state on the unit sphere. The spherical harmonics defined as $Y_{\ell,m}(\theta, \varphi) = \langle\theta, \varphi|\, \ell, m\rangle$ satisfy the differential equations

$$-\frac{1}{\sin(\theta)} \partial_\theta (\sin(\theta)\partial_\theta Y_{\ell,m}) - \frac{1}{\sin^2(\theta)} \partial_\varphi^2 Y_{\ell,m} = \ell(\ell+1) Y_{\ell,m} \tag{4.4}$$

$$-i\partial_\varphi Y_{\ell,m} = m Y_{\ell,m}. \tag{4.5}$$

Importantly, the second differential equation tells us that m (and consequently ℓ) must be an integer. Otherwise, $Y_{\ell,m}$ would not satisfy the required property $Y_{\ell m}(\theta, \varphi + 2\pi) = Y_{\ell m}(\theta, \varphi)$. This bit of information was missed in the purely algebraic treatment of the previous subsection.

The spherical harmonics are routinely used in many areas of applied mathematics. Explicit expressions for $Y_{\ell,m}$ for modest values of ℓ and m are in standard textbooks and on the web.

4.2 Spin

Elementary particles possess a property called spin which resembles angular momentum in various ways. The word 'spin' comes from the analogy with a classical spinning rigid body (which

carries angular momentum). However this analogy does not go very far. By their very nature, elementary particles cannot be broken down into more basic components – so what's spinning?

The spin operators are taken to satisfy the same algebra as the orbital angular momentum operators:

$$[\hat{S}_a, \hat{S}_b] = \sum_c i\hbar\varepsilon_{abc}\hat{S}_c. \tag{4.6}$$

All the results deduced from the algebraic relation carry over:

$$\begin{aligned}
\hat{S}^2 |s,m\rangle &= \hbar^2 s(s+1) |s,m\rangle \\
\hat{S}_z |s,m\rangle &= \hbar m |s,m\rangle \\
\hat{S}_+ |s,m\rangle &= \hbar\sqrt{s(s+1) - m(m+1)} |s,m+1\rangle \\
\hat{S}_- |s,m\rangle &= \hbar\sqrt{s(s+1) - m(m-1)} |s,m-1\rangle
\end{aligned}$$

where $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$. For spin it is customary to use s instead of ℓ.

In contrast to ℓ from orbital angular momentum, s is a fundamental ineradicable quantity for any elementary particle. For instance, the Higgs Boson has $s = 0$, the electron has $s = 1/2$, the photon has $s = 1$, while the graviton has $s = 2$. The value of s for an elementary particle is fixed by nature. On the other hand, there is nothing fundamental about ℓ.

4.2.1 Spin Half

We will now consider the simplest non-trivial case of $s = 1/2$. This case is particularly important because the methods apply to any 'two-level system'. A two-level system is a system living in a Hilbert space of dimension two. It is a quintessential quantum system with no immediate classical counterpart. The qubit, which will be discussed more later and which is the building block of a quantum computer, can naturally be thought of as a spin-half system.

We start by simplifying the notation as follows:

$$\begin{aligned}
|\uparrow\rangle &= |s = 1/2, m = 1/2\rangle \\
|\downarrow\rangle &= |s = 1/2, m = -1/2\rangle .
\end{aligned}$$

In words we call these two states 'spin up' and 'spin down' respectively. A general spin half state can be written as

$$|\psi\rangle = \psi_\uparrow |\uparrow\rangle + \psi_\downarrow |\downarrow\rangle .$$

It frequently proves useful to write this state as a vector:

$$\psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}$$

Such complex vectors are called spinors.

One may write 2×2 matrices corresponding to the spin operators as

$$S_a = \begin{pmatrix} \langle\uparrow| \hat{S}_a |\uparrow\rangle & \langle\uparrow| \hat{S}_a |\downarrow\rangle \\ \langle\downarrow| \hat{S}_a |\uparrow\rangle & \langle\downarrow| \hat{S}_a |\downarrow\rangle \end{pmatrix}.$$

The bra denotes the row while the ket denotes the column. Using the expressions from the previous subsection (check), one finds

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

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Example

To practice converting quantities to matrix form, let's consider the Hamiltonian $\hat{\mathcal{H}} = -B\hat{S}_z$ where B is real. Let's consider the evolution of a state that initially has the value $|\psi(t=0)\rangle = \cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)|\downarrow\rangle$. This describes a single spin under the presence of an external magnetic field.

The TDSE $i\hbar\partial_t |\psi\rangle = \hat{\mathcal{H}} |\psi\rangle$ can be written in matrix form as

$$i\hbar\partial_t \psi = \mathcal{H}\psi$$

where $\mathcal{H} = -BS_z$. This expression can be derived by inserting a resolution of the identity between $\hat{\mathcal{H}}$ and $|\psi\rangle$ and multiplying the equation on the left by $\langle\uparrow|$ and $\langle\downarrow|$. The time-evolution matrix is

$$\mathcal{U}(t) = e^{\frac{i}{\hbar}BS_z t}.$$

The expectation values of the spin operators can be directly worked out. They are found to be

$$\begin{aligned} \langle\psi(t)| \hat{S}_x |\psi(t)\rangle &= \psi^\dagger(t) S_x \psi(t) = \frac{\hbar}{2}\sin(\theta)\cos(Bt) \\ \langle\psi(t)| \hat{S}_y |\psi(t)\rangle &= -\frac{\hbar}{2}\sin(\theta)\sin(Bt) \\ \langle\psi(t)| \hat{S}_z |\psi(t)\rangle &= \frac{\hbar}{2}\cos(\theta). \end{aligned}$$

The spin precesses about the z-axis like a spinning top precesses when in a gravitational field. This is called Larmor precession.

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The Pauli matrices are defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

They are related to the spin-half matrices as $S_a = \frac{\hbar}{2}\sigma_a$. Any Hermitian 2×2 matrix M can be written in terms of Pauli matrices as

$$M = a\mathbb{1} + \mathbf{B} \cdot \boldsymbol{\sigma}$$

where a is a real number and $\mathbf{B}$ is a real vector. Also, $\boldsymbol{\sigma}$ is a vector composed of the Pauli matrices so that $\mathbf{B} \cdot \boldsymbol{\sigma} = B_x\sigma_x + B_y\sigma_y + B_z\sigma_z$.

In the following we discover some useful mathematical relations using the Pauli matrices.[2] The Pauli matrices satisfy the following multiplication rule which can be verified explicitly:

$$\sigma_a\sigma_b = \delta_{ab}\mathbb{1} + i\sum_c \varepsilon_{abc}\sigma_c.$$

From this we see that, for vectors $\mathbf{B}_1$ and $\mathbf{B}_2$,

$$(\mathbf{B}_1 \cdot \boldsymbol{\sigma})(\mathbf{B}_2 \cdot \boldsymbol{\sigma}) = \mathbf{B}_1 \cdot \mathbf{B}_2\mathbb{1} + i(\mathbf{B}_1 \times \mathbf{B}_2) \cdot \boldsymbol{\sigma}.$$

As a special case, when $\mathbf{B} \equiv \mathbf{B}_1 = \mathbf{B}_2$,

$$(\mathbf{B} \cdot \boldsymbol{\sigma})^2 = B^2\mathbb{1}.$$

Let's write $\mathbf{B}$ in terms of its magnitude and direction as $\mathbf{B} = B\mathbf{e}_B$ where $\mathbf{e}_B$ is a unit vector pointing along $\mathbf{B}$. This can be used to show that

$$e^{-i\mathbf{B}\cdot\boldsymbol{\sigma}} = \cos(B)\mathbb{1} - i\sin(B)\mathbf{e}_B \cdot \boldsymbol{\sigma}. \tag{4.7}$$

which is arrived at by expanding the exponential and recognising that the even terms are proportional to $\mathbb{1}$ while the odd terms are proportional to $\mathbf{e}_B \cdot \boldsymbol{\sigma}$ (recall Exercise 2.1). Such an expression is useful for, say, writing down the time-evolution matrix for a spin-half system.

Next, we write down the following identity

$$e^{-i\frac{\alpha}{2}\sigma_b}\sigma_a e^{i\frac{\alpha}{2}\sigma_b} = \sigma_a\cos(\alpha) + \frac{i}{2}\sin(\alpha)[\sigma_a, \sigma_b]. \tag{4.8}$$

which is valid for $a \neq b$. This can be derived directly by using (4.7) and the multiplication rule for Pauli matrices (check). A slightly longer derivation utilises only the commutation relations of the Pauli matrices (or spin-half matrices) and uses methods from the Chapter 3. Therefore relations similar to (4.8) exist for other quantities satisfying the angular momentum algebra.[3] Relation (4.7) on the other hand is specific to spin half systems.

Next let's try to diagonalise a general 2×2 Hamiltonian of the form $\mathcal{H} = \mathbf{B}\cdot\boldsymbol{\sigma}$ for arbitary real vector $\mathbf{B}$. For some θ and φ, $\mathbf{B}$ can be written as $\mathbf{B} = B(\sin(\theta)\cos(\varphi)\mathbf{i} + \sin(\theta)\sin(\varphi)\mathbf{j} + \cos(\theta)\mathbf{k})$. Next, letting

$$U = e^{-i\frac{\varphi}{2}\sigma_z}e^{-i\frac{\theta}{2}\sigma_y}$$

[2] Incidentally, the matrices $\mathbb{1}$, $i\sigma_x$, $i\sigma_y$, $i\sigma_z$ form a representation of the quaternion group.

[3] For instance, $e^{-i\frac{\alpha}{\hbar}\hat{L}_b}\hat{L}_a e^{i\frac{\alpha}{\hbar}\hat{L}_b} = \hat{L}_a\cos(\alpha) + \frac{i}{\hbar}\sin(\alpha)[\hat{L}_a, \hat{L}_b]$ for $a \neq b$. This operation rotates the angular momentum operators about one of the axes.

and using (4.8) twice, we have

$$U\sigma_z U^\dagger = \frac{1}{B}\mathbf{B}\cdot\boldsymbol{\sigma}.$$

Therefore our Hamiltonian can be written as

$$\mathcal{H} = BU\sigma_z U^\dagger.$$

The eigenvalues are $\pm B$ and the corresponding eigenvectors are

$$\phi_+ = U\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}\cos(\frac{\theta}{2})e^{-i\varphi/2}\\ \sin(\frac{\theta}{2})e^{i\varphi/2}\end{pmatrix} \tag{4.9}$$

and

$$\phi_- = U\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}-\sin(\frac{\theta}{2})e^{-i\varphi/2}\\ \cos(\frac{\theta}{2})e^{i\varphi/2}\end{pmatrix}.$$

4.2.2 Addition of spin

We have discussed earlier that the spin of an elementary particle is a fixed quantity (e.g. electrons always are spin half). What about composite objects? For instance, suppose we have an atom composed of protons, neutrons, and electrons. Does it make sense to assign a total spin to such a composite particle?

To shed light on this question, consider two separate spins, with spin operators $\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$ with $\hat{S}_1^2 = \mathbb{1}\hbar^2 s_1(s_1+1)$ and $\hat{S}_2^2 = \mathbb{1}\hbar^2 s_2(s_2+1)$. From these, we form the total spin operator as

$$\hat{\mathbf{S}} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2.$$

$\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$ act on different spins and so their components commute: $[S_{1a}, S_{2b}] = 0$. Also because $[\hat{S}_{1a}, \hat{S}_{1b}] = i\hbar\sum_c \varepsilon_{abc}\hat{S}_{1c}$ and $[\hat{S}_{2a}, \hat{S}_{2b}] = i\hbar\sum_c \varepsilon_{abc}\hat{S}_{2c}$, the total spin operator also satsifies the spin algebra:

$$[\hat{S}_a, \hat{S}_b] = i\hbar\sum_c \varepsilon_{abc}\hat{S}_c.$$

The results from the first section of the chapter apply to this. In particular:

$$\begin{aligned}
\hat{S}^2\,|s,m\rangle &= \hbar^2 s(s+1)\,|s,m\rangle\\
\hat{S}_z\,|s,m\rangle &= \hbar m\,|s,m\rangle\\
\hat{S}_+\,|s,m\rangle &= \hbar\sqrt{s(s+1)-m(m+1)}\,|s,m+1\rangle\\
\hat{S}_-\,|s,m\rangle &= \hbar\sqrt{s(s+1)-m(m-1)}\,|s,m-1\rangle
\end{aligned}$$

where m ranges from $-s$ to s in integer steps. The central question is: what are the possible values of s for the total spin?

To understand this problem better, we consider the case where $s_1 = s_2 = 1/2$. For this case, a basis for the system is

$$\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}.$$

In this notation, the first entry inside the ket denotes the state of the first spin while the second entry denotes the state of the second spin. The above is an eigenbasis of the commuting observables $\hat{S}_{1z}$ and $\hat{S}_{2z}$.

What we want is an eigenbasis of the commuting observables $\hat{S}^2$ and $\hat{S}_z$. Let's start by finding an eigenbasis of $\hat{S}_z$. These can be found essentially by inspection. There is only one state with $m = m_1 + m_2 = 1$, namely $|\uparrow\uparrow\rangle$. Similarly, there is only one state with $m = -1$ which is $|\downarrow\downarrow\rangle$. Finally, there are two states with $m = 0$, namely $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$.

