

Introduction to Quantum Mechanics

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Preface

To come.

Why Open Education?

This book and the supplementary material are released under a Creative Commons Attribution-ShareAlike 4.0 International License, which means you can do anything you want with this book: cut out stuff you don't need, use it to build an even better book, download it for free off the web, print it out yourself, give it to your friends (they want a copy, trust me), and anything else you can think of. The only stipulation is that you give credit where it's due, and release the derivative work under the same license.

Why did I choose this? Because I've taught university courses and have seen the issues with expensive textbooks: students not being able to afford them, students finding illegal PDF copies online and sharing them, the publishing companies fighting back with various schemes like renting digital copies, and so on. Especially in advanced physics, little textbooks can be so expensive, and yet I think textbooks are an important and necessary resource, and I want my students to all have a copy.

Thanks

To come.

Find a typo, mistake, or horrible misconception in this book? Let me know by creating a new issue at the GitHub page:

github.com/josephmacmillan/IntroductionToQuantumMechanics/issues.

Chapter 1

The Stern-Gerlach Experiment

1.1 Spin Angular Momentum

Let's start with something that is pretty much as far away from the quantum world as possible – the Earth and Sun. With its total motion, the Earth has two kinds of angular momentum: *orbital* angular momentum L from its orbit around the sun, and *spin* angular momentum S , resulting from its 24 hour rotation. Of course, the spin angular momentum in this case is due to adding up the orbital angular momentum $L_i = \mathbf{r}_i \times \mathbf{p}_i$ of each of the tiny pieces of the Earth, but we'll keep the distinction – it'll turn out that this is *not* the case in quantum systems.¹

The quantum version of this kind of system could be an electron in orbit around a proton – a hydrogen atom. The electron has orbital angular momentum just like the Earth (depending on what state it's in), and it also has spin angular momentum. Careful, though, as the electron doesn't rotate like the Earth – how can it when it has essentially no size or diameter to spin? Despite this, it has measurable intrinsic angular momentum, which we'll call *spin* S . Since spin is a vector, it has components (S_x, S_y, S_z), and thus to specify the spin of the electron we need to use three different numbers; keep this in mind for later.

I'd like to explore this idea of spin without the complication of orbital angular momentum, so let's put a stationary electron all by itself in a magnetic field \mathbf{B} . Since the electron isn't moving, the Lorentz force

$$\mathbf{F} = q\mathbf{v} \times \mathbf{B}$$

¹Note that the two kinds of angular momentum for the Earth point in different directions since the rotation axis of the Earth is tilted 23° from the orbital plane.

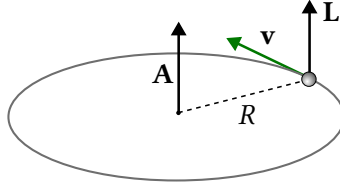


Figure 1.1: A charged particle in a circular orbit has a magnetic dipole moment.

is zero. But the electron's spin angular momentum gives it a magnetic dipole moment μ , and it's then possible for an *inhomogeneous* magnetic field to exert a force given by (see Griffiths *Introduction to Electrodynamics*, fifth edition, section 6.1.2)

$$\mathbf{F} = \nabla(\mu \cdot \mathbf{B}). \quad (1.1)$$

Now, we can calculate the magnetic dipole moment due to orbital angular momentum easily enough (we'll handle spin in a moment); Figure 1.1 shows a particle in a circular orbit of radius R and circular velocity \mathbf{v} . If we think of this as a current loop, the dipole moment is just the current I times the area A ,

$$\mu = IA.$$

The magnitude of the area vector is just $A = \pi R^2$ and the direction is perpendicular to the orbit, while the current will be the charge divided by the time it takes for the charge to make the orbit:

$$I = \frac{q}{T} = \frac{q}{2\pi R/v}.$$

The dipole moment is then

$$\mu = \left(\frac{1}{2} q v R, \text{ perpendicular to the orbit} \right).$$

It's more useful, though, to put this in terms of the angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, which for a circular orbit is

$$\mathbf{L} = (rmv, \text{ perpendicular to the orbit}).$$

Finally, then, the magnetic dipole moment arising from orbital angular momentum is

$$\mu = \frac{q}{2m} \mathbf{L}. \quad (1.2)$$

What changes for spin angular momentum? It turns out to be only slightly different, and we can write

$$\boldsymbol{\mu} = \frac{gq}{2m}\mathbf{S}, \quad (1.3)$$

where g is called the gyroscopic ratio or often just “ g -factor” and, for an electron, is *almost* $g = 2$.²

Let’s go back to our electron in an inhomogeneous field. Take the field to be constant in the x and y directions but *not* in the z direction. Then

$$\boldsymbol{\mu} \cdot \mathbf{B} = \mu_x B_x + \mu_y B_y + \mu_z B_z,$$

and since the first two terms are constant, equation (1.1) gives

$$\mathbf{F} = \nabla(\mu_z B_z) = \mu_z \frac{\partial B_z}{\partial z} \hat{z} = \frac{gq}{2m} \frac{\partial B_z}{\partial z} S_z \hat{z}. \quad (1.4)$$

The force on the electron in this case is directed along the z direction and proportional to the component of spin angular momentum S_z along that direction – the more the spin aligns with the z axis, the greater the force.

1.2 The Stern-Gerlach Experiment

In 1922 Otto Stern and Walther Gerlach used these ideas to measure the spin angular momentum of electrons. Their experiment is shown in Figure 1.2, and they actually used silver atoms rather than electrons. Why silver? The atoms are electrically neutral, so there won’t be any direct magnetic force on the atoms from the magnetic field, and the electronic configuration of silver is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 4d^{10} 5s^1$. Except for the outermost electron, all others are in closed shells, meaning we can ignore their contribution to the angular momentum of the silver atom. The outermost electron is in an s -orbit, which has no orbital angular momentum – so the only angular momentum of the entire silver atom is due to the spin of that one outer electron.

The Stern-Gerlach experiment proceeds as follows. First, the oven boils silver atoms off of a solid piece of silver; the atoms are “thermalized,” meaning they come out in all directions and with random spin orientations. A collimating slit produces a narrow beam of these atoms which pass between the magnets. The magnets are constructed to create an inhomogeneous magnetic field, with the inhomogeneity in the z direction;

²We don’t need to worry about this here, but each charged particle with spin has its own g -factor – the proton has $g = 5.58$, for example. These can be measured and in some cases calculated theoretically, but it requires quantum field theory to do it properly.

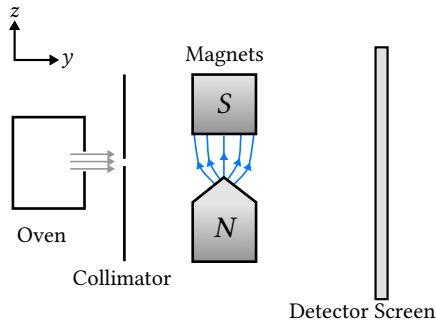


Figure 1.2: The Stern-Gerlach experiments, in which silver atoms are deflected by an inhomogeneous magnetic field.

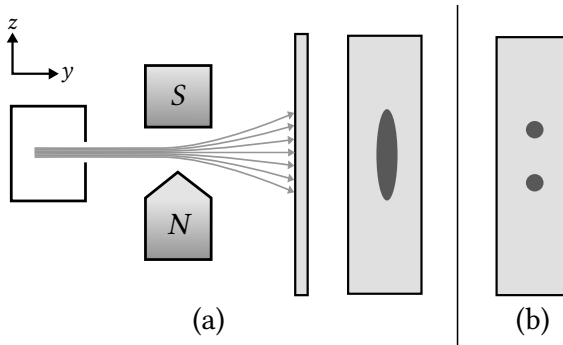


Figure 1.3: (a) Classically expected result. (b) Actual result showing quantization of spin angular momentum.

note that as shown the magnetic field gets stronger in the negative z direction, so $\partial B_z / \partial z$ is negative in equation (1.4). Because the charge on the electron is negative as well, the force on a silver atom passing through the field will be up along z if the spin has a positive z component, and down along $-z$ if the spin has a negative z component. Finally, the deflection of each atom is measured when they hit the detecting screen.

What do we expect? Well, as mentioned above, the oven thermalizes the atoms so the spin of the outer electron is in random directions. That means the force on each atom will be random as well – some atoms will get pushed up, some will get pushed down, and each with varying strength (up to some maximum for those spins that are entirely along z or $-z$). This expected result is shown in Figure 1.3 (a).

