II. The Schrödinger Equation

A. The Weirdness of Quantum Mechanics

The world is a strange place, but it wasn't until 1900, when Max Planck was studying the thermal spectrum of light (black body radiation) that we began to understand just how strange it was. Although this represented the formal start of modern quantum mechanics, it is easier to start in 1877, with Hertz's discovery of the photoelectric effect, which was explained in 1905 by Einstein. This effect demonstrated, in effect, that when you shine a light source of frequency f onto a piece of metal, the light acted not as if it were made of waves, but rather as if it were composed of tiny packets of energy hf, where h was a new constant called *Planck's constant*, given by

$$h = 6.626\times10^{-34}\ \mathrm{J}\cdot\mathrm{s} = 4.136\times10^{-15}\,\mathrm{eV}\cdot\mathrm{s} \tag{2.1}$$

This is the basis of the modern photomultiplier, a device that is capable of detecting individual particles of light, also known as *photons*. We aren't really interested in the inner workings of a realistic photomultiplier, but instead will simply treat it as an idealized detector that counts photons.

Although the formula $E = hf$ was the formula originally formulated by Planck, we will find it more useful to rewrite this by writing the frequency f in terms of the angular frequency $\omega = 2\pi f$, and then exchanging Planck's constant for the so-called reduced Planck constant.

$$\hbar \equiv \frac{h}{2\pi} = 1.0546\times10^{-34}\ \mathrm{J}\cdot\mathrm{s} = 6.582\times10^{-16}\,\mathrm{eV}\cdot\mathrm{s} \tag{2.2}$$

In terms of which the relationship between energy and angular frequency is given by

$$E = \hbar\omega \tag{2.3}$$

The basic problem with this discovery is that there was already ample evidence that light was electromagnetic waves (indeed, if they aren't waves, then what frequency are we discussing?). For example, the electric field of an electromagnetic wave traveling in the $+x$ direction would take the form

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0\cos(kx-\omega t) \quad \text{or} \quad \mathbf{E}(\mathbf{r},t) = \mathbf{E}_0\sin(kx-\omega t) \tag{2.4}$$

For technical mathematical reasons, which represent a convenience when studying electricity and magnetism, but will prove crucial here, it is common to combine these two real functions by multiplying the latter by i and then adding them to get the complex field

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0\exp\left[i(kx-\omega t)\right] \tag{2.5}$$

This form of the electric field (together with a corresponding magnetic field) can be shown to satisfy Maxwell's equations provided $\omega = ck$. With a little help from relativity, another important relationship can be worked out. For particles moving at the speed of light (such as photons), the energy and momentum are related by $E = cp$, where c is the speed of light and p is the momentum. Combining these two relations with (2.3), it is a moment's work to demonstrate

$$p = \hbar k \tag{2.6}$$

Waves have properties very different from particles; for example, particles have a very definite position, whereas waves tend to be spread out, or in essence, have some uncertainty in their position. The waves given by (2.4) or (2.5) have a very definite value of the wave number k, but they are infinite in extent, so that the position x has no definite value; indeed, for (2.5) the waves are distributed uniformly throughout all of space. Without going into too much detail here, it can be shown that you can combine waves with different wave numbers k to make a wave packet that is less spread out in space, but has an uncertainty in wave number k. Indeed, it is a classical result that for any wave, the uncertainties in the position x and wave number k must satisfy the inequality

$$(\Delta x)(\Delta k) \geq \tfrac{1}{2} \tag{2.7}$$

where Δx and Δk represent the uncertainty in the position and wave number respectively. These uncertainties will be defined much more precisely later in the course. If we combine this with (2.6), we obtain a corresponding relationship between the momentum and position of a photon, namely

$$(\Delta x)(\Delta p) \geq \tfrac{1}{2}\hbar \tag{2.8}$$

In contrast, particles are normally described by giving their position and momentum, and hence it is implicitly assumed in classical mechanics that the uncertainty in each of these quantities is zero.