Since $|\uparrow\uparrow\rangle$ is a non-degenerate eigenstate of $\hat{S}_z$ it will also be an eigenstate of $\hat{S}^2$. Let's figure out its eigenvalue. Using the relation (check) $\hat{S}_-\hat{S}_+ = \hat{S}^2 - \hat{S}_z^2 - \hbar\hat{S}_z$ we have

$$\hat{S}^2 |\uparrow\uparrow\rangle = (\hat{S}_z^2 + \hbar\hat{S}_z + \hat{S}_-\hat{S}_+) |\uparrow\uparrow\rangle .$$

Next we note that $\hat{S}_+ |\uparrow\uparrow\rangle = (\hat{S}_{1+} + \hat{S}_{2+}) |\uparrow\uparrow\rangle = 0$. Also remember that $|\uparrow\uparrow\rangle$ is an eigenstate of $\hat{S}_z$ with $m = 1$. Therefore,

$$\hat{S}^2 |\uparrow\uparrow\rangle = \hbar^2 1(1+1) |\uparrow\uparrow\rangle .$$

So for this state $s = 1$. We have found our first state in the total spin eigenbasis:

$$|s = 1, m = 1\rangle = |\uparrow\uparrow\rangle$$

We can now apply the lowering operator to find additional eigenstates. This lowers the value of m leaving s as it is. Applying once,

$$\hat{S}_- |\uparrow\uparrow\rangle = \hat{S}_{1-} |\uparrow\uparrow\rangle + \hat{S}_{2-} |\uparrow\uparrow\rangle = \hbar |\downarrow\uparrow\rangle + \hbar |\uparrow\downarrow\rangle .$$

Normalising we get

$$|s = 1, m = 0\rangle = \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle).$$

Applying $\hat{S}_-$ to this state and normalising gives

$$|s = 1, m = -1\rangle = |\downarrow\downarrow\rangle .$$

Finally, we form a state with $m = 0$ orthogonal to $|s = 1, m = 0\rangle$:

$$|\phi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$$

Since this is orthogonal to all of the other $|s,m\rangle$ states we have found so far it should be an eigenstate of $\hat{S}^2$. Let's find its eigenvalue. Remembering that $m=0$ for this state,

$$\hat{S}^2|\phi\rangle = (\hat{S}_z^2 + \hbar\hat{S}_z + \hat{S}_-\hat{S}_+)|\phi\rangle = \hat{S}_-\hat{S}_+|\phi\rangle = \hat{S}_-\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\uparrow\uparrow\rangle) = 0.$$

Therefore it must be that $s=0$ for this state. Therefore,

$$|s=0,m=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$$

In summary, combining two spin halfs, we can form states with total spin of either one or zero.

The more general result is the following. Suppose $\hat{\mathbf{S}}_1^2 = \hbar^2 s_1(s_1+1)\mathbb{1}$ and $\hat{\mathbf{S}}_2^2 = \hbar^2 s_2(s_2+1)\mathbb{1}$. Then the eigenvalues of $\hat{S}^2 = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)^2$ are $\hbar^2 s(s+1)$ where s takes on values from $|s_1 - s_2|$ to $s_1 + s_2$ in integer steps. For every s value there are $2s+1$ linearly independent eigenstates of $\hat{S}_z$ with eigenvalues ranging from $-s$ to s in integer steps. An approach for how to prove this result was given in lecture.

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Example

Suppose we have $s_1 = 1/2$ and $s_2 = 3/2$ and the Hamiltonian $\hat{\mathcal{H}} = \gamma\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2$. Such a Hamiltonian describes the so-called hyperfine interaction between a nuclear spin and an electronic spin. What are the eigenenergies of $\hat{\mathcal{H}}$?

The trick is to re-write this Hamiltonian as

$$\hat{\mathcal{H}} = \frac{\gamma}{2}(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)^2 - \frac{\gamma}{2}\hat{S}_1^2 - \frac{\gamma}{2}\hat{S}_2^2.$$

We can now read off the eigenenergies to be

$$E_s = \frac{\gamma}{2}\hbar^2 s(s+1) - \frac{9}{4}\gamma\hbar^2$$

where $s=1$ or $s=2$.

4.3 Elements of Quantum Technologies

4.3.1 Gates, circuits, and notation

Quantum technologies is an evolving and somewhat new field that aims to utilise the *principles* of quantum mechanics to create useful technologies. Under the quantum technologies umbrella are areas like quantum computing, quantum cryptography, quantum metrology, and others. It should be emphasized though that quantum mechanics itself has already found key applications during the past century in developing technologies that we now use every day. Such "quantum 1.0" advances include the transistor, the laser, MRI, and many others. Though the importance of these advances cannot be overstated, the more subtle aspects of quantum mechanics

usually was not central to their development. One can compute, say, the band gap of a semiconductor (relevant for the transistor) by directly solving the Schrödinger equation and more-or-less ignoring entanglement altogether. The newer area of quantum technologies, on the other hand, puts the more subtle aspects of quantum mechanics like entanglement and measurement-induced wavefuction collapse at the fore. Here, quantum states and how one can process the quantum information they contain are the primary concerns (and the Schrödinger equation itself is sometimes less relevant). This is the focus of quantum technologies or "quantum 2.0". It should be noted though that there is not always a crisp distinction between these two types of quantum nor does there need to be. It is all quantum mechanics which has an agreed-upon fundamental framework. The above should instead be thought of as a way of making a loose distinction between two overlapping areas.

To understand technical arguments involving quantum technologies, becoming familiar with an amount of new lingo is required. Once this is done, many of the concepts will be familiar. As mentioned earlier, spin-half systems can be viewed as qubits and vice versa. In the following, to get the full experience, we will make the presumably mild switch to the quantum information notation from our earlier notation. The spin-up and spin-down states are replaced by $|0\rangle$ and $|1\rangle$ to make the analogy with classical bits. The basis $\{|0\rangle, |1\rangle\}$ (and direct generalisations to multiple-qubit Hilbert spaces) is referred to as the **computational basis**. Finally, the Pauli matrices are replaced by X, Y, and Z.

The most important difference between classical bits and qubits is that qubits can exist in a superposition of states $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ whereas classical bits cannot. A handy way of visualising a quibit is to think of it as a point on the unit sphere, or **Bloch sphere**, using the method explained in 4.2.1. That is, the state $|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|1\rangle$, can be thought of as a point on the Bloch sphere with spherical coordiates (θ, φ). Compare this expression with Eq. 4.9 and notice we have multiplied the latter by the phase factor $e^{i\varphi/2}$. Note that (θ, φ) uniquely determines the qubit state up to an overall phase factor, assuming normalisation.

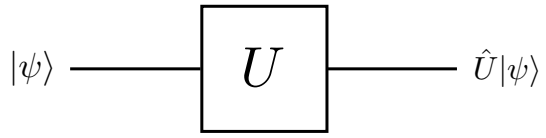
Now let's move on to discuss multiple qubit states. To be concrete we will focus on two-qubit states as the generalisation to more qubits is direct. Consider two qubits, the first in state $|\phi_1\rangle$ and the second in state $|\phi_2\rangle$. Multiple notations exist to represent the full state $|\phi\rangle$ of the two-qubit system: $|\phi\rangle = |\phi_1\phi_2\rangle = |\phi_1\rangle|\phi_2\rangle = |\phi_1\rangle \otimes |\phi_2\rangle$ where $\otimes$ denotes the tensor product. The three types of notation are often used interchangeably in the quantum information literature. While the notation involving the tensor product is the most precise, it can become cumbersome when working with many-qubit systems. The first notation, $|\phi_1\phi_2\rangle$, we used in our discussion on combining spins. The computational basis describing all two-quibit states is $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

Two-qubits states that cannot be written as a product (of the form $|a\rangle \otimes |b\rangle$ are said to be **entangled**. Examples of states that are not entangled are $|0\rangle|0\rangle$ and $|0\rangle|0\rangle + |0\rangle|1\rangle + |1\rangle|0\rangle + |1\rangle|1\rangle$ (why?). An example of an entangled state is $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. The key property of entanglement is that measurement of one subsystem (e.g. the first qubit) can influence the state of the second qubit. Entanglement is the key new property responsible for advantage (in terms of efficiency) of some quantum algorithms in comparison with classical ones.

We will now move on to consider particular examples of quantum algorithms. In essence a quantum algorithm involves the two following actions applied on a collection of qubits: unitary

operations and measurement. Quantum algorithms are often described pictorially as **quantum circuits** which are in turn composed of **quantum gates** connected by wires. Measurements are typically performed after a series of unitary operations are applied.

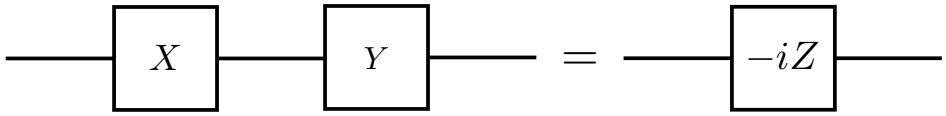
As a starting point, let's consider a circuit composed of a single-qubit gate. In general such a gate is determined uniquely by a 2×2 unitary matrix U and is represented pictorially as



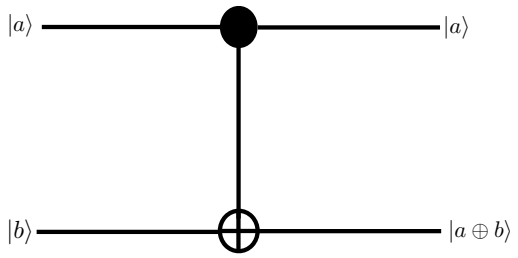
This diagram is to be read from left to right. It says that the state $|\psi\rangle$ is fed into a gate which applies a unitary operation and spits out the state $\hat{U}\,|\psi\rangle$. Note that we are being careful with hats – U is the matrix found from $\hat{U}$ by using the computational basis. It is worth noting that not all classical gates have a corresponding quantum gate since quantum gates are constrained (by physics) to be unitary. Pauli gates are obtained when U is replaced by one of the X, Y, Z Pauli operators. The X Pauli gate where $U = X$ is also known as the NOT gate because it maps $|0\rangle$ to $|1\rangle$ and vice versa. Another important operation is the Hadamard gate which is given by the matrix

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Notably if a state from the computational basis is fed into a Hadamard gate, a superposition state exits (the same is not true for the Pauli gates). Finally, we note that we can simplify quantum circuits using matrix multiplication, an example of which is given in the diagram below.



Now let's move onto two qubit gates. It turns out (as can be established using linear algebra) that any unitary operation on N qubits can be decomposed into a series of one and two qubit operations. One can then "programme" a quantum computer by arranging one and two-qubit gates in specific ways. An example of a two qubit gate is the CNOT (controlled not) gate. When acting on states in the computational two-qubit basis, the CNOT gate does the following: $|00\rangle \to |00\rangle$, $|01\rangle \to |01\rangle$, $|10\rangle \to |11\rangle$, and $|11\rangle \to |10\rangle$. In particular, the CNOT gate performs a NOT operation on the second qubit if the first qubit is in state 1, and does nothing to the second qubit if the first qubit is in state 0. Denoting the state of the first qubit as $|a\rangle$ and the state of the second qubit as $|b\rangle$ (so the two-qubit state is $|ab\rangle$) the controlled not gate is described pictorially as below where $\oplus$ denotes addition modulo two.



In the discussion so far, we have been focusing on what quantum gates do to states that are in the computational basis. However, we should note that we can use their **linearity** (which is always assumed on physical grounds) to determine how they act on arbitrary states. For instance, when acting on the superposition state $|ab\rangle + |cd\rangle$, where $|ab\rangle$ and $|cd\rangle$ are computational basis states, the CNOT gate yields $|a, a \oplus b\rangle + |c, c \oplus d\rangle$.

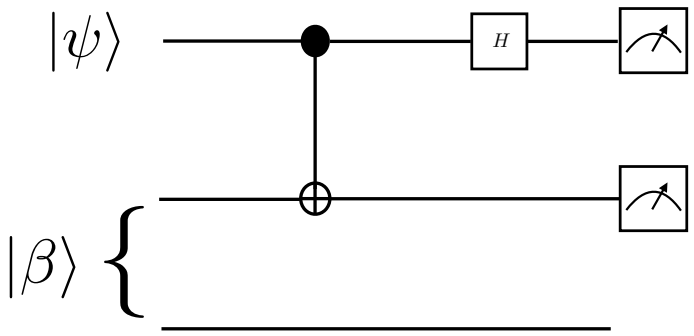
4.3.2 Teleportation

With these basic building blocks we can build up a circuit that does something neat: quantum teleportation. The setup is the following. Alice and Bob were together long ago and each took a single qubit from a so-called EPR pair (named after Einstein, Podolsky, and Rosen's early work on quantum mechanics) given by $|\beta\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$.[4] Bob is now in a far off place and Alice wishes to communicate to him the state of a single qubit she has in her possession but she is unaware of its particular state. To be clear, Alice has two qubits – a state which she wishes to transmit to Bob and her half of the EPR pair while Bob has one qubit – his half of the EPR pair. They also have a classical channel they can communicate over.

A first thought might be for Alice to send Bob information about the state through the classical channel. However, we must remember that measuring her state will irrevocably alter it. For instance if her state is $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ and she measures it in the computational basis, there's an $|\alpha|^2$ chance that she will measure state 0 and a $|\beta|^2$ chance to measure state 1. After the measurement, her state is either $|0\rangle$ or $|1\rangle$ (depending on the measurement outcome) so further measurements will not give anything useful. *If* (and this is an assumption) Alice had a way of consistently preparing the same state she could do repeated experiments on these identical states to reconstruct it. However, even if this is the case, she could only communicate to Bob over the classical channel an approximation of her state (both because it would take an infinite amount of measurements to determine the state exactly and because it would take an infinite amount of classical bandwidth to communicate α and β to all decimal places) and there are also concerns about the security of the classical channel.