But that's not at all what Stern and Gerlach saw; instead, as Figure

1.3 (b) shows, they detected only two locations where silver atoms hit the screen, corresponding to spin angular momentum values of either

$$S_z = +\frac{\hbar}{2} \quad \text{or} \quad S_z = -\frac{\hbar}{2}.$$

This is clear evidence of the *quantization* of angular momentum, something Niels Bohr suggested in 1913 when developing his model of the atom. Evidently, every silver atom boiled off with the outermost electron having only two values for S_z . Of course, this says nothing about the values of S_x or S_y , or even the magnitude of the spin S . And, actually, it turns out we can't even say they had these values of S_z when they were created – we can only say we measured S_z to be either one or the other; more on this later.

1.3 Extending the Experiments

Before we discuss this further, though, I want to introduce some notation:

$$|\psi\rangle \rightarrow \text{Represents the state of a quantum mechanical system.} \quad (1.5)$$

This notation is often called a “ket,” for reasons we’ll see later, and it includes all possible information you could know about a particular quantum system. Consider, for example, a silver atom that has been measured to have $S_z = +\hbar/2$. We could represent the state of the atom by

$$|+\rangle \rightarrow \text{State for which } S_z = +\hbar/2 \text{ has been measured,}$$

although it’s also common to use $|\uparrow\rangle$ or $|+z\rangle$. This state is usually called “spin up.” Similarly, the “spin down” state is represented by

$$|-\rangle \rightarrow \text{State for which } S_z = -\hbar/2 \text{ has been measured,}$$

or $|\downarrow\rangle$ or $|-z\rangle$. Any particle that, when measuring a component of its spin angular momentum, has only two possibilities for the results is called a *spin-1/2* particle; electrons, protons, and neutrons are all spin-1/2 particles.

Let’s run through a few extensions to the original Stern-Gerlach experiment. I’ve simplified the diagram of the original experiment in Figure 1.4 to highlight the important steps: a beam of spin-1/2 particles (whether silver atoms or something else) is created, all in state $|\psi\rangle$, and sent to a Stern-Gerlach device (the magnets) to have the spin of each particle measured. In the case of the original Stern-Gerlach experiment, if a beam of

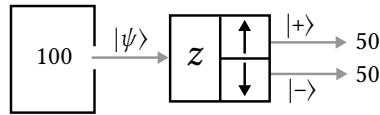


Figure 1.4: A simplified diagram of the original Stern-Gerlach experiment.

100 atoms were created, half of the atoms would be measured as spin up and half would be spin down.

Actually, we should be more careful – we can’t predict which atoms will be spin up and which will be spin down, and the process is inherently *random*. That means that we might get 49 spin up and 51 spin down, or 43 and 57, but if we increase the number of particles in the beam, we’ll get closer and closer to exactly 50% for each.

In these experiments, we can think of the Stern-Gerlach device as an *analyzer* – it measures something. But we can also think of it as a device for preparing a beam of particles all in the same known state; for example, each particle coming out of the top of the Stern-Gerlach device is in state $|+\rangle$, and we can use this knowledge to do further measurements.

1.3.1 Experiment 1

It may be a basic question, but it’s worth asking: once the particles are in state $|+\rangle$, for example, do they *stay* in that state? In Experiment 1 we’ll test this by connecting another Stern-Gerlach device as shown in Figure 1.5, and sure enough all particles that enter the second analyzer come out with the same $|+\rangle$ state, and none become spin down.

That’s a good thing: it means we can do repeated measurements and expect the same results. Science would be tricky to do if things were otherwise. But we should be a little careful, as quantum systems do evolve in time – we’ll learn about this later when we cover the Schrödinger equation – so the repeated measurement should be made right after the first.

What if we moved the second device to accept the spin down particles from the first? As you probably would guess, those particles would all be measured as being spin down, with no spin up particles at all.

1.3.2 Experiment 2

Now, we’ve been aligning the magnets in the Stern-Gerlach device so that the inhomogeneity in the magnetic field is along the z axis, but we could have just as easily rotated it (or changed our axes) so that it is in fact along

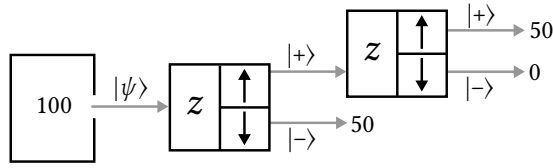


Figure 1.5: Experiment 1: the spin up particles are sent to a second analyzer, where they're found to still be spin up.

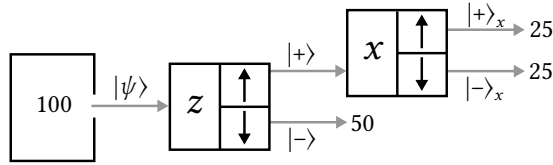


Figure 1.6: Experiment 2: the spin up particles are sent to a second analyzer that has been rotated so that it measures S_x .

the x direction. Does anything change? Well, no – the coordinate system is just our choice and can't affect the actual physics that's happening, so we could just replace every z in the discussion above with an x with no other change. But let's try something a little more interesting and combine a Stern-Gerlach device oriented along z with one oriented along x ; this is shown in Figure 1.6.

First, note the new notation; a particle in the state $|+\rangle_x$ has had its component of spin angular momentum along the x direction measured to be $S_x = +\hbar/2$. This is a different state than our previous spin up state (you might call it “spin up along x ” or something similar) and requires new notation. Note that I didn't bother with the z subscript for our S_z states; by convention, a ket without a subscript indicating direction will be along z .

The results are different this time, with half of the spin up particles sent into the second Stern-Gerlach device being spin up along x (so in state $|+\rangle_x$) and half being spin down along x (in state $|-\rangle_x$).

Remember what we're measuring here: the oven creates particles with a random spin orientation, and we measure half of those particles to have $S_z = +\hbar/2$, and then half of *those* particles to have $S_x = +\hbar/2$. We're missing the component of spin along the y direction, so you might think we just add a third device to measure S_y – and then we'd know all

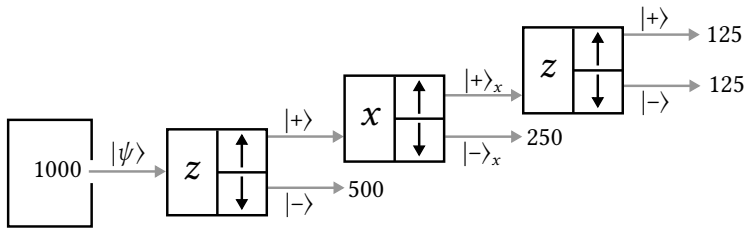


Figure 1.7: Experiment 3: the spin up particles are sent to a second analyzer that has been rotated so that it measures S_x , and then the particles in state $|+\rangle_x$ are sent to a third analyzer to have their spin component S_z measured again.

three components of spin and therefore the vector \mathbf{S} . But there's an interesting twist to this simple story that the next experiment will highlight.

1.3.3 Experiment 3

So, in Experiment 2, spin up (along z) particles have their spin along x measured, and half are found to be spin up along x . In Experiment 3, we take those particles that are spin up along both directions and send them into a third analyzer, this one oriented along z as shown in Figure 1.7. Just so that we're clear: none of the particles sent into this last analyzer were measured to have $S_z = -\hbar/2$. Despite this, half the particles analyzed by the last Stern-Gerlach device are found to be in state $|-\rangle$ along z .

What do we do to make of these experimental results? Evidently measuring S_x has *changed* the state of the particles; although they *were* in state $|+\rangle$, after the measurement of S_x they aren't any more.

Some more terminology: we call quantities that we can measure *observables*, and we say that S_z and S_x are *incompatible observables* – measuring one affects our knowledge of the other. Two other more famous incompatible observables are position and momentum from Heisenberg's uncertainty principle, although not all observables are incompatible – you could know a particle's position and spin S_z at the same time, for example.

Obviously we could have used S_y instead with no change to the results, so we run into a big problem measuring angular momentum: we need three components to specify it, but can never know more than one at a time! Actually, it turns out we can also know the *magnitude* S (we'll see why later), so at most we can specify the length and one component of the angular momentum vector.

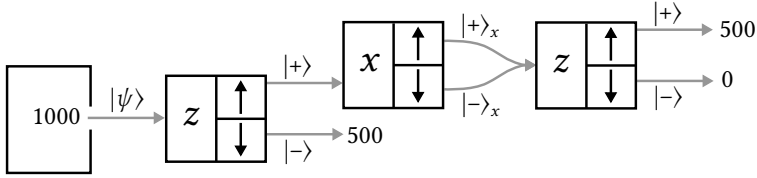


Figure 1.8: Experiment 4: We'll recombine the outputs from the S_x device without measuring anything and send that combined beam into an S_z device.