To help us understand some of the difficulties encountered as we move to a quantum picture of the world, a number of gedanken[1] experiments may help to clarify the situation. For example, consider a half-silvered mirror; that is, a mirror that lets some light through, but not all. Now, suppose we place a dim source in front of this half-silvered mirror, and shine a light on it, detecting the resulting waves using a pair of photomultipliers, as illustrated in Fig. 2-1. What happens in this experiment? Perhaps not surprisingly, the rate of photons appearing in each of the two detectors is exactly half the rate at which they strike the half-silvered mirror. If you inject the photons from the source very slowly, say one at a time, you find that the photons appear in either detector A or detector B – not in both, but always in one of them[2]. It is as if the half-silvered mirror sorts the photons one way or the other, even

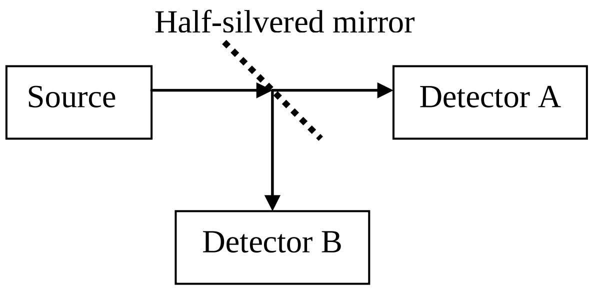

Figure 2-1. The half-silvered mirror somehow seems to selectively deflect each photon to only one of the two detectors, but the process seems to be completely random.

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[1] The German word "gedanken" means thought. A gedanken experiment is a thought experiment – one that is not necessarily going to be performed, but instead is used to illustrate a particular point.

[2] Actually, realistic detectors never have 100% efficiency, so in real experiments, some photons will *not* appear in either detector. Though this gedanken experiment cannot be perfectly performed, it is believed that nothing in principle makes such an experiment impossible.

though there is apparently no way to predict which way any single photon will go.

It is perhaps worth pointing out a couple of reasons for our confusion. If you work out the effects on the wave functions (2.4) or (2.5) of the half silvered mirror, you would find that the wave gets divided equally into two waves, one of which goes into each detector. But experimentally, each photon goes one way or the other. If you changed the half-silvered mirror for one that reflects some different fraction, you will find that the photons again each flow either one way or the other, though the probabilities will shift. Indeed, the probability of the photons going to one detector or the other is proportional to the intensity, which in the complex notation of (2.5) yields

$$P \propto \left|\mathbf{E}(\mathbf{r},t)\right|^2 = \mathbf{E}_0 \cdot \mathbf{E}_0^* \tag{2.8}$$

Indeed, since the power of a wave is proportional to this same quantity, and each of the photons has exactly the same energy (for a plane wave), this result is hardly surprising

Another experiment will clarify things even more. It is possible, with the addition of a couple of conventional mirrors and an additional half-silvered mirror, to create a configuration along the lines of Fig. 2-2. The light comes from the source, is divided in two by the half-silvered mirror. The light then continues to the two conventional mirrors, which then send it to a half-silvered mirror, which recombines the two waves. It is possible, if the distances are carefully controlled, to arrange things so that according to classical wave theory, the waves will combine perfectly at the second half-silvered mirror such that *all* of the light goes into detector A, and none of it goes into detector B. It is important to note that this happens, according to the wave theory, *only* if the light wave follows both paths; it is the interference of the two halves of the waves at the recombining half-silvered mirror that allows this effect: the two waves conspire to cancel out as they head towards detector B, and they conspire to add together (interfere constructively) as they head towards detector A.

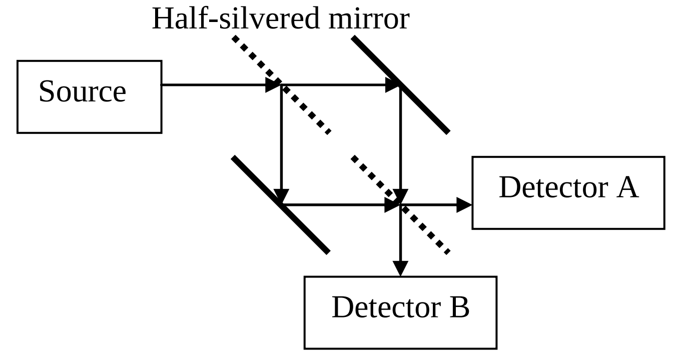

Figure 2-2. In this experiment, the light takes two paths to go from the source to the second half-silvered mirror. If the distances are set up carefully enough, all of the photons will appear in detector A, and none in detector B.

If we do this experiment with light that is low intensity, it is difficult to reconcile the wave and particle pictures. In this picture, half the photons will be deflected by the first half-silvered mirror, and half will pass through. Thus each photon will follow either the upper path or the lower path, not both, and therefore will reach the second half-silvered mirror from the upper path or the lower path, but not both. Since we already know that half-silvered mirrors reflect half the photons and pass the other half, we would expect the photons to again be divided in half, so in the end, there are four equally likely paths from the source to the detector, two of them ending up in detector A and two in detector B. But this is not what we find experimentally. We find, instead, that the photons all end up in detector A, and none of them in detector B. Recall, in the wave theory, this can only happen if the wave passes along *both* paths, but how can we explain this if we have only one particle at a time? It is as if the particle behaves like a wave between the first mirror and the second, and then behaves like a particle after passing through the second.