[4] An aside on how measurements work out for such a state which can be determined from quantum mechanics postulates. If Alice measures the state of the first qubit there's a 50% chance that it will be in state 0 and a 50% chance it will be in state 1. If Bob measures his state after Alice, he is certain to get the same outcome as Alice's measurement. That is, if Alice measures her qubit to be in state 0 then there's a 100% chance Bob will measure his qubit to be in state 0. Alice's measurement affects Bob's state which is one of the stranger things in quantum mechanics. One might think that this could violate relativity (transmission of information faster than the speed of light) but it does not.

Instead, she can teleport her qubit to Bob using the protocol given in the diagram below.



Alice starts by performing the CNOT operation on her qubit $|\psi\rangle$ (that she wishes to transmit to Bob) and her half of the EPR pair (recall that she shared the other part of the EPR pair with Bob long ago). Next she sends her first qubit through a Hadamard gate. The initial three-qubit state is $|\psi\rangle\,|\beta\rangle = \frac{1}{\sqrt{2}}(\alpha\,|000\rangle + \alpha\,|011\rangle + \beta\,|100\rangle + \beta\,|111\rangle)$. Operating on this state with the two gates, after a bit of algebra gives the state

$$\frac{1}{2}\,|0,0\rangle\,(\alpha\,|0\rangle + \beta\,|1\rangle) + \frac{1}{2}\,|0,1\rangle\,(\alpha\,|1\rangle + \beta\,|0\rangle) + \frac{1}{2}\,|1,0\rangle\,(\alpha\,|0\rangle - \beta\,|1\rangle) + \frac{1}{2}\,|1,1\rangle\,(\alpha\,|1\rangle - \beta\,|0\rangle)$$

where we have been using the notation like $|a,b,c\rangle = |a\rangle\,|bc\rangle = |ab\rangle\,|c\rangle$, as discussed before. Although this state appears complicated, properties of $|\psi\rangle$ are lurking in the third qubit (which is Bob's). The resemblances can be made clearer by writing this state as

$$\frac{1}{2}\,|0,0\rangle\,|\psi\rangle + \frac{1}{2}\,|0,1\rangle\,\hat{X}\,|\psi\rangle + \frac{1}{2}\,|1,0\rangle\,\hat{Z}\,|\psi\rangle + \frac{1}{2}\,|1,1\rangle\,\hat{X}\hat{Z}\,|\psi\rangle\,.$$

The next step is for Alice to measure her two qubits in the computational basis and to communicate the outcome of this measurement to Bob over the classical channel. Bob will then know what to do to "fix up" his qubit. For instance, if Alices measurement returns "10", then Bob's state after the measurement is $\hat{Z}\,|\psi\rangle$. After Alice sends the news that she measured "10" to Bob, Bob then knows he needs to apply a Z-gate to his qubit. Then presto, Bob has the exact state $|\psi\rangle$ in his possession. What was originally Bob's half of the EPR pair has become the teleported state after a series of unitary operations and a measurement.

4.3.3 Quantum cryptography

Similar tricks utilising the principles of quantum mechanics can help Bob and Alice transmit information in other ways. In the following we will describe the the BB84 protocol that is one of the most well known protocols in quantum cryptography. The goal is for Alice and Bob to securely share a private key of random numbers which can be used to encrypt a message to be sent over a public channel. It works as follows. Alice generates a list of N randomly chosen negative ones and positive ones $A = (a_1, a_2, \ldots a_N)$. If $a_n = 1$, Alice randomly chooses between

the two states $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|0\rangle$ to send to Bob (note these are eigenstates of either X or Z with eigenvalue 1). If $a_n = -1$, Alice randomly chooses between the two states $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ and $|1\rangle$ to send to Bob (note these are eigenstates of either X or Z with eigenvalue -1). Physically, this is most often done by using photons, where information of the quantum states is encoded through polarization.[5] Upon receipt of the qubits, Bob measures either $\hat{Z}$ or $\hat{X}$, choosing such axes in a random way. Bob records his results in the list $B = (b_1, b_2, \ldots b_N)$. Note that if Alice's and Bob's axes happen to coincide for a particular qubit then (if there is no tampering involved) $a_n = b_n$. On the other hand, if their axes are different then $a_n = b_n$ only half of the time on average and this is not very useful.

Next Alice and Bob exchange information of the axes they used to send / measure photons publicly but keep secret their lists A and B. They then strike from their lists entries for which different axes were used to form the smaller lists A' and B'. If there has been no tampering then $A' = B'$. The final step is to check if the qubits have been tampered with in their journey from Alice to Bob. To do so, Alice and Bob will sacrifice n randomly-chosen entries from their lists A' and B' by communicating the values they obtained over a classical channel. If all of these agree, then they will know with confidence exponential in n that their communication is secure. They then strike these sacrificed bits from their list to form lists A'' and B'' where it should be true that $A'' = B''$. This forms the private key which can be used to encrypt a message sent over a public channel. If, on the other hand, some of the sacrificed bits disagree, they abort the process and start from scratch.

4.3.4 Quantum computers

The most famous quantum computing algorithms that can theoretically offer great speedup in comparison with the classical state-of-the-art are those of Shor and Grover. Shor's algorithm provides a means to factor a prime number in polynomial time. Grover's algorithm offers clear theoretical advantage to the problem of unstructured search. Describing the details of these algorithms, however, will require more time than we have. If interested, there are many places to learn about their details like the books by Nielson/Chuang and Mermin.

Here we will describe a simpler algorithm due to Deutsch and Jozsa that was one of the first showing a clear quantum speedup. However, the importance of the problem that it can solve quickly is probably fairly limited. The setup is this. Fix a positive integer n. Say we have a function $f : \{0, 1, \ldots 2^n - 1\} \to \{0, 1\}$ which we know is either *balanced* or *constant*. By constant we mean that it always returns the same output regardless of input. By balanced we mean $\sum_{l=0}^{2^n-1}(-1)^{f(\ell)} = 0$. That is, if f is balanced it returns 0 half the time and 1 half the time. The objective is to determine if the function is balanced or constant by calling it as few times as possible. Classically, we can just start calling the function for various inputs. If we ever get two distinct outputs we know at that moment with certainty that it is balanced. But if we do not get

[5] At this point you may be asking why we went through all of the trouble in the previous example on teleportation if qubits can be transmitted so easily by photons in such a way. The difficulty is that Alice simply sending Bob a photon in state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ is inherently insecure. They do not know if there is a third party between them tampering with the state. We are going to focus here on how to mitigate the potential presence of such a third party.

two distinct outputs, we have to keep going until we have used half of the possible inputs to say which type of function it is with complete confidence.

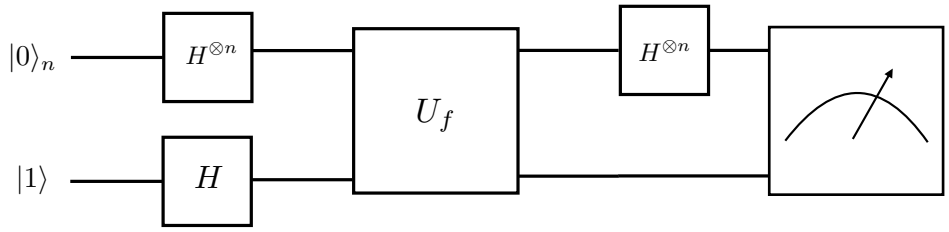
Now we describe the quantum algorithm which solves this problem with only a single call of the function, and demonstrates the power of quantum parallelism. Since we are now switching to quantum, we demand that f knows how to handle states in a superposition. First, we can represent the possible inputs of the function using computational basis states of an n-qubit system using a base-two binary representation. That is, let the input integer ℓ in binary notation be $\ell_1\ell_2\ldots\ell_n$ so that $\ell = \ell_1 2^{n-1} + \ell_2 2^{n-2} + \ldots + \ell_n$. For notational simplicity, we write the n-qubit state as

$$|\ell\rangle_n = |\ell_1\ell_2\ldots\ell_n\rangle\,.$$

Next we require a unitary gate $\hat{U}_f$ which does the following operation on $n+1$ qubit states:

$$\hat{U}_f\left(|\ell\rangle_n|a\rangle\right) = |\ell\rangle_n|a\oplus f(\ell)\rangle$$

where $|a\rangle$ is a single-qubit state in the computational basis and $\oplus$ denotes mod-2 addition. We send the input state $|0\rangle_n|1\rangle$ into quantum circuit given below.



In the diagram, the notation $H^{\otimes n}$ means that a Hadamard gate is applied separately to each qubit of an n-qubit system. While the above circuit undoubtedly does clever things, we will refrain from directly commenting on them. Instead, we will focus on the mechanics of what the gates do at various points in the circuit. The following steps exclude some detail which are useful to work through. When in doubt it may be helpful to restrict to the case $n = 1$. After the first set of Hadamards are applied, one obtains

$$|0\rangle_n|1\rangle \to \frac{1}{2^{(n+1)/2}}\sum_{\ell=0}^{2^n-1}\sum_{p=0}^{1}(-1)^p|\ell\rangle_n|p\rangle\,.$$

Then after U_f is applied one finds

$$\frac{1}{2^{(n+1)/2}}\sum_{\ell=0}^{2^n-1}\sum_{p=0}^{1}(-1)^p|\ell\rangle_n|p\oplus f(\ell)\rangle = \frac{1}{2^{(n+1)/2}}\sum_{\ell=0}^{2^n-1}\sum_{p=0}^{1}(-1)^{p-f(\ell)}|\ell\rangle_n|p\rangle\,.$$

Next apply the n-qubit Hadamard to find

$$|\psi\rangle = \frac{1}{\sqrt{2}}\frac{1}{2^n}\sum_{q,\ell=0}^{2^n-1}\sum_{p=0}^{1}(-1)^{p-f(\ell)}(-1)^{q\cdot\ell}|q\rangle_n|p\rangle\,.$$

In this, $q \cdot \ell = q_1\ell_1 + q_2\ell_2 + \ldots + q_n\ell_n$ where $\ell_1\ell_2 \ldots \ell_n$ and $q_1q_2 \ldots q_n$ are the binary representations of ℓ and q.

Finally the measurement. We measure the Hermitian operator $\hat{P} = |\phi\rangle \langle\phi|$ where $|\phi\rangle = |0\rangle_n \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. So we compute:

$$\langle\phi|\,\psi\rangle = \frac{1}{2^n} \sum_{\ell=0}^{2^n-1} (-1)^{-f(\ell)} = \frac{1}{2^n} \sum_{\ell=0}^{2^n-1} (-1)^{f(\ell)}.$$

From this, we see that we are guaranteed that we will get 0 for the measurement outcome if the function is balanced while we will always get 1 if the function is constant. Therefore the sought-after information about the function was obtained after calling it only once.

4.3.5 Closing remarks

- This section is meant to give a flavour of the developments in quantum technologies. No comprehensive reference list to the literature has been given. We also dug into a few technical calculations involving gates to really understand how some algorithms work from the ground up and perhaps inspire some tinkering with new ones.

- A number of experiments successfully demonstrating quantum encryption have been performed. Similarly, quantum teleportation has been achieved using a number of different experimental platforms. Such ideas have so far not been widely adopted commercially. This is probably because the status-quo is functioning adequately. But perhaps we will eventually see banks using quantum encryption methods to secure accounts. The physics Nobel Prize in 2022 was awarded to pioneers in this area.

- Great progress continues to be made in developing commercially viable quantum computers. The main bottleneck is scalability. To run game-changing algorithms like those of Shor or Grover on problems where classical computers cannot help requires cleanly processing thousands of qubits. However, errors due to environmental noise have limited scaling up to so many qubits. To combat this, error correcting protocols are sought. Nevertheless being able to run Shor or Grover on difficult problems still appears to be well in the future.

- Over the past few years there have been several claims of quantum advantage, also known as quantum supremacy. Demonstrating quantum advantage means solving a problem on a quantum computer that cannot be solved on a classical computer in a practical amount of time. Though this is a major milestone, the problems solved are rather special and have unknown relevance elsewhere. There has been some back and forth: some high-profile publications claiming quantum advantage were later simulated using classical computers.

- It is often said that during the past few years we have entered the noisy intermediate-scale quantum computer (NISQC) era. This involves having quantum computers composed of tens to hundreds of qubits that do not have reliable fault tolerance. A key current question is identifying important problems that current NISQC devices can help with.

- It is still unclear what the best hardware for a quantum computer will be. Private companies as well as research groups in academia are betting on a variety of different platforms. A few receiving attention are photonics, superconducting Josephson junctions, trapped ions, and Rydberg atoms. There is also a major drive to create qubits that are inherently protected against decoherence using topological properties of their states.

4.4 Exercises

Exercise 4.1 *Verify that the spin-half matrices satisfy* $[S_a, S_b] = i\hbar \sum_c \varepsilon_{abc} S_c$.