1.3.4 Experiment 4

For this last experiment, we need to make some changes to the Stern-Gerlach device measuring S_x . The details aren't too important as to how, but rather than measuring the spin S_x observable, we'll recombine the two beams – one pushed up by the magnetic field and one pushed down – and send that combined beam into the last Stern-Gerlach device aligned along the z direction. But now the results are different, and we find that every particle is spin up along z . It seems as though the middle device no longer has an effect on the initial $|+\rangle$ state of the particle; apparently it's the act of *measurement itself* that alters the state, not the push by the magnetic field. This is similar to the famous results from the double slit experiment – measuring which slit the particle goes through destroys the interference pattern.

Problems

Problem 1.1 – Electron spin. This whole chapter is about electron spin, but of course the electron doesn't really spin around like a top. But let's pretend for a moment that an electron really is a tiny sphere, of radius

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2}$$

(the so-called classical electron radius), and that it spins around its axis with angular momentum $S_z = \hbar/2$. How fast would a point on the “equator” be moving? Does this model make sense?

Chapter 2

The Quantum State Vector

2.1 Basis States

In the previous chapter I introduced the ket $|\psi\rangle$, and said that it represents a *state* of a quantum mechanical system. But what exactly is it? It's hard to define, since by its nature it's abstract – in some ways, it's meant to represent everything we could possibly know about a particular quantum system. If we wanted to be technical I could tell you that it's a vector in complex Hilbert space, but I'm not sure that will help. Instead, I think it's best to draw an analogy with something you know well: vectors in three dimensional position space. Before we do that, though, I want to also introduce a *different* way of representing a quantum space, called (for reasons we'll see shortly) a “bra”:

$\langle\psi \rightarrow$ Represents the state of a quantum mechanical system.

 (2.1)

Our job in this chapter is to get a good working idea of what a ket and bra actually are and how we use them in quantum mechanics.

I'm sure you recall some of the basics of how we write vectors – that is, normal old vectors in Cartesian coordinates – in physics. We can use the unit vectors

$$\hat{x}, \quad \hat{y}, \quad \hat{z}$$

(or, if you prefer, \hat{i} , \hat{j} , and \hat{k}) to specify the three coordinate directions. These unit vectors can be used to write any other vector in this coordinate system, so for example the vector \mathbf{A} can be written as

$$\mathbf{A} = A_x \hat{x} + A_y \hat{y} + A_z \hat{z},$$

where A_x , A_y , and A_z and so on are the components of the vector along those directions. The unit vectors are called *complete* if they can be used to write every possible vector in this way.

In addition, these are *unit* vectors, which means that have a length of exactly one (with no dimensions). Mathematically we could express this using the dot product,

$$\hat{x} \cdot \hat{x} = 1, \quad \hat{y} \cdot \hat{y} = 1, \quad \hat{z} \cdot \hat{z} = 1.$$

We say that a vector is *normalized* if this is the case – that the dot product with itself is one.

Of course, these unit vectors are also *orthogonal* – they have 90° between them – which we could also write in terms of dot products as

$$\hat{x} \cdot \hat{y} = 0, \quad \hat{y} \cdot \hat{z} = 0, \quad \hat{z} \cdot \hat{x} = 0.$$

Taken together, we can use the term *orthonormal* for vectors that are both normalized and orthogonal.

The quantum state vectors $|+\rangle$ and $|-\rangle$ play a similar role as the unit vectors, but for spin-1/2 systems; because these states correspond to measuring spin up and spin down along the z axis, these kets form what we'll call the " S_z basis." And like \hat{x} , \hat{y} , and \hat{z} , they're complete, so that any general spin-1/2 state can be written down in terms of them:

$$|\psi\rangle = a|+\rangle + b|-\rangle. \quad (2.2)$$

The values a and b – which can be complex numbers, so be careful – in a loose sense¹ tell you how much of the general state $|\psi\rangle$ is made up of the spin up state (a) how much is made up of the spin down state (b).

Remember I introduced the bra $\langle\psi|$ above? Well, in the S_z basis the state could also be written as

$$\langle\psi| = a^*\langle+| + b^*\langle-|. \quad (2.3)$$

Those stars indicate the *complex conjugate*. It's important to realize that not only are the two representations of the state – the ket $|\psi\rangle$ and the bra $\langle\psi|$ – different (one obviously involves the complex conjugate of the other), but they're not even the same kind of mathematical object. That said, either provides a full representation of the same state.

Okay, so what about these funny names, *ket* and *bra*? They come about because of how we write the *inner product* – the analog to the dot

¹Careful with taking this too far; we'll see exactly what a and b tell us soon.

product we used above for the unit vectors. We stick the bra first, then the ket, like so:

$$\langle \text{bra} | \text{ket} \rangle.$$

Can you see what the whole thing spells? I think this is supposed to be a joke, so feel free to laugh; we're stuck with the notation, though, which Paul Dirac invented in 1939, and which we now call *Dirac notation*.

With the inner product defined, we can now write out the normalization condition for our basis vectors,

$$\langle + | + \rangle = \langle - | - \rangle = 1, \quad (2.4)$$

as well as orthogonalization,

$$\langle + | - \rangle = \langle - | + \rangle = 0. \quad (2.5)$$

Actually, in quantum mechanics, it's not just the basis vectors that are normalized; *every* quantum state must be normalized:

$$\boxed{\langle \psi | \psi \rangle = 1.} \quad (2.6)$$

I know I keep saying this, but we'll see why this must be the case later.

Example 2.1 – Normalization. Consider the state

$$|\psi\rangle = A(|+\rangle + 2i|-\rangle). \quad (2.7)$$

Is the state normalized? Check:

$$\begin{aligned} \langle \psi | \psi \rangle &= 1 \\ \Rightarrow A^* (\langle + | - 2i \langle - |) A (| + \rangle + 2i | - \rangle) &= 1 \end{aligned}$$

Expanding out the brackets and using the orthonormality conditions above gives

$$5|A|^2 = 1, \quad (2.8)$$

where $|A|^2 \equiv A^* A$ is the “complex square.” Now, the complex square will always be a real number, which we can see easily if we write the general complex number A in polar form as

$$A = r e^{i\theta},$$

where r (the *amplitude*) and θ (the *phase*) are both real numbers. Then

$$|A|^2 = A^* A = r e^{-i\theta} r e^{i\theta} = r^2.$$

That means the normalization condition above in equation (2.8) can't give us any information about the phase θ , only the amplitude. As it will turn out, that's okay – an overall phase in a quantum state doesn't mean anything physically, and we'll see why in due time – so by convention we take it to be zero, and set the constant to

$$A = \frac{1}{\sqrt{5}}.$$

With this value of A , the state is normalized.

Example 2.2 – Inner products. Consider another state given by

$$|\phi\rangle = \frac{3}{5}|+\rangle - \frac{4}{5}|-\rangle. \quad (2.9)$$

Notice that this state is already normalized (check it!). What is the inner product between state $|\psi\rangle$ and $|\phi\rangle$?