Exercise 4.2 *Find the three* 3×3 *spin-one matrices.*

Exercise 4.3 *Consider a spin-*s *spin. Define an anti-unitary operator as* $\hat{T} = e^{-i\pi \hat{S}_y/\hbar}\hat{K}$. *Here* $\hat{K}$ *is the antiunitary operator introduced in the previous chapter which acts trivially on the eigenbasis of* $\hat{S}_z$. *Show that this operator satisfies* $\hat{T}\hat{S}_a\hat{T}^{-1} = -\hat{S}_a$. *Furthermore, show that* $\hat{T}^2 = \mathbb{1}$ *when* s *is an integer and* $\hat{T}^2 = -\mathbb{1}$ *when* s *is a half integer.*

Exercise 4.4 *Suppose we have* $s_1 = 1/2$ *and* $s_2 = 3/2$ *and the Hamiltonian* $\hat{\mathcal{H}} = \gamma \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2$. *Find explicit expressions for the eigenstates of this Hamiltonian. Choose the eigenstates to also be eigenstates of* $\hat{S}_{1z} + \hat{S}_{2z}$ *which commutes with this Hamiltonian.*

Exercise 4.5 *Explicitly show that* $\sigma_a\sigma_b = \delta_{ab}\mathbb{1} + i\sum_c \varepsilon_{abc}\sigma_c$. *Using this, derive equation (4.8).*

Exercise 4.6 *Let* ψ *be a two-component normalised spinor. Let* $\mathbf{n} = \psi^\dagger \boldsymbol{\sigma} \psi$. *Show that* $\mathbf{n}$ *is a unit vector.*

Exercise 4.7 *Suppose the state* $|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\varphi}|1\rangle$ *is fed through a single-qubit* X*-gate and then measured in the computational basis. What is the probability of the system being in state* $|0\rangle$ *after the measurement?*

Exercise 4.8 *The two-qubit swap operation does the following:* $\hat{U}|\phi_1\phi_2\rangle = |\phi_2\phi_1\rangle$ *for arbitrary singles qubits states* $|\phi_1\rangle$ *and* $|\phi_2\rangle$ *. Explain why this operation is unitary. Find an explicit matrix representation of* $\hat{U}$ *in the computational basis.*

Exercise 4.9 *The following exercise relates to the Deutsch-Jozsa algorithm. Show that* $\hat{U}_f$ *is a unitary operation. Show that* $\hat{H}^{\otimes n}|0\rangle_n = \frac{1}{2^{n/2}}\sum_{\ell=0}^{2^n-1}|\ell\rangle_n$.

Exercise 4.10 *Alice and Bob each take a qubit from the singlet state* $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$. *This is the same state considered in our discussion of spin, but we are using the quantum information notation. Alice measures the single-qubit operator* $\hat{A} = |\phi\rangle\langle\phi| - \left|\tilde{\phi}\right\rangle\left\langle\tilde{\phi}\right|$ *with her half of the pair where* $|\phi\rangle$ *is some single-qubit state and* $\left\langle\tilde{\phi}\middle|\,\phi\right\rangle = 0$. *What are the two possible experimental outcomes when measuring* $\hat{A}$*? What is the probability that Alice's measurement of* $\hat{A}$ *will return 1? Suppose Alice measures* 1. *Next Bob performs a measurement of the same operator. What is the probability that he also measures* 1. *This suggests that the spin-singlet state can be written (up to phase) as* $\frac{1}{\sqrt{2}}(\left|\phi\tilde{\phi}\right\rangle - \left|\tilde{\phi}\phi\right\rangle)$. *Is this true?*

4.A Appendix: Aspects of quantum measurement

In this Appendix we will briefly discuss measurement in quantum mechanics and how it relates to classical probability theory. Quantum mechanics is more general than standard probability theory as it deals with potentially complex probability amplitudes, also known as wave functions.

Suppose we have two Hilbert spaces of dimension N and M spanned respectively by orthonormal bases $\{|\phi_n\rangle : n = 1, \dots N\}$ and $\{|\xi_\ell\rangle : \ell = 1, \dots . M\}$. Now combine these two Hilbert spaces (via tensor product) to obtain a larger Hilbert space of dimension NM spanned by orthonormal basis $\{|\phi_n\rangle \otimes |\xi_\ell\rangle\}$. We'll think of the two original Hilbert spaces (of dimensions N and M) as subsystems of the larger Hilbert space in what follows and use typical shorthand notation such as $|\phi_n \xi_\ell\rangle = |\phi_n\rangle \otimes |\xi_\ell\rangle$

Now let's consider doing measurements with respect to an orthonormal basis. Take the state of the system to be $|\psi\rangle$. The probability of measuring the system to be in the state $|\phi_n \xi_\ell\rangle$ we all know is:

$$P(n, \ell) = |\langle \phi_n \xi_\ell | \psi \rangle|^2.$$

If we determine that the system is in state $|\phi_n \xi_\ell\rangle$ then post-measurement, the state of the system "collapses" to $|\psi'\rangle = |\phi_n\rangle \otimes |\xi_\ell\rangle$.

Now let's suppose instead that we are only measuring one of the two subsystems. The probability of measuring the state of the first subsystem to be $|\phi_n\rangle$ is:

$$P(n) = \sum_\ell P(n, \ell) = \langle \psi | \hat{P}_n \otimes \mathbb{1} | \psi \rangle$$

where $\hat{P}_n = |\phi_n\rangle \langle \phi_n|$ is a projection operator (not to be confused with probability). Suppose upon measurement we determine the first subsystem to be in state $|\phi_n\rangle$. To determine then the state post measurement, we project into this state and normalise:

$$|\psi'\rangle = \frac{\hat{P}_n \otimes \mathbb{1} |\psi\rangle}{\sqrt{\langle \psi | \hat{P}_n \otimes \mathbb{1} |\psi\rangle}}$$

Similar relations follow if we consider measuring the other subsystem.

Now with the above we can even discuss conditional probability. Using the expression immediately above for the post-measurement state we can determine what is the probability for the second subsystem to be in state $|\xi_\ell\rangle$ *provided* the first subsystem is measured to be in state $|\phi_n\rangle$. It is

$$P(\ell | n) = |\langle \phi_n \xi_\ell | \psi' \rangle|^2 = P(n, \ell)/P(n).$$

Chapter 5

Approximation Schemes

In this Chapter we discuss approximation schemes used in quantum mechanics.

5.1 Time-independent perturbation theory (non-degenerate case)

Suppose that we are confronted with a Hamiltonian of the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda \hat{V}.$$

We know how to diagonalise $\hat{\mathcal{H}}_0$ but not the full $\hat{\mathcal{H}}$. Suppose additionally that λ is a small parameter. For such systems we turn to perturbation theory.

To set the notation we take, as usual,

$$\hat{\mathcal{H}} \left|\phi_n\right\rangle = E_n \left|\phi_n\right\rangle .$$

For the 'unperturbed' system (assumed to be solvable) we take

$$\hat{\mathcal{H}}_0 \left|n\right\rangle = \varepsilon_n \left|n\right\rangle .$$

In the above equations n labels the eigenenergies/eigenstates. The collection of eigenstates $\{|n\rangle\}$ is taken to be orthonormal (i.e. normalised in the usual way).

Let's now fix a particular state (n value) and ask how it changes as we 'turn the perturbation on'. We assume that we have the following series expressions in λ:

$$\left|\phi_n\right\rangle = \left|\phi_n^{(0)}\right\rangle + \lambda \left|\phi_n^{(1)}\right\rangle + \lambda^2 \left|\phi_n^{(2)}\right\rangle + \dots$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

where $E_n^{(i)}$ and $\left|\phi_n^{(i)}\right\rangle$ are independent of λ. We assume that the unperturbed eigenvalue ε_n is **non-degenerate** (the degenerate case requires a separate treatment). We take the (unconventional) normalisation condition $\left\langle \phi_n^{(0)} \middle| \phi_n \right\rangle = 1$. Since this normalisation is taken to hold for

arbitrary λ, it requires $\left\langle \phi_n^{(0)} \middle| \phi_n^{(i)} \right\rangle = 0$ for $i \neq 0$. Requiring these to reduce to the unperturbed states when $\lambda \to 0$ requires $\left| \phi_n^{(0)} \right\rangle = |n\rangle$ and $E_n^{(0)} = \varepsilon_n$.

Now let's insert our perturbative expansions into the Schrödinger equation $\hat{\mathcal{H}} |\phi_n\rangle = E_n |\phi_n\rangle$ and equate powers of λ. The order λ^0 piece gives us nothing new. The order λ^1 piece gives us:

$$\hat{\mathcal{H}}_0 \left| \phi_n^{(1)} \right\rangle + \hat{V} |n\rangle = \varepsilon_n \left| \phi_n^{(1)} \right\rangle + E_n^{(1)} |n\rangle .$$

This is a useful equation. Multiplying by $\langle n|$ gives us the first order correction to the energy:

$$E_n^{(1)} = \langle n| \hat{V} |n\rangle .$$

Next we apply $\langle n'|$ for $n' \neq n$. This gives

$$\langle n'| \phi_n^{(1)} \rangle = \frac{\langle n'| \hat{V} |n\rangle}{\varepsilon_n - \varepsilon_{n'}}.$$

Due to our normalisation condition, we have $\langle n| \phi_n^{(1)} \rangle = 0$. Therefore,

$$\left| \phi_n^{(1)} \right\rangle = \sum_{n'} |n'\rangle \langle n'| \phi_n^{(1)} \rangle = \sum_{n' \neq n} \frac{\langle n'| \hat{V} |n\rangle}{\varepsilon_n - \varepsilon_{n'}} |n'\rangle .$$

This is the first order correction to the eigenket.

Next we consider the λ^2 piece in the Schrödinger equation. This reads

$$\hat{\mathcal{H}}_0 \left| \phi_n^{(2)} \right\rangle + \hat{V} \left| \phi_n^{(1)} \right\rangle = E_n^{(2)} \left| \phi_n^{(0)} \right\rangle + E_n^{(1)} \left| \phi_n^{(1)} \right\rangle + E_n^{(0)} \left| \phi_n^{(2)} \right\rangle .$$

Multiplying by $\langle n|$ gives

$$E_n^{(2)} = \langle n| \hat{V} \left| \phi_n^{(1)} \right\rangle = \sum_{n' \neq n} \frac{|\langle n'| \hat{V} |n\rangle|^2}{\varepsilon_n - \varepsilon_{n'}}.$$

This is the second order correction to the eigenenergy. Though we could clearly continue on in this way, we will stop here.

5.2 Time-independent perturbation theory (degenerate case)

In this section, we will handle the case where the state for which we wish to find perturbative corrections is degenerate. We will derive an *effective* Hamiltonian that acts within this space of degenerate subspace of unperturbed states. The eigenenergies of this effective Hamiltonian give the corrected eigenenergies of the system (to second order).

We take a similar setup as before, but now allow ε_n to be degenerate. In particular, we take N orthonormal states with

$$\hat{\mathcal{H}}_0 |n, r\rangle = \varepsilon_n |n, r\rangle$$

where r runs from 1 to N. The degenerate case is slightly more involved than the non-degenerate case for the following reason. In the previous section, the zeroth order unperturbed state was clearly $\left|\phi_n^{(0)}\right\rangle = |n\rangle$. However now for the degenerate case it will generally be some linear combination of the degenerate states: $\left|\phi_n^{(0)}\right\rangle = \sum_r c_r |n, r\rangle$. The key in degenerate perturbation theory is finding the correct linear combination of these unperturbed states so that the states continuously change as the perturbation is 'turned on'.

We next introduce the projection operators

$$\hat{P} = \sum_r |n, r\rangle \langle n, r|$$

and

$$\hat{Q} = \mathbb{1} - \hat{P}.$$

The operator $\hat{P}$ projects into the set of degenerate states while the operator $\hat{Q}$ projects into everything else. For the exact eigenstate $|\phi_n\rangle$ we write

$$|\phi_n\rangle = \mathbb{1} |\phi_n\rangle = \hat{P} |\phi_n\rangle + \hat{Q} |\phi_n\rangle .$$

Now let $\left|\phi_n^{(0)}\right\rangle = \hat{P} |\phi_n\rangle$. Clearly this will be a linear combination of the degenerate states. We next take a similar normalisation convention as we did for the non-degenerate case: $\left\langle \phi_n^{(0)} \middle| \phi_n \right\rangle = 1$. We also assume, as before, that we can expand in λ as follows:

$$|\phi_n\rangle = \left|\phi_n^{(0)}\right\rangle + \lambda \left|\phi_n^{(1)}\right\rangle + \lambda^2 \left|\phi_n^{(2)}\right\rangle + \dots$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots .$$

Acting with $\hat{P}$ from the left on the Schrödinger equation gives:

$$\varepsilon_n \hat{P} |\phi_n\rangle + \lambda \hat{P} \hat{V} |\phi_n\rangle = E_n \hat{P} |\phi_n\rangle \tag{5.1}$$

Acting in a similar way with $\hat{Q}$ gives

$$\hat{Q} \hat{\mathcal{H}}_0 |\phi_n\rangle + \lambda \hat{Q} \hat{V} |\phi_n\rangle = E_n \hat{Q} |\phi_n\rangle .$$

Rearranging gives

$$\hat{Q}(E_n - \hat{\mathcal{H}}_0) |\phi_n\rangle = \lambda \hat{Q} \hat{V} |\phi_n\rangle . \tag{5.2}$$

Multiplying both sides of this equation by

$$\hat{Q}(E_n - \hat{\mathcal{H}}_0)^{-1} = \sum_{n' \neq n} \frac{1}{E_n - \varepsilon_{n'}} |n'\rangle \langle n'|$$

(sum is taken over states not degenerate with ε_n) gives

$$\hat{Q}\left|\phi_n\right\rangle = \lambda\hat{Q}(E_n - \hat{\mathcal{H}}_0)^{-1}\hat{V}\left|\phi_n\right\rangle. \tag{5.3}$$

Substituting $\left|\phi_n\right\rangle = \hat{P}\left|\phi_n\right\rangle + \hat{Q}\left|\phi_n\right\rangle$ into the second term on the LHS of equation (5.1) gives

$$\varepsilon_n\hat{P}\left|\phi_n\right\rangle + \lambda\hat{P}\hat{V}\hat{P}\left|\phi_n\right\rangle + \lambda^2\hat{P}\hat{V}\hat{Q}(E_n - \hat{\mathcal{H}}_0)^{-1}\hat{V}\left|\phi_n\right\rangle = E_n\hat{P}\left|\phi_n\right\rangle. \tag{5.4}$$

Everything is exact up to this point. However, equation (5.4) is difficult to tackle since the eigenvalue E_n appears on both sides of the equation. Let's be satisfied with a simpler but approximate equation. In particular, we require that (5.4) is only accurate to second order in λ. With such a requirement, we can replace the term multiplying λ^2 with its $\lambda = 0$ value. With this we have (remembering $\left|\phi_n^{(0)}\right\rangle = \hat{P}\left|\phi_n\right\rangle$)

$$\hat{\mathcal{H}}_{\text{eff}}\left|\phi_n^{(0)}\right\rangle = E_n\left|\phi_n^{(0)}\right\rangle$$

where

$$\hat{\mathcal{H}}_{\text{eff}} = \hat{P}\left[\varepsilon_n + \lambda\hat{V} + \lambda^2\hat{V}\hat{G}\hat{V}\right]\hat{P}$$

and

$$\hat{G} = (\varepsilon_n - \hat{\mathcal{H}}_0)^{-1}\hat{Q}.$$

This effective Hamiltonian acts non-trivially only within the subspace of degenerate states and is expressible entirely in terms of known quantities. Its eigenvalues give the desired results: corrected eigenenergies for the originally degenerate states that are accurate to second order in λ. The results from non-degenerate perturbation theory are also contained in this treatment (check).

What about the corrections to the eigenstates? For this we can use equation (5.3). Looking at the term of order λ^1 from this equation gives

$$\left|\phi_n^{(1)}\right\rangle = \hat{Q}(\varepsilon_n - \hat{\mathcal{H}}_0)^{-1}\hat{V}\left|\phi_n^{(0)}\right\rangle.$$

Therefore, the eigenket that is accurate to first order in λ is

$$\left|\phi_n\right\rangle = \left|\phi_n^0\right\rangle + \lambda\hat{Q}(\varepsilon_n - \hat{\mathcal{H}}_0)^{-1}\hat{V}\left|\phi_n^{(0)}\right\rangle.$$

5.3 Time-dependent perturbation theory

Now we move on to the case where the perturbation has time dependence. In particular, we focus on Hamiltonians of the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda\hat{V}(t).$$

The interaction picture, developed at the end of Chapter 2 is ideally suited for handling problems like this. The evolution operator in the interaction picture satisfies

$$i\hbar\partial_t\hat{\mathcal{U}}_I = \lambda\hat{V}_I\hat{\mathcal{U}}_I$$

with $\hat{\mathcal{U}}_I(t=0) = \mathbb{1}$. It therefore can be written as a Dyson series (essentially the same calculation as we did for $\hat{\mathcal{U}}(t)$ in Section 2.1):

$$\hat{\mathcal{U}}_I(t) = T_t e^{\frac{-i\lambda}{\hbar}\int_0^t dt'\hat{V}_I(t')} = \mathbb{1} - i\frac{\lambda}{\hbar}\int_0^t dt'\hat{V}_I(t') + \left(\frac{-i\lambda}{\hbar}\right)^2\int_0^t dt'\hat{V}_{\rm I}(t')\int_0^{t'} dt''\hat{V}_{\rm I}(t'') + \dots.$$

This is our perturbative expansion in λ!

We will be particularly interested in the following scenario. Define the eigenstates / eigenenergies of $\hat{\mathcal{H}}_0$ as usual:

$$\hat{\mathcal{H}}_0\left|n\right\rangle = \varepsilon_n\left|n\right\rangle.$$

Suppose we start in a particular eigenstate $|n\rangle$ at $t=0$. What is the probability for the system to end up in state $|n'\rangle$ after time t? Denoting this probability as $P_{n\to n'}$ we have

$$P_{n\to n'} = \left|\left\langle n'\right|\hat{\mathcal{U}}(t)\left|n\right\rangle\right|^2.$$

It is straightforward to establish that these probabilities satisfy the sum rule:

$$\sum_{n'} P_{n\to n'} = 1$$

as they should.

Often such expressions are difficult to compute exactly. In such cases we can resort to perturbation theory. Let's focus on the case $n \neq n'$ (noting that the case $n = n'$ can be obtained from the sum rule). For this,

$$\left\langle n'\right|\hat{\mathcal{U}}(t)\left|n\right\rangle = \left\langle n'\right|\hat{\mathcal{U}}_0(t)\hat{\mathcal{U}}_I(t)\left|n\right\rangle = e^{i\varepsilon_{n'}t/\hbar}\left\langle n'\right|\hat{\mathcal{U}}_I(t)\left|n\right\rangle = e^{i\varepsilon_{n'}t/\hbar}\frac{-i\lambda}{\hbar}\int_0^t dt'\left\langle n'\right|\hat{V}_I(t')\left|n\right\rangle$$

where we have dropped the (presumably small) terms in the Dyson series of order λ^2 and above. Working on the integrand in this expression,

$$\left\langle n'\right|\hat{V}_I(t')\left|n\right\rangle = \left\langle n'\right|\hat{\mathcal{U}}_0^\dagger(t')\hat{V}(t')\hat{\mathcal{U}}_0(t')\left|n\right\rangle = \left\langle n'\right|\hat{V}(t')\left|n\right\rangle e^{-i(\varepsilon_n-\varepsilon_{n'})t'/\hbar} = V_{n'n}(t')e^{-i\omega_{nn'}t'}$$

where we have introduced the notation $V_{n'n}(t') = \left\langle n'\right|\hat{V}(t')\left|n\right\rangle$ and $\hbar\omega_{nn'} = \varepsilon_n - \varepsilon_{n'}$. With this,

$$\left\langle n'\right|\hat{\mathcal{U}}(t)\left|n\right\rangle = e^{i\varepsilon_{n'}t/\hbar}\frac{-i\lambda}{\hbar}\int_0^t dt' V_{n'n}(t')e^{-i\omega_{nn'}t'}.$$

Finally, we can determine an expression for $P_{n\to n'}$ to lowest non-trivial order in λ:

$$P_{n\to n'} = \frac{\lambda^2}{\hbar^2}\left|\int_0^t dt' V_{n'n}(t') e^{-i\omega_{nn'}t'}\right|^2 \tag{5.5}$$

which is our main result.

****

Example

Consider the Hamiltonian

$$\hat{\mathcal{H}} = \varepsilon\left|1\right\rangle\left\langle 1\right| + \lambda\frac{\Omega}{2}\left(\left|1\right\rangle\left\langle 0\right| e^{-i\omega t} + \left|0\right\rangle\left\langle 1\right| e^{i\omega t}\right)$$

where ω, ε, and Ω are positive real parameters and $\{\left|0\right\rangle, \left|1\right\rangle\}$ forms an orthonormal basis. This is a simplified model of an atom interacting with radiation. The effective model for the atom alone is $\hat{\mathcal{H}}_0 = \varepsilon\left|1\right\rangle\left\langle 1\right|$ (much simpler than Hydrogen!). Ω is proportional to the external electric field and ω gives the frequency of the radiation. Additionally, the so-called rotating wave approximation has been employed but we will not go into any details of this. Such Hamiltonians are the bread and butter of atomic, molecular, and optical physicists (especially experimentalists!).

Suppose we start in the ground state of $\hat{\mathcal{H}}_0$. What is $P_{0\to 1}$ to lowest non-trivial order in λ? Computing the answer is just a matter directly applying equation (5.5) (and doing the integral). The result is

$$P_{0\to 1} = \frac{\lambda^2\Omega^2}{(\varepsilon - \hbar\omega)^2}\sin^2\left(\frac{\varepsilon/\hbar - \omega}{2}t\right).$$

The probability exhibits oscillations. This is physical and these are known as Rabi oscillations. One can see that the oscillations have largest amplitude when $\hbar\omega$ becomes close to ε (known as resonance). For the case when we are right at resonance, our formula tells us

$$P_{0\to 1} = \frac{\lambda^2\Omega^2}{4\hbar^2}t^2.$$

While this expression is accurate for small t, our perturbation theory will inevitably break down for larger values of t since $P_{0\to 1}$ will eventually become comparable to 1. A more extensive treatment of this model shows that there will be Rabi oscillations at resonance as well.

5.4 The Adiabatic Limit

We now consider the case where the time dependence of $\hat{\mathcal{H}}(t)$ is 'slow'. This is the so-called adiabatic limit. How do wave functions evolve under such a time-dependent Hamiltonian? To analyse this problem it is helpful to use the instantaneous eigenstates and eigenenergies of $\hat{\mathcal{H}}$:

$$\hat{\mathcal{H}}\left|\phi_n\right\rangle = \varepsilon_n\left|\phi_n\right\rangle.$$

This looks like the TISE, but shouldn't be called that because it depends on time! Suppose that at a given time, say $t = 0$, the system is in the instantaneous ground state: $|\psi(t = 0)\rangle = |\phi_0(t = 0)\rangle$. Our intuition tells us that, if the time-dependence of the Hamiltonian is slow, then at later times we should have $|\psi(t)\rangle \approx e^{i\beta_0} |\phi_0(t)\rangle$ where $e^{i\beta_0}$ is some phase factor. Think about gradually (adiabatically) moving a cup of coffee so that it doesn't slosh about.

With this thought, let's consider starting in the nth instantaneous eigenstate at time $t = 0$ (almost always this is the ground state but let's be open minded). Let's insert the ansatz $|\psi(t)\rangle = e^{i\beta_n(t)} |\phi_n(t)\rangle$ into $i\hbar\partial_t |\psi\rangle = \hat{\mathcal{H}} |\psi\rangle$ and see what happens. We find

$$-\hbar\dot{\beta}_n |\phi_n\rangle + i\hbar \left|\dot{\phi}_n\right\rangle = \varepsilon_n |\phi_n\rangle .$$

Overhead dots correspond to time derivatives. Applying $\langle\phi_n|$ to this equation gives

$$\dot{\beta}_n = -\varepsilon_n/\hbar + i \langle\phi_n| \dot{\phi}_n\rangle.$$

Integrating (noting $\beta_n(0) = 0$) we have

$$\beta_n = -\alpha_n + \gamma_n$$

where

$$\alpha_n(t) = \int_0^t dt' \varepsilon_n(t')/\hbar$$

and

$$\gamma_n(t) = \int_0^t dt' i \langle\phi_n(t')| \dot{\phi}_n(t')\rangle.$$

$\alpha_n(t)$ is known as the dynamical phase while $\gamma_n(t)$ is known as the Berry phase. So our adiabatic solution is

$$|\psi(t)\rangle = e^{i\gamma_n(t)} e^{-i\alpha_n(t)} |\phi_n(t)\rangle .$$

While this turns out to be correct, the alert reader will notice that important details have been swept under the rug. In particular, we did not look at the other components of the TDSE, obtained by applying $\langle\phi_{n'}|$ for $n' \neq n$. At present we have no good reason, apart from our intuition, to believe that these other components will be unimportant.

We need to be more careful. Let's consider the situation where the system starts in the ground state at time $t = 0$. We will further assume that the ground state is non-degenerate. The instantaneous eigenstates form a complete basis, so we can expand $|\psi(t)\rangle$ for later times as

$$|\psi(t)\rangle = \sum_n a_n e^{-i\alpha_n(t)} e^{i\gamma_n(t)} |\phi_n(t)\rangle .$$

where a_n are some time-dependent coefficients. The reason the two phase factors are not absorbed into a_n is for later convenience. Our initial condition requires $a_0(0) = 1$ and $a_n(0) = 0$

for $n \neq 0$. If our intuition is correct, then the a_n coefficients for later times should stay very close to their initial values.

Inserting this $|\psi(t)\rangle$ into the TDSE and applying $\langle\phi_m|$ on the left we find the relatively compact expression (check)

$$\dot{a}_m = i \sum_{n \neq m} A_{mn} e^{-i(\alpha_n - \alpha_m)} e^{i(\gamma_n - \gamma_m)} a_n. \tag{5.6}$$

where

$$A_{mn} = i \langle \phi_m | \dot{\phi}_n \rangle$$

Everything is exact so far.

We will be happy to find an approximate solution to (5.6). What we will do in the following is typically called adiabatic perturbation theory. We can write (5.6) in integral form as

$$a_m(t) = a_m(0) + i \int_0^t dt' \sum_{n \neq m} A_{mn}(t') e^{-i(\alpha_n(t') - \alpha_m(t'))} e^{i(\gamma_n(t') - \gamma_m(t'))} a_n(t').$$

Next we can apply the same procedure we used to derive the Dyson series to arrive at a series expansion for $a_m(t)$. Stopping at first order,

$$a_m(t) = a_m(0) + i \int_0^t dt' \sum_{n \neq m} A_{mn}(t') e^{-i(\alpha_n(t') - \alpha_m(t'))} e^{i(\gamma_n(t') - \gamma_m(t'))} a_n(0).$$

Obviously we could go to higher order if higher accuracy was needed. We want to argue that the corrections to $a_m(0)$ are small in the adiabatic limit.