Using Dirac notation we can write each state in their S_z basis and “foil” it out to get

$$\begin{aligned} \langle\psi|\phi\rangle &= \left(\frac{1}{\sqrt{5}}\langle+| - \frac{2i}{\sqrt{5}}\langle-| \right) \left(\frac{3}{5}|+\rangle - \frac{4}{5}|-\rangle \right) \\ &= \frac{3}{5\sqrt{5}} + \frac{8i}{5\sqrt{5}}. \end{aligned}$$

Notice what happens if we reverse the order of the inner product:

$$\begin{aligned} \langle\phi|\psi\rangle &= \left(\frac{3}{5}\langle+| - \frac{4}{5}\langle-| \right) \left(\frac{1}{\sqrt{5}}|+\rangle + \frac{2i}{\sqrt{5}}|-\rangle \right) \\ &= \frac{3}{5\sqrt{5}} - \frac{8i}{5\sqrt{5}}. \end{aligned}$$

This is precisely the complex conjugate of the first inner product; in fact, in general for any two state vectors $|\alpha\rangle$ and $|\beta\rangle$ we have

$$\boxed{\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*}. \quad (2.10)$$

2.2 Matrix Notation

Dirac notation is fun and expressive, but there's another way to write out a quantum state that can be a little more practical for calculations. Take a look at the form of some general state, which in Dirac notation is

$$|\psi\rangle = a|+\rangle + b|-\rangle. \quad (2.11)$$

Now, the kets $|+\rangle$ and $|-\rangle$ are the basis states as we've mentioned, and a and b are two complex numbers that tell you – again, loosely – how much of each basis state makes up the state $|\psi\rangle$. We can “pick out” these numbers with an inner product; for example,

$$\langle +|\psi\rangle = \langle +|(a|+\rangle + b|-\rangle) = a\langle +|+\rangle + b\langle +|-\rangle = a.$$

Notice how the bra $\langle +|$ acts past the numbers a and b to stick to the kets, and that to make the last equality we used orthonormality. Likewise, the inner product

$$\langle -|\psi\rangle = b.$$

As long as we know the basis we're in, any state can be specified by only those two numbers a and b . So let's use just them and write the state as a *column vector*,

$$|\psi\rangle \rightarrow \begin{pmatrix} a \\ b \end{pmatrix}. \quad (2.12)$$

I'm using an arrow (\rightarrow) rather than an equal sign since we're mixing notations here; the ket $|\psi\rangle$ is written in Dirac notation, and the column vector is what we'll call *matrix notation*. We could also write the column vector as

$$|\psi\rangle \rightarrow \begin{pmatrix} \langle +|\psi\rangle \\ \langle -|\psi\rangle \end{pmatrix}, \quad (2.13)$$

which mixes the two notations even further but makes it clear what basis the state is written in. It also makes it clear that the basis states themselves are just unit column vectors:

$$|+\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (2.14)$$

But what about the bra – how do we represent that? With a bit of thought, you might agree that they should be *row vectors*, so that the general state is written as

$$\langle \psi| \rightarrow (a^* \quad b^*) \quad (2.15)$$

or

$$\langle\psi| \rightarrow (\langle\psi|+ \quad \langle\psi|-).$$
 (2.16)

We're really leveraging all this notation – the row vector elements are the complex conjugate of the numbers a and b , so in equation (2.16) I've swapped the order of the two states in the inner product.

Example 2.3 – Inner products, again. Let's go back to the previous example and recompute the inner product $\langle\psi|\phi\rangle$ but using matrix notation. Each state can now be written as

$$|\psi\rangle = \begin{pmatrix} 1/\sqrt{5} \\ 2i/\sqrt{5} \end{pmatrix} \quad \text{and} \quad |\phi\rangle \rightarrow \begin{pmatrix} 3/5 \\ -4/5 \end{pmatrix}.$$

Remember the bra is the row vector (with complex conjugate elements) and the ket the column, so the inner product works out perfectly:

$$\langle\psi|\phi\rangle \rightarrow \begin{pmatrix} 1/\sqrt{5} & -2i/\sqrt{5} \end{pmatrix} \begin{pmatrix} 1/\sqrt{5} \\ 2i/\sqrt{5} \end{pmatrix} = \frac{3}{5\sqrt{5}} + \frac{8i}{5\sqrt{5}}.$$

This is of course the same result we got last time, but if you're like me you find it a little easier to multiply matrices than foil out in Dirac notation.

Problems

Problem 2.1 – Spin-1/2 States. Consider these different spin-1/2 states, given in Dirac notation by

$$\begin{aligned} |\psi_1\rangle &= 3|+\rangle + 4|-\rangle \\ |\psi_2\rangle &= |+\rangle + 2i|-\rangle \\ |\psi_3\rangle &= 3|+\rangle - e^{i\pi/3}|-\rangle \\ |\psi_4\rangle &= 3|+\rangle - 5i|-\rangle. \end{aligned}$$

- Normalize each state.
- Write each state in matrix notation.
- Write the bra of each ket; write the bras in matrix notation, too.
- Find a (normalized) ket that is orthogonal to each state.

- (e) Compute the following inner products, using either Dirac notation or matrix notation: $\langle\psi_1|\psi_2\rangle$, $\langle\psi_3|\psi_4\rangle$, $\langle\psi_4|\psi_1\rangle$, and $\langle\psi_3|\psi_2\rangle$.

Problem 2.2 – A Three-State System. So far we’ve only looked at the fairly simple two-state spin-1/2 system. For this problem, consider a system which has *three* orthonormal basis states, given by

$$|a_1\rangle, |a_2\rangle, \text{ and } |a_3\rangle.$$

- (a) What would these kets look like in matrix notation?
 (b) Normalize the state

$$|\psi_1\rangle = |a_1\rangle - 2|a_2\rangle + 5|a_3\rangle.$$

- (c) Take the inner product of $|\psi_1\rangle$ with the state

$$|\psi_2\rangle = i|a_1\rangle + 3|a_2\rangle - 2|a_3\rangle.$$

(you’ll have to normalize that state first, of course).

Chapter 3

Amplitude and Probability

3.1 The S_x and S_y Spin States

In the previous chapter we talked about the two basis states – for what we’re calling the S_z basis – and wrote them in Dirac and matrix notation as

$$|+\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (3.1)$$

But since these are basis states, *any* other state can be written in terms of them, including the states corresponding to measuring $S_x = +\hbar/2$ and $S_x = -\hbar/2$ that we discussed back in Experiment 2 in Section 1.3.2. I’ll show you how to figure this out later, and for now I’ll just tell you the states:

$$|+\rangle_x = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle \rightarrow \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \quad (3.2)$$

and

$$|-\rangle_x = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}|-\rangle \rightarrow \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}. \quad (3.3)$$

Of course we can also rotate the Stern-Gerlach device so that we measure the spin along the y -direction, in which case we’d have the associated states $|+\rangle_y$ and $|-\rangle_y$. In the S_z basis, they can be written as

$$|+\rangle_y = \frac{1}{\sqrt{2}}|+\rangle + \frac{i}{\sqrt{2}}|-\rangle \rightarrow \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} \quad (3.4)$$

and

$$|-\rangle_y = \frac{1}{\sqrt{2}}|+\rangle - \frac{i}{\sqrt{2}}|-\rangle \rightarrow \begin{pmatrix} 1/\sqrt{2} \\ -i/\sqrt{2} \end{pmatrix}. \quad (3.5)$$

Now that we know how to write these states down, we can talk more about the inner product and its role in quantum mechanics.

3.2 Calculating Probability

Suppose you have a particle in the state $|\psi\rangle$, and you want to measure some quantity associated with the particle – maybe its spin, but it could be anything, so I’ll call it A for now. In quantum mechanics we call this quantity an *observable*. Further suppose that there a number of different possibilities that you might measure: a_1, a_2, a_3 , and so on. Then the probability of measuring the particular value a_n is

$$\mathcal{P}_{a_n} = |\langle a_n | \psi \rangle|^2. \quad (3.6)$$

The bra in that equation corresponds to the state associated with measuring the value a_n ; the ket would be $|a_n\rangle$.

This is the one of the most important ideas in quantum mechanics, and is central to what’s called the Born rule or the generalized statistical interpretation. The underlying idea – which we’ll come back to at the end of this chapter – is that the theory of quantum mechanics can’t predict exactly what value an experiment will produce (it can’t tell you, when you measure A , if you will get a_1 or a_2 or something else) but only the probability of measuring each (so maybe 50% of the time you’ll measure a_1 , 25% of the time a_2 , and so on).

Let’s try applying this to our measurements of spin. If we want to measure the value of S_z , for example, the probability that we would get the value $S_z = +\hbar/2$ could be calculated by

$$\mathcal{P}_+ = |\langle + | \psi \rangle|^2,$$

and the probability of measuring $S_z = -\hbar/2$ is

$$\mathcal{P}_- = |\langle - | \psi \rangle|^2,$$

Of course, with only two possibilities, we’d have to have

$$\mathcal{P}_+ + \mathcal{P}_- = 1$$

so that we have 100% chance of measuring something.

One last thing: notice the role of the inner product, which in this context is called the *amplitude*, and complex squaring the amplitude gives us the probability. Remember that the complex conjugate of an inner product flips the order, so the full complex square can be written

$$\langle a_n | \psi \rangle^2 = (\langle a_n | \psi \rangle)^* \langle a_n | \psi \rangle = \langle \psi | a_n \rangle \langle a_n | \psi \rangle. \quad (3.7)$$

Example 3.1 – Calculating probability. Suppose our particle is in the state $|+\rangle$. In this state, of course, there's a 100% chance of measuring $S_z = +\hbar/2$, as we can see with the calculation

$$\mathcal{P}_+ = |\langle + | + \rangle|^2 = 1.$$

But what's the probability of measuring $S_x = +\hbar/2$? This is easier to calculate using matrix notation:

$$\mathcal{P}_{+x} = |{}_x\langle + | + \rangle|^2 \rightarrow \left| \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right|^2 = \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2}.$$

So there's a 50% chance of measuring spin up along the x -direction.