Using our initial conditions for the a_m coefficients, we have

$$a_0(t) = a_0(0) = 1$$

which is encouraging. For $m \neq 0$ we have

$$a_m(t) = i \int_0^t dt' A_{m0}(t') e^{-i(\alpha_0(t') - \alpha_m(t'))} e^{i(\gamma_0(t') - \gamma_m(t'))}. \tag{5.7}$$

Is the correction to $a_m(t)$ above small? To answer this we should be more precise about what me mean by 'slow'. Slow compared to what? The other natural quantities having units of rate (1/time) are the spacings between the energy levels of $\hat{\mathcal{H}}$ (divided by $\hbar$). We refine our condition to mean slow compared to $(\varepsilon_0 - \varepsilon_m)/\hbar$ where $m \neq 0$. For such a case the term $e^{-i(\alpha_0(t') - \alpha_m(t'))}$ will oscillate much more rapidly than the others in (5.7). Using approximation techniques for

dealing with rapidly oscillating integrals[1] we find

$$a_m(t) = \left(\frac{-\hbar}{\varepsilon_0 - \varepsilon_m} A_{m0} e^{-i(\alpha_0 - \alpha_m)} e^{i(\gamma_0 - \gamma_m)} \right]_0^t .$$

Using the relation

$$\langle \phi_m | \dot{\phi}_0 \rangle = \frac{\langle \phi_m | \dot{\hat{\mathcal{H}}} | \phi_0 \rangle}{\varepsilon_0 - \varepsilon_m}$$

which can be arrived at by taking the time derivative of $\langle \phi_m | \hat{\mathcal{H}} | \phi_0 \rangle$ (check) we have

$$a_m(t) = -i \left(\frac{\hbar \langle \phi_m | \dot{\hat{\mathcal{H}}} | \phi_0 \rangle}{(\varepsilon_0 - \varepsilon_m)^2} e^{-i(\alpha_0 - \alpha_m)} e^{i(\gamma_0 - \gamma_m)} \right]_0^t .$$

We now see that the adiabatic limit corresponds to

$$\left| \frac{\hbar \langle \phi_m | \dot{\hat{\mathcal{H}}} | \phi_0 \rangle}{(\varepsilon_0 - \varepsilon_m)^2} \right| \ll 1.$$

Let's consider the case where $\dot{\hat{\mathcal{H}}} = 0$ at the initial time for simplicity (this is often the relevant physical case). For this, we have the rather nice expression for the time-dependent state with first order correction:

$$|\psi\rangle = e^{-i\alpha_0} e^{i\gamma_0} \left[|\phi_0\rangle - i \sum_{n \neq 0} \frac{\hbar \langle \phi_n | \dot{\hat{\mathcal{H}}} | \phi_0 \rangle}{(\varepsilon_0 - \varepsilon_n)^2} |\phi_n\rangle \right].$$

In summary, suppose we start with an instantaneous ground state of a time-dependent system. If the rate of time variations of this system is much smaller than the 'gap' between the ground state and excited states (instantaneous) divided by $\hbar$, then the system is well approximated by

$$|\psi\rangle = e^{-i\alpha_0} e^{i\gamma_0} |\phi_0\rangle .$$

We refer to this as the adiabatic limit. If necessary, corrections to this expression can be incorporated systematically through the methods described above.

[1] For instance, what is $I(t) = \int_0^t dt' e^{-i\omega t'} f(t')$ in the limit of large ω for well-behaved $f(t)$? To find out this limiting behaviour, we can integrate by parts:

$$I(t) = \int_0^t dt' f(t') \frac{i}{\omega} \frac{d}{dt'} e^{-i\omega t'} = \frac{i}{\omega}(e^{-i\omega t} f(t) - f(0)) - \int_0^t dt' \frac{i}{\omega} e^{-i\omega t'} \frac{d}{dt'} f(t').$$

Continuing in this manner will generate a series expansion in $1/\omega$:

$$I(t) = \frac{i}{\omega}(e^{-i\omega t} f(t) - f(0)) + \frac{1}{\omega^2}(f'(t) e^{-i\omega t} - f'(0)) + \ldots .$$

In this section we are happy with the lowest order expression.

5.4.1 Berry phase

In this section, we consider the Berry phase for the situation where the Hamiltonian at time $t = 0$ and $t = T$ is the same: $\hat{\mathcal{H}}(0) = \hat{\mathcal{H}}(T)$. Let's focus on a single instantaneous eigenstate of this Hamiltonian which satisfies

$$|\phi(T)\rangle = |\phi(0)\rangle .$$

The Berry phase is then

$$\gamma = i \int_0^T dt \, \langle \phi | \, \dot{\phi} \rangle = \int_0^T dt A(t)$$

where $A(t) = i \langle \phi | \, \dot{\phi} \rangle$.

In the following we will outline a few important properties of this Berry phase. First we note that $A(t)$ and hence γ are real. This follows from the normalisation of $|\phi\rangle$ for all times (check). Next, we note that eigenstates of $\hat{\mathcal{H}}$ are only defined up to a phase factor. That is, the state $|\phi'\rangle = e^{-i\alpha} |\phi\rangle$ is an equally valid eigenstate of $\hat{\mathcal{H}}$. Provided that $\alpha(T) = \alpha(0) + 2\pi n$ for integer n, then $|\phi'(T)\rangle = |\phi'(0)\rangle$. This is called 'gauge freedom'. If we could always pick a γ so that the Berry phase vanishes, this story would not be very interesting. With the new eigenstates we have

$$\gamma' = i \int_0^T dt \, \langle \phi' | \, \dot{\phi'} \rangle = \int_0^T dt \dot{\alpha} + i \int_0^T dt \, \langle \phi | \, \dot{\phi} \rangle = \gamma + 2\pi n.$$

So through this method we can only change the Berry phase by integer multiples of 2π. We say that the Berry phase is gauge invariant modulo 2π.

The Berry phase is a geometrical quantity. The classic example is the case of a spin-half particle under a slowly varying magnetic field of constant magnitude: $\hat{\mathcal{H}} = -\mathbf{B}(t) \cdot \boldsymbol{\sigma}$ where $\mathbf{B}(0) = \mathbf{B}(T)$. The normalised vector $\mathbf{B}/B$ traces out a closed curve on the unit sphere as t advances from 0 to T. Though we will not work out the details, the Berry phase for this situation is $-1/2$ times the area of the portion of the unit sphere bounded by this curve (modulo 2π).

Finally, the relevance of the Berry phase is not confined to systems in the adiabatic limit. For instance, the Berry phase (and related quantities like the so-called Berry curvature and Berry connection) plays a central role in the physics of the so-called topological insulators and topological superconductors which have been receiving considerable attention in recent years.

5.5 Exercises

Exercise 5.1 *Suppose we add the perturbation $\hat{V} = -\gamma \hat{x}$ to the Harmonic oscillator Hamiltonian $\hat{\mathcal{H}}_0 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2$. The full Hamiltonian reads $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda\hat{V}$. What are the first and second order (in λ) corrections to the eigenenergies of $\hat{\mathcal{H}}$?*

Exercise 5.2 *Consider the Hamiltonian of Exercise 2.6 with a λ added for convenience: $\hat{\mathcal{H}} = (\varepsilon + g)\hat{a}^\dagger\hat{a} + \frac{\lambda}{2}g(\hat{a}\hat{a} + \hat{a}^\dagger\hat{a}^\dagger)$. Compute the first and second order corrections (in λ) to the ground state energy of this system.*

Exercise 5.3 *Consider the Hamiltonian*

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega\hat{x}^2 + \lambda\gamma\hat{x}\theta(t).$$

Here $\theta(t)$ is the step function where $\theta(t) = 0$ for $t < 0$ and $\theta(t) = 1$ for $t \geq 0$. Such a model corresponds to a Harmonic oscillator that experiences an abrupt displacement at time $t = 0$. Suppose the system is in the ground state of the harmonic oscillator for $t < 0$. What is the probability, to lowest non-trivial order in λ, for the system to transition to the first excited state for positive times?

Exercise 5.4 *Consider the matrix Hamiltonian $\mathcal{H} = -\mathbf{B}\cdot\boldsymbol{\sigma}$ where*

$$\mathbf{B}(t) = B(\sin(\theta)\cos(\omega t), \sin(\theta)\sin(\omega t), \cos(\theta)).$$

Suppose at $t = 0$, the system is in the instantaneous ground state $\psi(0)$. Obtain a condition on ω for which adiabatic theory will be applicable. In the adiabatic limit, compute the state after a complete cycle: $\psi(T)$ where $T = 2\pi/\omega$.

Bonus (more difficult): obtain the exact solution of this problem (using e.g. a time-dependent unitary transformation). Compare this with the approximate adiabatic solution.

Exercise 5.5 *Longer problem that ties together different parts of the chapter. In this problem we consider the time-dependent Hamiltonian given by*

$$\hat{\mathcal{H}} = \varepsilon(|1\rangle\langle 1| - |0\rangle\langle 0|) + f(t)\lambda\Omega(|1\rangle\langle 0| + |0\rangle\langle 1|) = \hat{\mathcal{H}}_0 + \lambda\hat{V}(t).$$

where ε and Ω are positive constants and λ is our usual perturbative parameter. $\{|0\rangle, |1\rangle\}$ form an orthonormal basis. The time-dependent function appearing in the Hamiltonian is defined as $f(t) = e^{\eta t}$ for $t < 0$ and $f(t) = 1$ for $t \geq 0$ where η is a positive constant. Adjusting η allows us to control how quickly the second term in the Hamiltonian is 'turned on'.

Suppose that in the 'distant past', $t \to -\infty$, the system is in the ground state $|0\rangle$ of the Hamiltonian. In this problem we will focus on computing the probability $P_{0\to 1}$ for the system to be in the state $|1\rangle$ at time $t > 0$.

(a) Limit of small λ. Using time-dependent perturbation theory, show that to lowest non-trivial order in λ,

$$P_{0\to 1} = \frac{\lambda^2\Omega^2}{\hbar^2}\left|\frac{1}{2i\varepsilon/\hbar + \eta} + \frac{1}{2i\varepsilon/\hbar}(e^{2i\varepsilon t/\hbar} - 1)\right|^2.$$

Hint: recall the result from time-dependent perturbation theory

$$P_{0\to 1} = \frac{\lambda^2}{\hbar^2}\left|\int_{-\infty}^{t} dt' \langle 1|\hat{V}(t')|0\rangle e^{-i(\varepsilon_0-\varepsilon_1)t'/\hbar)}\right|^2.$$

(b) Limit of large η. In the limit when $\eta \to +\infty$, $f(t)$ becomes a step function. That is $f(t) = 0$ for $t < 0$ and $f(t) = 1$ for $t \geq 0$. Taking $f(t)$ to be a step function, compute the probability $P_{0\to 1}$ exactly. Show that it agrees with the result of (a) in the limit of small λ and large η.

(c) Now consider the opposite limit of η approaching zero (slow turn-on). Show that in this limit

$$P_{0\to 1} = \frac{1}{2}\left(1 - \frac{\varepsilon}{\sqrt{\varepsilon^2 + \lambda^2\Omega^2}}\right).$$

Argue that this result is consistent with that of (a).

Chapter 6

Multiple-Particle Systems

In this final Chapter, we consider multiple-particle systems in quantum mechanics. The notation of second quantisation will be introduced, which is typically the most efficient way to treat such systems. This topic could easily fill up an entire module. This Chapter just gives a taste of the subject.

6.1 Two-particle systems

To start, let us consider the simple situation of two particles with the same mass coupled to the same external potential. To be more concrete, let's take the external potential to be that of a harmonic oscillator $V(\hat{x}) = \frac{1}{2}m\omega^2\hat{x}^2$. The Hamiltonian describing such a system is:

$$\hat{\mathcal{H}} = \frac{\hat{p}_1^2}{2m} + V(\hat{x}_1) + \frac{\hat{p}_2^2}{2m} + V(\hat{x}_2) = \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2.$$

As these are independent particles, the operators with subscript 1 commute with those having subscript 2. We can immediately write down the eigenfunctions of this system. They are

$$|\phi_n\phi_m\rangle\,.$$

In this notation n denotes the state of the first particle while m denotes the state of the second particle. In the position basis, this state is $\langle x_1x_2|\,\phi_n\phi_m\rangle = \phi_n(x_1)\phi_m(x_2)$ which is the product of two *single-particle eigenstates*. These states satisfy the following rule for inner products:

$$\langle\phi_n\phi_m|\,\phi_{n'}\phi_{m'}\rangle = \langle\phi_n|\,\phi_{n'}\rangle\,\langle\phi_m|\,\phi_{m'}\rangle.$$

The eigenenergy corresponding to $|\phi_n\phi_m\rangle$ is $E_n + E_m = \hbar\omega(n + m + 1)$.

That's all simple enough. Now we introduce the notion of indistinguishable (or identical) particles which is a concept that enters quantum mechanics at the postulate level. Here, 'indistinguishable' is taken in the strongest possible sense of the word. It means that no experiment can distinguish between the two particles. Suppose we have two indistinguishable particles (e.g.

two spin up electrons) described by the wave function $\psi(x_1, x_2)$. Naively one might say that the quantity

$$|\psi(x_1, x_2)|^2 dx_1 dx_2$$

is the probability of electron one being between x_1 and $x_1 + dx_1$ and electron two being between x_2 and $x_2 + dx_2$. However, this would mean that we can differentiate between the two electrons. We cannot do this. We cannot paint one red and the other blue. Instead, we say that this quantity is the probability of *an* electron being between x_1 and x_1+dx_1 and *another* electron being between x_2 and $x_2 + dx_2$. An immediate consequence is that

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2.$$

Now let's consider a Hamiltonian describing the evolution of our two-identical-particle system, say the one we wrote down at the beginning of this section. Such a Hamiltonian is necessarily invariant under the interchanges $\hat{x}_1 \leftrightarrow \hat{x}_2$ and $\hat{p}_1 \leftrightarrow \hat{p}_2$. This interchange can be implemented with the exchange operator $\hat{\mathscr{P}}$. This operator satisfies the follow properties

$$\begin{aligned}
\hat{\mathscr{P}}\hat{x}_1\hat{\mathscr{P}} = \hat{x}_2, \quad \hat{\mathscr{P}}\hat{x}_2\hat{\mathscr{P}} = \hat{x}_1 \\
\hat{\mathscr{P}}\hat{p}_1\hat{\mathscr{P}} = \hat{p}_2, \quad \hat{\mathscr{P}}\hat{p}_2\hat{\mathscr{P}} = \hat{p}_1 \\
\hat{\mathscr{P}}\left|x_1x_2\right\rangle = \left|x_2x_1\right\rangle, \quad \hat{\mathscr{P}}\left|p_1p_2\right\rangle = \left|p_2p_1\right\rangle, \quad \hat{\mathscr{P}}\left|\phi_n\phi_m\right\rangle = \left|\phi_m\phi_n\right\rangle \\
\hat{\mathscr{P}}^2 = \mathbb{1}.
\end{aligned}$$

An explicit representation of this operator is

$$\hat{\mathscr{P}} = \int dx_1 dx_2 \left|x_1x_2\right\rangle \left\langle x_2x_1\right|.$$

The statement of our Hamiltonian being invariant under exchange is $\hat{\mathscr{P}}\hat{\mathcal{H}}\hat{\mathscr{P}} = \hat{\mathcal{H}}$ or $[\hat{\mathscr{P}}, \hat{\mathcal{H}}] = 0$. Therefore, the exchange operator and our Hamiltonian can be simultaneously diagonalised. Since the exchange operator squares to one, its eigenvalues will be either 1 or -1 (check). Furthermore, eigenstates of the exchange operator satisfy our criterion established earlier for identical particles. Writing the exchange operator in the position basis, we will either have $\mathscr{P}\psi(x_1, x_2) = \psi(x_2, x_1) = \psi(x_1, x_2)$ or $\mathscr{P}\psi(x_1, x_2) = \psi(x_2, x_1) = -\psi(x_1, x_2)$. For both scenarios, we have $|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2$.

Let's see how the corresponding joint eigenstates work out. The states $|\phi_n\phi_m\rangle$ and $|\phi_m\phi_n\rangle$ are degenerate eigenstates of $\hat{\mathcal{H}}$. However, unless $n = m$, these clearly will not be eigenstates of $\hat{\mathscr{P}}$. To obtain eigenstates of $\hat{\mathscr{P}}$ we take the following linear combinations:

$$\begin{aligned}
|\phi_+\rangle &= \frac{1}{\sqrt{2}}\left(|\phi_n\phi_m\rangle + |\phi_m\phi_n\rangle\right) \\
|\phi_-\rangle &= \frac{1}{\sqrt{2}}\left(|\phi_n\phi_m\rangle - |\phi_m\phi_n\rangle\right).
\end{aligned}$$

The corresponding exchange eigenvalues are $+1$ and -1 respectively. In the former case, we say that the particles are bosons while in the latter case we say that the particles are fermions.

At this point, it might seem very strange that we are giving the particles names according to the state that we 'put them in'. In the past we didn't introduce any silly terminology like calling a particle in the ground state of the harmonic oscillator an alpha particle and a particle in the first excited state of the harmonic oscillator a beta particle. The important thing to note is the following. Suppose that our particles start in a state with exchange eigenvalue 1. Since these particles are identical, any possible Hamiltonian in Nature with which these particles evolve must commute with $\hat{\mathscr{P}}$. Therefore, the state describing these two particles will have exchange eigenvalue of 1 forevermore. In particular, conversion between $|\phi_+\rangle$ and $|\phi_-\rangle$ will not happen. Hence it is sensible to give the particles different names.

It follows from the above that we cannot put two identical fermions into the same single-particle state. That is, if $n = m$, we have

$$|\phi_-\rangle = \frac{1}{\sqrt{2}} \left(|\phi_n \phi_n\rangle - |\phi_n \phi_n\rangle \right) = 0.$$

This is the **Pauli exclusion principle** which is foundational.

The **Spin-Statistics Theorem** gives an important connection between the above and spin. It states that particles with half-integer spin are fermions while particles with integer spin are bosons. For example, since electrons have spin half, they are fermions. The result of this theorem is simple, but its proof requires incorporating relativity. We offer a quote from R.P. Feynman about this theorem:

'It appears to be one of the few places in physics where there is a rule which can be stated very simply, but for which no one has found a simple and easy explanation. The explanation is deep down in relativistic quantum mechanics. This probably means that we do not have a complete understanding of the fundamental principle involved.'

6.2 Many-particle systems

Having considered the two-particle system as a warm up, we now move on to the general case. For an N-particle system, we have the **symmetrisation postulate**. This says that any state $|\psi\rangle$ describing a system of N identical particles will satisfy one of the following conditions:

1. $\hat{\mathscr{P}}_{nm} |\psi\rangle = |\psi\rangle \ \forall\, n, m \ (n \neq m)$ (identical bosons)
2. $\hat{\mathscr{P}}_{nm} |\psi\rangle = -|\psi\rangle \ \forall\, n, m \ (n \neq m)$ (identical fermions)

where $\hat{\mathscr{P}}_{nm} = \hat{\mathscr{P}}_{mn}$ exchanges the nth and mth particles. The first case corresponds to a collection of identical bosons while the second case corresponds to a collection of identical fermions.

It is fine to accept the above postulate for what it is and move on. In the following two paragraphs, though, we will attempt to motivate it using the notion of indistinguishable particles. Suppose we are interested in measuring observable A corresponding to the Hermitian operator $\hat{A} = \hat{Q} - |\psi\rangle \langle\psi|$ where $\hat{Q} = 1 - |\psi\rangle \langle\psi|$. Outcomes of experiments measuring this quantity will

yield either +1 or -1. Suppose our system is in state $|\psi\rangle$. Then the probability of experimental outcome -1 is $|\langle\psi|\psi\rangle|^2 = 1$. Due to particles being indistinguishable, if our system is in state $|\xi\rangle = \hat{\mathscr{P}}_{nm}|\psi\rangle$, we must have the same experimental outcome, namely $|\langle\psi|\xi\rangle|^2 = 1$. This, in turn, means that $\hat{\mathscr{P}}_{nm}|\psi\rangle = \lambda_{nm}|\psi\rangle$ where $|\lambda_{nm}| = 1$. Since the exchange operators square to one further constrains the possible values λ_{nm}: they can either be +1 or -1.

We have so far concluded that a state describing N identical particles must be an eigenstate of all of the $N(N-1)/2$ exchange operators and the corresponding eigenvalues will either be +1 or -1. Can we have "mixed statistics", meaning some of the exchange eigenvalues will be +1 while others -1? The answer turns out to be no. Suppose we know one of the exchange eigenvalues, λ_{nm}. This is actually enough to determine all of the other exchange eigenvalues. Consider ℓ distinct from n and m. Convince yourself that $\hat{\mathscr{P}}_{n\ell} = \hat{\mathscr{P}}_{\ell m}\hat{\mathscr{P}}_{nm}\hat{\mathscr{P}}_{\ell m} = \hat{\mathscr{P}}_{nm}\hat{\mathscr{P}}_{\ell m}\hat{\mathscr{P}}_{nm}$ (maybe think of that three-cup game where you are trying to confuse the other player by permuting them). Applying these operators to the state we get $\lambda_{n\ell} = (\lambda_{\ell m})^2\lambda_{nm} = (\lambda_{nm})^2\lambda_{\ell m}$ which means that $\lambda_{n\ell} = \lambda_{nm} = \lambda_{\ell m}$. Next we can apply the same argument for ℓ' distinct from ℓ, n, m to see that $\lambda_{n\ell} = \lambda_{n\ell'} = \lambda_{\ell\ell'}$. So, in summary, we have $\lambda_{nm} = \lambda_{n\ell} = \lambda_{\ell m} = \lambda_{\ell\ell'}$ and since ℓ and ℓ' are arbitrary we are done. Therefore, we have reached the conclusion from the beginning of this section.

As an aside, it is worth noting that throughout we have always assumed that the exchange operators square to one which has led us to the conclusion that there are two particle types: fermions and bosons. This is always correct in our three-dimensional world. However, there can be exotic scenarios arising in two spatial dimensions where the exchange operators do not square to one. At the root of this is the fact that there are homotopically distinct ways of exchanging particles (often called braiding) in two dimensions. This has led to the theoretical prediction of so-called anyons ('any' replaces 'Fermi' or 'Bose'). Anyon physics is currently an active area of research, in part due to their potential use in quantum computing hardware as a topological qubit.

Let us extend the example we looked at in the previous section to the case of N particles. The Hamiltonian becomes

$$\hat{\mathcal{H}} = \sum_{n=1}^{N}\left(\frac{1}{2m}\hat{p}_n^2 + V(\hat{x}_n)\right).$$

What is the ground state of this system? The Pauli principle does not apply to bosons. So we may put all the bosons into the lowest energy single-particle state. The ground state, in the position basis, is

$$\phi_{\text{bosons}}(x_1, x_2, \ldots, x_N) = \phi_0(x_1)\phi_0(x_2)\ldots\phi_0(x_N)$$

which has eigenenergy $E = NE_0$. On the other hand, we cannot put two identical fermions into the same single-particle state. The ground state for this situation is:

$$\phi_{\text{fermions}}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}}\det\begin{pmatrix} \phi_0(x_1) & \phi_0(x_2) & \ldots & \phi_0(x_N) \\ \phi_1(x_1) & \phi_1(x_2) & \ldots & \phi_1(x_N) \\ \vdots & & & \vdots \\ \phi_{N-1}(x_1) & \phi_{N-1}(x_2) & \ldots & \phi_{N-1}(x_N) \end{pmatrix}$$

which has eigenenergy $E = E_0 + E_1 + \ldots E_{N-1}$. With the properties of the determinant, we can tell that this fermionic wave function is completely antisymmetric under exchange of any pair of coordinates. The above is known as a Slater determinant.

6.3 Second quantisation

Suppose we have N particles and M single-particle states, $\{|\phi_n\rangle\}$. For the previous example of the harmonic oscillator, M is infinite, but for the present purpose it is useful to take finite M. First let us consider the situation where the particles are distinguishable. The Hilbert space for this system will have dimension

$$D_{\text{dist}} = M^N.$$

For instance, we can take basis elements to be of the form

$$|\phi_{n_1}\phi_{n_2}\ldots\phi_{n_N}\rangle\,.$$

where the n_i's can take on values from 1 to M. Only a small subspace of this Hilbert space will correspond to acceptable bosonic or fermionic states. It turns out that the completely symmetric (bosonic) subspace has dimension

$$D_{\text{bosons}} = \left(\begin{array}{c} N+M-1 \\ M-1 \end{array}\right)$$

while the completely antisymmetric (fermionic) subspace has dimension

$$D_{\text{fermions}} = \left(\begin{array}{c} M \\ N \end{array}\right).$$

For the case $M = N = 2$, which we have essentially already done, we have $D_{\text{dist}} = 4$, $D_{\text{bosons}} = 3$, and $D_{\text{fermions}} = 1$.

As we start to consider larger values of N and M, the difference in the size between the original Hilbert space and the (anti)symmetric subspace is becomes vast. Basis elements of the form $|\phi_{n_1}\phi_{n_2}\ldots\phi_{n_N}\rangle$ are most suitable for the case of distinguishable particles. For the case of a collection of identical fermions (or bosons), on the other hand, one can can easily write down unphysical states in this basis (that is, states without the appropriate symmetries). The language of second quantisation, to be discussed now, gives us an economical way of restricting to the correct subspace.

The vacuum state, denoted by $|0\rangle$, is the state with no particles present. This is normalised to one, as usual. We next introduce the so-called field operator: $\hat{\Psi}(x)$. When acting on the vacuum state, we have

$$\begin{aligned}\hat{\Psi}(x)\,|0\rangle &= 0 \\ \hat{\Psi}^\dagger(x)\,|0\rangle &= |x\rangle\,.\end{aligned}$$

The field operator $\hat{\Psi}(x)$ removes a particle at position x while $\hat{\Psi}^\dagger(x)$ creates a particle at position x. The vacuum is the state with no particles, so when acted upon by the field operator we obtain zero. For the bosonic case, the field operators are taken to satisfy the following algebraic relations

$$[\hat{\Psi}(x), \hat{\Psi}^\dagger(x')] = \delta(x - x')$$
$$[\hat{\Psi}(x), \hat{\Psi}(x')] = 0.$$

For the fermionic case, the operators are taken to satisfy

$$\{\hat{\Psi}(x), \hat{\Psi}^\dagger(x')\} = \delta(x - x')$$
$$\{\hat{\Psi}(x), \hat{\Psi}(x')\} = 0$$

where the curly brackets denote the 'anticommutator': $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$. In the following, we will treat the fermionic and bosonic cases together (as much as possible). In order to do so, we introduce the temporary notation: $[\hat{A}, \hat{B}]_\eta = \hat{A}\hat{B} - \eta\hat{B}\hat{A}$ where η is either -1 or 1. So $[\hat{A}, \hat{B}]_\eta$ gives either the commutator or anticommutator. For bosons we put $\eta = 1$ while for fermions we put $\eta = -1$.