We went over this already back in the Stern-Gerlach Experiment 1 (Section 1.3.1) and Experiment 2 (Section 1.3.2) – this is the theory that explains the results we went over then. So we might as well go over Experiment 3, too (Section 1.3.3), in which we had a beam of particles in the state $|+\rangle_x$ entering a Stern-Gerlach device aligned to measure S_z . Question: how many particles will we measure to have $S_z = +\hbar/2$? Well, the probability of measuring spin up along z is

$$\mathcal{P}_+ = |\langle + | + \rangle_x|^2 \rightarrow \left| \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \right|^2 = \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2}.$$

So 50% of the particles should have $S_z = +\hbar/2$ (and presumably the other 50% are spin down).

3.3 Indeterminant States

Let's return to an issue that I've been trying to avoid. As usual, pretend we have a particle in some general state $|\psi\rangle$, and suppose we want to measure the observable S_z . We know from our Stern-Gerlach discussions that the state *changes* once a measurement is made – we say the state *collapses* to the state that corresponds to the measurement we made. For example, if a particle is in state $|\psi\rangle$ and we measure $S_z = +\hbar/2$, the state has collapsed to the new state $|+\rangle$. This, though, is not the issue I've been dancing around.

Instead, consider this question: what is the value of the S_z *just before* we make the measurement? I know what it is after measurement – it's $+\hbar/2$ – and I can check by measuring S_z again (and I'll get the same value

as long as the state hasn't been disturbed in some way). But what's S_z – the component of spin angular momentum along the z -direction – *before* that first measurement?

This is a more difficult question to answer than you might think since our theory doesn't quite provide an answer for us – the fact that the state collapses upon measurement means that we don't really know the value of S_z before the collapse. There are three possibilities we must consider:¹

1. The obvious possibility is that the spin was $S_z = +\hbar/2$ just before measurement, too – that's what we measure it to be, after all. This is called the *realist* position. There's just one problem, though – if the particle has $S_z = +\hbar/2$ all along, why couldn't quantum mechanics tell us that? This suggests that it's an *incomplete theory* – we're missing something that would allow us to calculate directly the answer to this question.
2. Another option is a little more drastic – maybe the particle did not have a value for S_z . Not that it's zero or we don't know the value – but that it does not have a definite value for its spin angular momentum. This is called *indeterminacy* – the state is indeterminant with respect to its value of S_z – and this interpretation of quantum mechanics is called the *Copenhagen interpretation*.
3. I guess we could also just refuse to answer – the theory doesn't allow us to answer, so maybe it's not a good question to ask. This is called the *agnostic* position.

In 1964 John Bell showed that it actually makes an observable difference whether a particle has a value of an observable (even if it's unknown) or if it's indeterminant. Although I won't get into the details of Bell's work here,² the conclusion is pretty remarkable: it's the Copenhagen interpretation that is the correct one. Actually, I should be a little more careful, since there are extensions of quantum mechanics (called nonlocal hidden variable theories) that can maintain the realist position, as well as interpretations (like the popular many-worlds interpretation) that fall outside of the simple picture I've gone over here. But those are also outside the scope of this book, so going forward we'll adopt the Copenhagen interpretation in which observables might not have precise values before measurement.

¹From Griffiths' *Introduction to Quantum Mechanics*, section 1.2

²See Griffiths *Introduction to Quantum Mechanics* section 12.2.

Problems

Problem 3.1 – Orthogonality. Show that the states $|+\rangle_x$ and $|-\rangle_x$ are orthogonal. Do the same for the states $|+\rangle_y$ and $|-\rangle_y$.

Problem 3.2 – S_z and S_x Measurements. Consider the two normalized states

$$|\psi_1\rangle = \frac{2}{\sqrt{13}}|+\rangle + \frac{3i}{\sqrt{13}}|-\rangle \quad \text{and} \quad |\psi_2\rangle = \frac{2}{\sqrt{13}}|+\rangle_x + \frac{3i}{\sqrt{13}}|-\rangle_x.$$

- If you measure the observable S_z on each state, what are the possible results you would measure, and with what probability would you measure each?
- If you measure the observable S_x on each state, what are the possible results you would measure, and with what probability would you measure each?

Problem 3.3 – Measurements. Using a Stern-Gerlach device rotated at some angle, you're able to prepare a beam of particles all in the state (we'll see later on how you can do this)

$$|\psi\rangle = 3|+\rangle + 5i|-\rangle.$$

- What is the normalized state?
- If you were to measure S_z , what are the possible results and their probabilities?
- Suppose you measured S_z on the beam of particles, and some of them were found to be $-\hbar/2$. If you then made a measurement of S_y on just those particles, what are the possible results and their probabilities?

Problem 3.4 – An Overall Phase.

- First, consider this normalized state:

$$|\psi_1\rangle = \frac{4}{5}|+\rangle + \frac{3i}{5}|-\rangle.$$

What is the probability of measuring $S_y = +\hbar/2$ for a particle in this state?

- (b) Next, we can change the state by introducing an *overall phase factor*,

$$|\psi_2\rangle = -(\frac{4}{5}|+\rangle + \frac{3i}{5}|-\rangle) = -\frac{4}{5}|+\rangle - \frac{3i}{5}|-\rangle.$$

What is the probability of measuring $S_y = +\hbar/2$ for a particle in this state? What affect does the overall phase factor have on the measurement?

- (c) We can also change the state by introducing a *relative phase factor*,

$$|\psi_3\rangle = \frac{4}{5}|+\rangle - \frac{3i}{5}|-\rangle.$$

What is the probability of measuring $S_y = +\hbar/2$ for a particle in this state? What affect does the relative phase factor have on the measurement?

Problem 3.5 – An Overall Phase Part 2.

- (a) Show that you can write the overall phase from Problem 3.4 (b) as

$$|\psi_2\rangle = e^{i\delta}(\frac{4}{5}|+\rangle + \frac{3i}{5}|-\rangle).$$

What is the value of δ ?

- (b) Show that an overall phase for *any* measurement on a general state $|\psi\rangle$ has no affect on the probability. This is a fact we'll exploit every so often – that an overall phase has no affect on a physical measurement.

Problem 3.6 – A Three-State System. Remember our three-state system from Problem 2.2? We had three orthonormal basis states, given by

$$|a_1\rangle, |a_2\rangle, \text{ and } |a_3\rangle.$$

Here, each state corresponds to a measurement of an observable A .

- (a) Suppose the system is prepared in the state

$$|\psi\rangle = |a_1\rangle - 2|a_2\rangle + 5|a_3\rangle.$$

You then measure the observable A on this state; what are the possible results and probabilities of each?

Chapter 4

Observables and Operators

4.1 Operators and Measurement

We’ve already seen lots of examples of *observables* – the spin components S_x , S_y , and S_z are all examples of things that we can observe, as are things like position and momentum. In the language of quantum mechanics:

A physical observable A is represented by an operator \hat{A} .

Wait, what exactly is an operator? At the risk of being too simplistic, it’s something that *operates* on a quantum state, producing a new state. Mathematically we can write this operation like

$$\hat{A}|\psi\rangle = |\phi\rangle.^1 \quad (4.1)$$

Actually, although in general the operator \hat{A} produces a new state, sometimes the state it operates on is special and *doesn’t* change:

$$\hat{A}|\psi\rangle = a|\psi\rangle. \quad (4.2)$$

Instead of making a new state, it gives back the same state, but multiplied by a number a . If you’re familiar with linear algebra, you might recognize equation (4.2) as an *eigenvalue equation*, with a playing the role of the eigenvalue and the ket $|\psi\rangle$ being the eigenvector. The eigenvalue is very important:

The only possible result of a measurement of an observable A is one of the eigenvalues a_n of the corresponding operator \hat{A} .

¹Although the hat on the operator is standard, many textbooks drop it to reduce clutter in notation. I think it’s important to be able to easily distinguish an observable and an operator at a glance, especially for newcomers.

4.1.1 The Operator \hat{S}_z

That's a lot to take in on first reading, so let's do a full example. We'll return to the observable S_z , which must have a corresponding operator \hat{S}_z . We'll figure out how we can write this in a moment, but you might have realized we already know the eigenvalues of this operator: they must be $\hbar/2$ and $-\hbar/2$, since we know measurements of S_z always return one of those two numbers.

That means that the eigenvalue equations – two of them for two eigenvalues – could be written as

$$\hat{S}_z|+\rangle = \frac{\hbar}{2}|+\rangle \quad \text{and} \quad \hat{S}_z|-\rangle = -\frac{\hbar}{2}|-\rangle. \quad (4.3)$$

We can get a sense of what the operator \hat{S}_z is by thinking of this in matrix notation – the states $|+\rangle$ and $|-\rangle$ are column vectors, meaning \hat{S}_z must be represented as a 2×2 matrix (nothing else, when multiplied by a column vector, gives another column vector). I don't know what the elements of the matrix are, so I'll write it out for now as

$$\hat{S}_z \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

To find the unknown elements a , b , c , and d (which could be complex), we can go back to the eigenvalue equations, this time in matrix notation. For the eigenvalue $\hbar/2$, we have

$$\hat{S}_z|+\rangle = \frac{\hbar}{2}|+\rangle \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (4.4)$$

Multiplying out the left side gives

$$\begin{pmatrix} a \\ c \end{pmatrix} = \begin{pmatrix} \hbar/2 \\ 0 \end{pmatrix},$$

so we know that $a = \hbar/2$ and $c = 0$. The other eigenvalue equation, for $-\hbar/2$, similarly gives $b = 0$ and $d = -\hbar/2$. The operator \hat{S}_z , in matrix notation, is

$$\hat{S}_z \rightarrow \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.5)$$

There's a few things here we should notice – in particular that \hat{S}_z is a *diagonal* matrix, with the eigenvalues as the diagonal elements. Also note that the eigenvectors (the states $|+\rangle$ and $|-\rangle$) are unit vectors. Both of these things arise because of the basis we're using – it's the S_z basis! In other words, in its own basis – where the basis states are the eigenstates of the basis operator – an operator will be diagonal with the eigenvalues along that diagonal.

4.2 Matrix Representation

In fact, any operator can be represented as a matrix; sticking with the S_z basis, we can write a general operator \hat{A} as a 2×2 matrix

$$\hat{A} \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \quad (4.6)$$

Now for something a little new. Consider the calculation $\langle + | \hat{A} | + \rangle$. What exactly does this mean? First we apply the operator \hat{A} to the ket $|+\rangle$, getting a new state, and then apply the bra $\langle + |$ to that new state:

$$\langle + | (\hat{A} | + \rangle) \rightarrow (1 \quad 0) \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (1 \quad 0) \begin{pmatrix} a \\ b \end{pmatrix} = a.$$

So the ultimate result is just a number – a in this case. Similarly, you can show that $\langle + | \hat{A} | - \rangle = b$, and so on. That means we could be able to write our operator in matrix notation as

$$\hat{A} \rightarrow \begin{pmatrix} \langle + | \hat{A} | + \rangle & \langle + | \hat{A} | - \rangle \\ \langle - | \hat{A} | + \rangle & \langle - | \hat{A} | - \rangle \end{pmatrix}. \quad (4.7)$$

This is just notation, but useful since we can see explicitly what the basis is.

It's easy enough to generalize this to any system; the matrix representation might have a different size than 2×2 (it might even be infinite), but the idea is the same. In general we can write

$$\hat{A} \rightarrow \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (4.8)$$

where $a_{ij} = \langle i | \hat{A} | j \rangle$ and $|i\rangle$ and $|j\rangle$ are the basis states. In this context we'll often call the a_{ij} s matrix elements.

4.3 The Operators \hat{S}_x and \hat{S}_y

The matrix representation of the other two spin component operators are given by

$$\hat{S}_x \rightarrow \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (4.9)$$

and

$$\hat{S}_y \rightarrow \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (4.10)$$

These are both written in the S_z basis (notice that they're not diagonal). If you'd like to know where these came from, feel free to work through the Stern-Gerlach results in Problem XXX. What I'd rather do right now is ask the question: *if we were to measure, say, S_y on some particular state, what are the possible results we could get?* We already know the answer in this case, but a lot of quantum mechanics boils down to figuring out the answer to this question for a variety of different observables and corresponding operators, so it's worth going through the process in detail.

The answer, as mentioned above, is given by the eigenvalues of the operator. You probably already know how to find eigenvalues from your linear algebra course, but let's do it together nice and slow. First, the eigenvalue equation is

$$\hat{S}_y |\lambda\rangle = \lambda |\lambda\rangle, \quad (4.11)$$

where λ does double duty here, standing for the unknown eigenvalue as well as the corresponding eigenstate. This might seem confusing at first, but we'll get used to it.

We find the eigenvalues by solving the characteristic (or secular) equation, which looks like

$$\det[\mathbf{S}_y - \lambda \mathbf{I}] = 0. \quad (4.12)$$

The bolded letter \mathbf{S}_y denote the matrix representation of the operator, and \mathbf{I} is the identity matrix. Filling in the matrices gives

$$\left| \begin{pmatrix} 0 & -i\hbar/2 \\ i\hbar/2 & 0 \end{pmatrix} - \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \right| = 0,$$

or, after simplifying,

$$\left| \begin{pmatrix} -\lambda & -i\hbar/2 \\ i\hbar/2 & -\lambda \end{pmatrix} \right| = 0.$$

Work out the determinant to get

$$\lambda^2 - \left(\frac{\hbar}{2}\right)^2 = 0$$

so that, finally, we can see that the two eigenvalues – as expected! – are $\lambda_1 = \hbar/2$ and $\lambda_2 = -\hbar/2$. These two values are the only possible results we would get if we measured S_y on any spin state.

What about the eigenstates? To find these, we go back to the original eigenvalue equation (4.11) and plug in each eigenvalue in turn. For $\lambda = \hbar/2$, we have

$$\hat{S}_y|\lambda\rangle = \frac{\hbar}{2}|\lambda\rangle.$$

Writing the unknown state $|\lambda\rangle$ in matrix notation,

$$|\lambda\rangle \rightarrow \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad (4.13)$$

our job is to find the value of α and β that satisfy the eigenvalue equation. Here we go:

$$\hat{S}_y|\lambda\rangle = \frac{\hbar}{2}|\lambda\rangle \rightarrow \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \alpha \\ \beta \end{pmatrix},$$

so

$$\begin{pmatrix} -i\beta \\ i\alpha \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

This is really two equations for α and β , but they're the same equation – we don't have enough information to get both values right now. But we can at least solve for β in terms of α and get

$$\beta = i\alpha,$$

making the eigenstate so far

$$|\lambda\rangle = |+\rangle_y \rightarrow \alpha \begin{pmatrix} 1 \\ i \end{pmatrix}. \quad (4.14)$$

How, then, do we get the last unknown α ? Well, every state must be normalized, so

$${}_y\langle + | + \rangle_y = 1. \quad (4.15)$$

In matrix notation, this becomes

$$|\alpha|^2 \begin{pmatrix} 1 & -i \end{pmatrix} \begin{pmatrix} 1 \\ i \end{pmatrix} = |\alpha|^2 (2) = 1,$$

so we'll take

$$\alpha = \frac{1}{\sqrt{2}}$$

and therefore

$$|+\rangle_y = \frac{1}{\sqrt{2}}|+\rangle + \frac{i}{\sqrt{2}}|-\rangle \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}. \quad (4.16)$$

Feel free to go through the same process to get the spin down eigenstate; it turns out to be

$$|-\rangle_y = \frac{1}{\sqrt{2}}|+\rangle - \frac{i}{\sqrt{2}}|-\rangle \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}. \quad (4.17)$$

Problem XXX will get you to go through the process for S_x .