Moving on to two-particle states we make the following identifications:

$$\hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)\,|0\rangle = \frac{1}{\sqrt{2}}(|x_1x_2\rangle + \eta\,|x_2x_1\rangle).$$

Note that due to the algebraic relations from above we have $\hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2) = \eta\hat{\Psi}^\dagger(x_2)\hat{\Psi}^\dagger(x_1)$.

It is often useful to expand the field operator in a basis. We take $\{\phi_n(x)\}$ to be an orthonormal basis of our (single-particle) Hilbert space. For example, we could take these to be the Harmonic oscillator eigenstates. Letting

$$\hat{c}_n = \int dx \phi_n^*(x)\hat{\Psi}(x),$$

we then have

$$\hat{\Psi}(x) = \sum_n \phi_n(x)\hat{c}_n.$$

The $\hat{c}_n$ operators then satisfy (check)

$$[\hat{c}_n, \hat{c}_{n'}^\dagger]_\eta = \delta_{nn'}$$
$$[\hat{c}_n, \hat{c}_n']_\eta = 0.$$

The particle number operator is defined to be

$$\hat{N} = \int dx \Psi^\dagger(x)\Psi(x) = \sum_n \hat{c}_n^\dagger\hat{c}_n.$$

We are now in a position to provide a recipe for writing a system in the second-quantised notation. Take a collection of N identical particles evolving under the 'first quantised' Hamiltonian:

$$\hat{\mathcal{H}}_{\text{1st}} = \sum_{n=1}^{N} \left(\frac{1}{2m} \hat{p}_n^2 + V(\hat{x}_n) \right) + \frac{1}{2} \sum_{n \neq n'} V_{\text{int}}(\hat{x}_n - \hat{x}_{n'}). \tag{6.1}$$

Here, we are allowing the particles to interact with one another through the potential V_{int}. Writing the single-particle Hamiltonian in the position basis we have $\mathcal{H}_0(x) = \frac{-\hbar^2}{2m}\partial_x^2 + V(x)$. The second quantised Hamiltonian describing this system is:

$$\hat{\mathcal{H}}_{\text{2nd}} = \int dx \hat{\Psi}^\dagger(x) \mathcal{H}_0(x) \hat{\Psi}(x) + \frac{1}{2} \int dx dx' V_{\text{int}}(x - x') \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x') \hat{\Psi}(x') \hat{\Psi}(x). \tag{6.2}$$

A direct correspondence between the first and second quantised Hamiltonians can be established with the relation

$$\langle x_1 x_2 \dots x_N | \, \hat{\mathcal{H}}_{\text{2nd}} \, |\phi\rangle = \mathcal{H}_{\text{1st}} \phi(x_1, x_2, \dots x_N)$$

where $\mathcal{H}_{\text{1st}}$ is (6.1) in the position basis and $|x_1 x_2 \dots x_N\rangle = \hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)\dots\hat{\Psi}^\dagger(x_N)\,|0\rangle$. The above relation can be obtained by exploiting the commutation relations of the field operators but we will not provide an explicit derivation here.[1]

To start, let's consider the case where $V_{\text{int}} = 0$. For this, things become rather simple when we expand the field operator in the eigenbasis of $\mathcal{H}_0(x)$. We have

$$\hat{\mathcal{H}} = \sum_n E_n \hat{c}_n^\dagger \hat{c}_n.$$

This is the Hamiltonian considered in the previous section in second quantised notation. For the bosonic case, the ground state is

$$|\phi\rangle_{\text{bosons}} = \frac{1}{\sqrt{N!}} (\hat{c}_0^\dagger)^N \, |0\rangle \, .$$

For the fermionic case, the ground state is

$$|\phi\rangle_{\text{fermions}} = \hat{c}_0^\dagger \hat{c}_1^\dagger \dots \hat{c}_{N-1}^\dagger \, |0\rangle \, .$$

Note that, for the fermionic case, the Pauli exclusion principle is automatically enforced. This is because the fermionic creation operators anticommute. For instance $\hat{c}_0^\dagger \hat{c}_0^\dagger = -\hat{c}_0^\dagger \hat{c}_0^\dagger = 0$.

Next, let's consider the case where there are interactions. Interactions are notorious for making many-particle problems difficult to solve. To simplify matters, we consider the situation of a bosonic system under tight harmonic confinement and weak interactions. For such a scenario, it can be appropriate to use just a single basis state for the field operator: $\hat{\Psi}(x) = \phi_0(x)\hat{c}_0$. That

[1] A thorough treatment is given in Appendix A.2 and A.3 of the Statistical Mechanics textbook by K. Huang.

is, we are considering a collection of interacting bosons in the ground state of the Harmonic oscillator potential. Inserting this expression for the field operator yields

$$\hat{\mathcal{H}} = \varepsilon_0 \hat{c}_0^\dagger \hat{c}_0 + \frac{1}{2} U \hat{c}_0^\dagger \hat{c}_0^\dagger \hat{c}_0 \hat{c}_0$$

where $U = \int dx dx' V_{\text{int}}(x - x') |\phi_0(x)|^2 |\phi_0(x')|^2$. The second term above describes the interactions. We considered the dynamics induced by this term back in Chapter 2 in our example of the collapse-revival phenomenon.

This formalism carries over naturally to more general systems. For instance, for a collection of electrons in three spatial dimensions we take the field operator to be $\hat{\Psi}_\sigma(\mathbf{r})$ where σ is either $\uparrow$ or $\downarrow$. The state $\hat{\Psi}_\uparrow^\dagger(\mathbf{r}) |0\rangle$ corresponds to a single spin up electron localised at $\mathbf{r}$. Note that the spin up electrons are *distinguishable* from the spin down electrons. The generalised field operators satisfy the following relations:

$$[\hat{\Psi}_\sigma(\mathbf{r}), \hat{\Psi}_{\sigma'}^\dagger(\mathbf{r}')]_\eta = \delta(x - x')\delta(y - y')\delta(z - z')\delta_{\sigma\sigma'}$$
$$[\hat{\Psi}_\sigma(\mathbf{r}), \hat{\Psi}_{\sigma'}(\mathbf{r}')]_\eta = 0.$$

6.4 Lattice Models

In this section, we will consider second-quantised lattice models arrived at by using the so-called tight-binding approximation. We wish to understand the behaviour of a collection of identical particles in a periodic potential $V(x)$. In the limit where this potential is weak, the single-particle eigenstates will be (nearly) plane waves. We are interested in the opposite regime – the so-called tight-binding regime. Here, it is best to use localised (in position space) orthonormal basis functions situated at the minima of $V(x)$. Furthermore, in order to obtain a good approximation to the low-energy behaviour of the system, this basis need not be complete. Often a sufficiently good approximation involves keeping only one basis function per minimum of $V(x)$. The details (there are quite a few – it can be a very sophisticated technique) of the tight-binding approximation are outside of the scope of this course.[2]

An example of a model arrived at through this scheme is the following

$$\hat{\mathcal{H}} = -w \sum_n \left(\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{c}_{n+1}^\dagger \hat{c}_n \right).$$

This model corresponds to particles hopping on a one-dimensional lattice. The operator $\hat{c}_n^\dagger$ creates a particle at lattice site n. This model is rather intuitive.

Let us now restrict to the case of fermions. Let's consider periodic boundary conditions where $\hat{c}_{n+M} = \hat{c}_n$ where M is the number of lattice sites in the system. To put this Hamiltonian in diagonal form, we introduce the operators

$$\hat{c}_k = \frac{1}{\sqrt{M}} \sum_n e^{-ikn} \hat{c}_n$$

[2]Treatments of the tight-binding approximation are given in most textbooks on solid-state physics. The book *Atomic and Electronic Structure of Solids* by E. Kaxiras is recommended.

where k is restricted to integer multiples of $2\pi/M$ and the sum is from $n = 1$ to $n = M$. This relation can be inverted as

$$\hat{c}_n = \frac{1}{\sqrt{M}} \sum_k e^{ikn} \hat{c}_k$$

where the summation is over values $k = \frac{2\pi}{M}, \frac{2\pi}{M}2, \ldots, \frac{2\pi}{M}M$. The Fourier-transformed operators also satisfy fermionic relations:

$$\{\hat{c}_k, \hat{c}_{k'}\} = 0$$
$$\{\hat{c}_k, \hat{c}^\dagger_{k'}\} = \delta_{kk'}.$$

Note also that these operators are periodic in k: $\hat{c}_{k+2\pi} = \hat{c}_k$.

With these quantities, our Hamiltonian takes on a diagonal form (check)

$$\hat{\mathcal{H}} = \sum_k E_k \hat{c}^\dagger_k \hat{c}_k.$$

where $E_k = -2w\cos(k)$. To find the N-particle ground state we can do what we did before – fill up the single particle states one by one until there are no particles left. The resulting ground state is

$$|\phi\rangle = \prod_{|k|\leq k_F} \hat{c}^\dagger_k |0\rangle$$

where k_F is the k-value of the most energetic particle. Such a state is called a filled 'Fermi sea'.

6.4.1 Fermionic Hubbard model

Recalling that interactions yield quartic terms in the creation / destruction operators, we see that the above Hamiltonian is for a non-interacting system. In the following example, we consider an interacting lattice model. We consider a collection of spin-half fermions (electrons) hopping on a square lattice. The interactions between the fermions is accounted for by including an onsite repulsive term. Such a system is described by the so-called Hubbard model

$$\hat{\mathcal{H}} = -w \sum_{<nn'>\sigma} \hat{c}^\dagger_{n\sigma} \hat{c}_{n'\sigma} + U \sum_n \hat{\rho}_{n\uparrow} \hat{\rho}_{n\downarrow}$$

where $\hat{\rho}_{n\sigma} = \hat{c}^\dagger_{n\sigma} \hat{c}_{n\sigma}$. The subscript n labels the vertices of the square lattice. The first summation in this Hamiltonian includes only hopping between nearest-neighbour lattice sites.

Despite many years of investigation, and despite the model's simplicity, its solution (for arbitrary w and U and particle number) has remained elusive. Numerical methods used to investigate it suffer from problems (like the so-called 'sign problem' of quantum Monte Carlo). It is a fairly high-stakes problem too. The Hubbard model is thought to describe the superconductors with the highest transition temperatures to date, the so-called high T_c superconductors.

6.5 Exercises

Exercise 6.1 *Show that the inner product between the state* $\hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)\,|0\rangle$ *and the state* $\hat{\Psi}^\dagger(x_1')\hat{\Psi}^\dagger(x_2')\,|0\rangle$ *is* $\delta(x_1-x_1')\delta(x_2-x_2')+\eta\delta(x_1-x_2')\delta(x_2-x_1')$ *where* $\eta=1$ *for the bosonic case while* $\eta=-1$ *for the fermionic case.*

Exercise 6.2 *Consider a collection of spinless bosons in one spatial dimension interacting through the potential* $V_{\text{int}}(x-x')=g\delta(x-x')$*. Show that the Heisenberg equation of motion for the field operator with dynamics governed by the Hamiltonian (6.2) is*

$$i\hbar\partial_t\hat{\Psi}_{\text{H}}=\mathcal{H}_0\hat{\Psi}_{\text{H}}+g\hat{\Psi}_{\text{H}}^\dagger\hat{\Psi}_{\text{H}}\hat{\Psi}_{\text{H}}.$$

Exercise 6.3 *Consider the two-mode bosonic model:*

$$\hat{\mathcal{H}}=-w(\hat{c}_1^\dagger\hat{c}_2+\hat{c}_2^\dagger\hat{c}_1)+U(\hat{c}_1^\dagger\hat{c}_1-\hat{c}_2^\dagger\hat{c}_2)^2$$

where w *and* U *are positive parameters,* $[\hat{c}_n,\hat{c}_{n'}^\dagger]=\delta_{nn'}$*, and* $[\hat{c}_n,\hat{c}_{n'}]=0$*. Find the ground state of this system for* $N=2$ *particles.*

Exercise 6.4 *(more difficult) Consider the two-site fermionic Hubbard model:*

$$\hat{\mathcal{H}}=-w\sum_\sigma(\hat{c}_{1\sigma}^\dagger\hat{c}_{2\sigma}+\hat{c}_{2\sigma}^\dagger\hat{c}_{1\sigma})+U(\hat{\rho}_{1\uparrow}\hat{\rho}_{1\downarrow}+\hat{\rho}_{2\uparrow}\hat{\rho}_{2\downarrow})$$

where w *and* U *are positive parameters,* $\{\hat{c}_{n\sigma},\hat{c}_{n'\sigma'}^\dagger\}=\delta_{nn'}\delta_{\sigma\sigma'}$*, and* $\{\hat{c}_{n\sigma},\hat{c}_{n'\sigma'}\}=0$*. Find its ground state for the cases of* $N=2$ *particles. It is helpful to recognise that the operator* $\sum_n(\hat{c}_{n\uparrow}^\dagger\hat{c}_{n\uparrow}-\hat{c}_{n\downarrow}^\dagger\hat{c}_{n\downarrow})$ *commutes with this Hamiltonain.*

Appendix A

Answers/Solutions to exercises