4.4 Spin in a General Direction, \hat{S}_n

At this point I just want to give you some more operators and figure out their eigenvalues and eigenstates, partly so we can get the practice and partly so we can use them again later. First up, suppose we rotate our usual Stern-Gerlach device to some random orientation so that the magnetic field points in the direction of \mathbf{n} as shown in Figure XXX. The angles θ (the polar angle) and ϕ (the azimuthal angle) are the usual spherical coordinates, and we'll make \mathbf{n} a unit vector so it has a length of one. That means in terms of the Cartesian unit vectors \hat{x} , \hat{y} , and \hat{z} , we can write

$$\mathbf{n} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}. \quad (4.18)$$

Suppose we measure the spin of a particle along this direction; let's call the observable S_n , where

$$S_n = \mathbf{S} \cdot \mathbf{n} = S_x \sin \theta \cos \phi + S_y \sin \theta \sin \phi + S_z \cos \theta. \quad (4.19)$$

The operator associated with this observable is, of course, the exact same except with hats on the operators, so we have²

$$\hat{S}_n = \hat{\mathbf{S}} \cdot \mathbf{n} = \hat{S}_x \sin \theta \cos \phi + \hat{S}_y \sin \theta \sin \phi + \hat{S}_z \cos \theta. \quad (4.20)$$

To write this operator in matrix notation, we just fill in the matrices for \hat{S}_x , \hat{S}_y , and \hat{S}_z and add them together to get

$$\hat{S}_n \rightarrow \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix} \quad (4.21)$$

(see Problem XXX).

This is a new operator we've never seen before, and anytime we're faced with a new operator, we should always find its eigenvalues and eigenstates – remember, the eigenvalues of the operator answer the question of what we get when we measure the observable, so they're pretty

²Okay, we have to be a little careful now distinguishing unit vectors from operators, both of which have hats. Things should be clear from context.

important, and we'll see that the eigenstates play just as important a role. But wait – we *already* know the eigenvalues! They *have* to be $\hbar/2$ and $-\hbar/2$, just like \hat{S}_x or any other component. After all, changing the direction of the magnetic field by rotating the device is the exact same operation as changing our coordinate system, and that should affect the actual results we get.

So, fine, we know the eigenvalues (you can check that we're correct in Problem XXX); what about the eigenstates? You need more practice than I do, so try on your own (that's Problem XXX again), and I'll give you just the answers for now. The eigenstates are (with notation that should be clear by now; the ket $|+\rangle_n$ is the state that goes with $+\hbar/2$ and similarly for the eigenvalue $-\hbar/2$)

$$|+\rangle_n = \cos(\theta/2) |+\rangle + \sin(\theta/2) e^{i\phi} |-\rangle \quad (4.22)$$

and

$$|-\rangle_n = \sin(\theta/2) |+\rangle - \cos(\theta/2) e^{i\phi} |-\rangle. \quad (4.23)$$

Remember, all this is explicitly in the S_z basis.

By the way, if you were wondering how we make some “general spin state” $|\psi\rangle$ with some specific set of coefficients, this is how: orient the Stern-Gerlach device at just the correct angles θ and ϕ that give you those coefficients. Problem XXX will ask you to do this.

4.5 The \hat{S}^2 Operator

All of the spin operators we've seen so far have been *components* of the spin angular momentum *vector*. We know that we can't simultaneously know all three components, but it turns out we can measure the total magnitude of the spin; in fact, we usually work with the square,

$$S^2 = S_x^2 + S_y^2 + S_z^2. \quad (4.24)$$

At the risk of repeating things, the operator \hat{S}^2 is of course

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2, \quad (4.25)$$

and we can determine what it looks like in the S_z basis using matrix notation. Substituting from equations (4.5), (4.9), and (4.10), we see that

$$\hat{S}^2 \rightarrow \left[\frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right]^2 + \left[\frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right]^2 + \left[\frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right]^2 \quad (4.26)$$

or

$$\hat{S}^2 \rightarrow \frac{3}{4} \hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (4.27)$$

But this matrix is just the identity matrix!

Problems

Problem 4.1 – Orthogonality. Show that the states $|+\rangle_x$ and $|-\rangle_x$ are orthogonal. Do the same for the states $|+\rangle_y$ and $|-\rangle_y$.

Chapter 5

Examples of Discrete Systems

5.1 An Electron in a Magnetic Field

To come.

5.2 Neutrino Oscillations

Neutrinos – little neutral particles created in huge numbers during nuclear reactions – were long thought to be massless. But during the 1980s and 1990s the *solar neutrino problem* became undeniable: neutrino detection experiments on Earth were missing about half of the expected number of neutrinos made in the core of the sun during hydrogen burning. There were only two possibilities: either our model of the sun was way off¹ or something happened to the neutrinos on their way to us.

The correct explanation turned out to be something called *neutrino oscillations*, and the theory earned the Nobel prize. In short, *electron* neutrinos are created in the core of the sun, but on their way to Earth some of them turn into *muon* neutrinos – don’t worry too much about the names or why there’s more than one kind of neutrino; the main idea is that neutrinos can oscillate back and forth between these two different types (actually, there’s a *third* type, a tau neutrino, but we’ll ignore that for simplicity).

As a slightly simplified model for neutrino mixing, we’ll suppose the state of any neutrino – I’ll call this the “flavour state,” since particle physicists call the type of particle its flavour for some reason – can be written as

¹One of my undergraduate professors was a solar physicist, and according to him there was no way the solar models could be that wrong, so really there’s only one possible explanation – something was wrong with our understanding of neutrinos.

a superposition of an electron neutrino state and a muon neutrino state:

$$|\nu\rangle = a|e\rangle + b|\mu\rangle. \quad (5.1)$$

This is a two-state system, something we've already studied in detail, so the physics of neutrinos is pretty much the same as spin-1/2 systems or photon polarizations. To see how neutrinos oscillate, though, we'll have to calculate how this state evolves in time, meaning we'll need the Hamiltonian of the system.

The Hamiltonian, of course, is just the total energy, so we'll start with the relativistic energy of any particle (unfortunately, neutrinos are inherently relativistic objects – it's hard to slow them down),

$$E = \sqrt{p^2 c^2 + m^2 c^4}.$$

Although neutrinos were originally thought to be massless, it turns out we'll need to give them a very small mass in order for them to oscillate. That said, it will be a *very* small mass, so it's reasonable to think that their rest energy (mc^2) will be much smaller than their momentum (the pc term), in which case we can write

$$E = pc \left(1 + \frac{m^2 c^4}{p^2 c^2} \right)^{1/2} \approx pc \left(1 + \frac{m^2 c^4}{2 p^2 c^2} \right),$$

or

$$E = pc + \frac{m^2 c^3}{2p}. \quad (5.2)$$

For reasons we won't see until we solve the whole problem, I'm going to write the Hamiltonian as

$$\hat{H} \rightarrow \begin{pmatrix} pc + (m_1^2 + m_2^2)c^3/4p & (m_1^2 - m_2^2)c^3/4p \\ (m_1^2 - m_2^2)c^3/4p & pc + (m_1^2 + m_2^2)c^3/4p \end{pmatrix} \quad (5.3)$$

where m_1 and m_2 are two different masses. You might think that m_1 is the mass of the electron neutrino and m_2 is that of the muon neutrino, but that's not quite the case; hold tight and we'll see what that means.

Before we find the energy eigenvalues and eigenstates, consider for a moment what the Hamiltonian would look like if the neutrinos were in fact *massless*; then

$$\hat{H} \rightarrow \begin{pmatrix} pc & 0 \\ 0 & pc \end{pmatrix}.$$

This matrix is diagonal, so the possible energies are easy to read off: they're both the same, $E = pc$ as we'd expect for a massless relativistic particle.

The eigenstates of the matrix are just the flavour basis states, $|e\rangle$ and $|\mu\rangle$, so the implication is that both neutrinos have the same energy. More importantly, though, the flavour states – which are also the energy eigenstates – are stationary states, so neutrino oscillations simply wouldn't happen. Once an electron neutrino is created during a reaction, it will stay an electron neutrino forever. Actually, it's possible to have massive neutrinos and still have the flavour states be stationary, as long as the masses are the same. In this case the matrix remains diagonal and we reach the same conclusions; evidently it's the *different* masses of the two neutrinos that lead to oscillations.

Okay, let's find the energies of the full Hamiltonian. For ease of writing stuff out, I'm going to write the Hamiltonian as

$$\hat{H} \rightarrow \begin{pmatrix} h & g \\ g & h \end{pmatrix},$$

where $h = pc + (m_1^2 + m_2^2)c^3/4p$ and $g = (m_1^2 - m_2^2)c^3/4p$. The characteristic equation is

$$\begin{vmatrix} h - E & g \\ g & h - E \end{vmatrix} = 0,$$

which has solutions

$$E_1 = h + g = pc + (m_1^2 + m_2^2)c^3/4p + (m_1^2 - m_2^2)c^3/4p = pc + m_1^2 c^3/2p \quad (5.4)$$

and

$$E_2 = h - g = pc + (m_1^2 + m_2^2)c^3/4p - (m_1^2 - m_2^2)c^3/4p = pc + m_2^2 c^3/2p. \quad (5.5)$$

Now you can see why I chose the exact Hamiltonian I did – we get exactly the energies we expect based on equation 5.2. As long as the masses are different, these are two distinct energies.

Now that we have the energy eigenvalues, we can get the corresponding states as well. For $E = E_1 = h + g$, the eigenvalue equation is

$$\hat{H}|E_1\rangle = E_1|E_1\rangle,$$

or, in matrix notation,

$$\begin{pmatrix} h & g \\ g & h \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = (h + g) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

Solving gives $\beta = \alpha$, and after normalizing to find $\alpha = 1/\sqrt{2}$, the eigenstate is

$$|E_1\rangle = \frac{1}{\sqrt{2}}|e\rangle + \frac{1}{\sqrt{2}}|\mu\rangle. \quad (5.6)$$

Similarly, the eigenstate associated with energy $E_2 = h - g$ is

$$|E_2\rangle = \frac{1}{\sqrt{2}}|e\rangle - \frac{1}{\sqrt{2}}|\mu\rangle. \quad (5.7)$$

This is where things get interesting and a little weird. According to particle physics, a neutrino is created either as an electron neutrino (state $|e\rangle$) or as a muon neutrino (state $|\mu\rangle$). But the energy states are a superposition of these flavour states – evidently the electron neutrino, say, just doesn't *have* a definite energy. Put another way – because the energies depend on the two different masses – we can say the an electron neutrino does not have a definite mass; the m_1 isn't an m_{ν_e} . Alternatively, if we manage to measure the energy (or mass) of an electron neutrino, it's no longer an electron neutrino – its state collapses to one of the superpositions above and it doesn't have a definite flavour.

We can see how this leads to neutrino oscillations and solves the solar neutrino problem by supposing that, at the centre of the sun, an electron neutrino is created. The initial state is then

$$|\nu(0)\rangle = |e\rangle. \quad (5.8)$$

I think it's fair to call this neutrino an electron neutrino at this point.

To find the state at a later time, we need to first switch to the energy basis. For fun, I'll do that by multiplying the state by the identity operator:

$$|\nu(0)\rangle = \hat{1}|e\rangle = (|E_1\rangle\langle E_1| + |E_2\rangle\langle E_2|)|e\rangle.$$

Notice that I wrote the identity operator in the energy basis – this is the mechanism that switches basis for us. Working out the inner products gives

$$|\nu(0)\rangle = \frac{1}{\sqrt{2}}|E_1\rangle + \frac{1}{\sqrt{2}}|E_2\rangle \quad (5.9)$$

as you might expect; although it's fair to say this is an electron neutrino, we definitely can't say what the energy of the particle is – it simply doesn't have one.

Now we can tack on the exponential time factors to find the state at a later time in the usual way. We get

$$|\nu(t)\rangle = \frac{e^{-iE_1t/\hbar}}{\sqrt{2}}|E_1\rangle + \frac{e^{-iE_2t/\hbar}}{\sqrt{2}}|E_2\rangle.$$

Finally, I'll switch back to the flavour basis, although this time I'll do it using equations (5.6) and (5.7) directly rather than using the identity operator:

$$|\nu(t)\rangle = \frac{e^{-iE_1t/\hbar}}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|e\rangle + \frac{1}{\sqrt{2}}|\mu\rangle\right) + \frac{e^{-iE_2t/\hbar}}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|e\rangle - \frac{1}{\sqrt{2}}|\mu\rangle\right).$$

Using $E_1 = h + g$ and $E_2 = h - g$ and simplifying things, we get

$$|v(t)\rangle = \frac{1}{2}e^{-iht/\hbar} \left[\left(e^{-igt/\hbar} + e^{igt/\hbar} \right) |e\rangle + \left(e^{-igt/\hbar} - e^{igt/\hbar} \right) |\mu\rangle \right].$$

You might recognize cosine and sine in there, so we'll simplify further, but also note that there's an overall phase factor out in front – we'll drop that since it doesn't mean anything physically. Finally, the state at time t is

$$|v(t)\rangle = \cos(gt/\hbar)|e\rangle - i \sin(gt/\hbar)|\mu\rangle. \quad (5.10)$$

Take a look at what happens at time

$$\tau = \frac{\pi\hbar}{g} = \frac{\pi p\hbar}{4c^3} \frac{1}{m_1^2 - m_2^2},$$

at that point the cosine term goes to zero and the sine term becomes one and our state is

$$|v(\tau)\rangle = |\mu\rangle.$$

The electron neutrino has oscillated into a muon neutrino!

This is the explanation for the solar neutrino problem, although the full theory is a bit more complex since there are actually three different neutrino flavours. But the main idea is still the same – the flavour states are not the energy eigenstates, and are therefore not stationary – they instead oscillate amongst themselves.

Chapter 6

The Finite Square Well

6.1 Bound States

What happens if the walls of our “box” weren’t quite so high? Let’s find out – suppose we have a particle in a *finite* square well, defined by the potential energy

$$V(x) = \begin{cases} V_0, & x < -a \\ 0, & -a < x < a \\ V_0, & x > a, \end{cases} \quad (6.1)$$

where V_0 is a positive constant – the depth of the well as shown in Figure 6.1. Notice one other difference from the infinite version as well: the well has been centered at $x = 0$ so the width of the well is actually $2a$; we’ll see why in a little bit.

Actually, probably the biggest difference between the infinite square well and the finite well is what kind of states are allowed. Classically, for

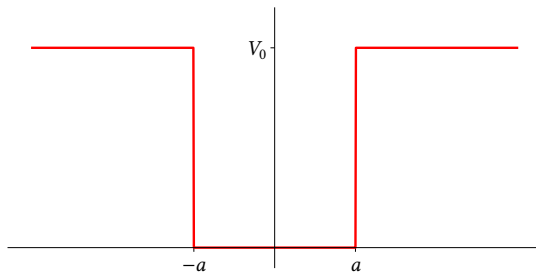


Figure 6.1: The potential energy of the finite square well.

the infinite square well, the particle in the box was always contained and could never escape, regardless of the energy of the particle. In the finite well, though, if $E > V_0$ the particle would not be trapped in the box and would instead escape to infinity. As we discussed back in Chapter 8, this case would be an *unbound state*, and unbound states have some additional complications in quantum mechanics – we’ll save those for a later chapter. In the meantime, we’ll only look for bound energy eigenstates, where

$$E < V_0 \quad (\text{bound states}),$$

but keep in mind that we’ll be missing some of the eigenstates. One consequence of this is that the energy eigenstates we find here won’t be *complete*.

Luckily, finding the bound states is pretty easy. For $x < -a$, to the left of the well, the energy eigenvalue equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\phi}{dx^2} + V_0\phi = E\phi,$$

or, cleaning it up a bit,

$$\frac{d^2\phi}{dx^2} = q^2\phi, \quad (6.2)$$

where

$$q = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \quad (6.3)$$

Notice that q is always *real* since we’re requiring that $E < V_0$. This should be a recognizable differential equation; the general solution looks like

$$\phi(x) = Ae^{qx} + Be^{-qx} \quad (x < -a). \quad (6.4)$$

Similarly, for $x > a$, the potential energy is again $V = V_0$ so our solution is the same, although we’ll have to use different constants:

$$\phi(x) = Fe^{qx} + Ge^{-qx} \quad (x > a). \quad (6.5)$$

Finally, in the well itself we have $V = 0$, so the solution is the exact same as the infinite square well. We can write the energy eigenvalue equation as

$$\frac{d^2\phi}{dx^2} = -k^2\phi, \quad (6.6)$$

where

$$k = \frac{\sqrt{2mE}}{\hbar} \quad (6.7)$$

is once again real and positive. The general solution is

$$\phi(x) = C \sin(kx) + D \cos(kx) \quad (-a < x < a). \quad (6.8)$$

At the risk of repeating myself unnecessarily, I'll write out the full solution as a piecewise function; it helps to see it all together:

$$\phi(x) = \begin{cases} Ae^{qx} + Be^{-qx}, & x < -a \\ C \sin(kx) + D \cos(kx), & -a < x < a \\ Fe^{qx} + Ge^{-qx}, & x > a. \end{cases} \quad (6.9)$$

Now all we have to do is find all six constants A , B , C , D , F , and G , plus of course our allowed energy E , which is buried inside q and k . To do that we use *boundary conditions* as usual.

6.2 Boundary Conditions