To clarify the situation, imagine replacing one of the two conventional mirrors in Fig. 2-2 by something that absorbs photons, say, another photomultiplier, as shown in Fig. 2-3. In this configuration, the system acts exactly as predicted if photons are particles: half of them are deflected by the first half-silvered mirror into detector C, and the other half are subdivided by the second mirror into half, so that ultimately one-fourth of them end up in detectors A and B. But when the second mirror is replaced, the photons disappear again. In this case, *adding* a path by which the particles could reach detector B causes a *decrease* in the photons arriving there.

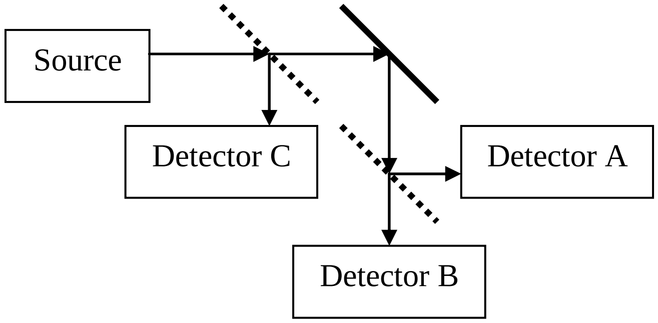

Figure 2-3: When you replace one of the two mirrors with a detector, the system behaves as one would expect for particles, with half the particles going into detector C, and one-fourth each into A and B.

It is important to remember that the interference described in Fig. 2-2 can only occur if the two path lengths are carefully controlled. In particular, if one of the mirrors is repositioned by, say, a modest fraction of a wavelength of light, the interference will be imperfect or even completely destroyed, and many photons will make it into detector B. Fortunately, modern optical equipment can easily be adjusted much more accurately than a fraction of a wavelength, so this experiment (or comparable equivalent experiments) can easily be performed.

What we would like to do is find an experiment where we can actually catch quantum mechanics in the act, so to speak, where we can *both* measure the path that the light took (upper or lower?) and also we can create interference effects, such as are shown in Fig. 2-2. This proves to be surprisingly difficult. For example, consider the following minor modification of Fig. 2-2: replace one (or both) of the conventional mirrors with a very lightweight mirror; indeed, let's make it so light that when a single photon bounces off of it, it will cause the mirror to recoil with some measurable velocity.[3] Now, we inject a single photon into the apparatus, let it pass through and check whether it registered in detector A or B. We also carefully measure the momentum of one of the mirrors after the experiment is done, to see whether the photon rebounded from it, transferring momentum to it. If we set up the distances accurately, then the photon should always appear in detector A, never in B, and if necessary, we can repeat the experiment several times to check that it actually never *does* appear in B. In the mean

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[3] Not surprisingly, this experiment is *only* a gedanken experiment; such a small recoil from a macroscopic mirror cannot actually be measured. What *is* surprising is that this experiment will prove to be *theoretically* impossible as well. Fundamentally, any such experiment is doomed to failure.

time, for each repetition of the experiment, we can check which path the photon took. Since the interference *requires* that the photon take both paths, and measuring the recoil of the mirror *requires* that the photon take one path or the other, it seems we should be able to catch nature in a bind. What will happen?

The answer turns out to be surprisingly subtle. Recall, as I have said before, that the mirror must be placed very carefully to make sure the interference works; indeed, it must be positioned much better than a wavelength. In other words, if there is some uncertainty in the mirror's position, because we were sloppy in setting up the experiment, we had be very careful that this uncertainty satisfies $(\Delta x)_m \ll \lambda$, or using the relationship $k\lambda = 2\pi$, we must have

$$k(\Delta x)_m \ll 2\pi \tag{2.9}$$

where k is the wave number of the light, and Δx is the uncertainty in the position of the mirror.

Of course, we are also trying to measure an incredibly tiny momentum change in the mirror. When it reflects a single photon, the photon transfers a momentum of order $\hbar k$ to the mirror. We must be certain there are no other forces on the mirror that are larger, for example, errant breezes. This can generally be controlled by placing the experiment in vacuum, etc., but we must *in addition* be very careful that the tiny mirror is not moving with any significant momentum initially, otherwise we might mistake this initial motion for the effects of the recoil of the photon. In particular, we had better make sure that the momentum is known with an accuracy smaller than the momentum of the photon, so we need

$$(\Delta p)_m < \hbar k \tag{2.10}$$

We see, therefore, that the initial momentum and position of the mirror must *both* be known to high accuracy, or the experiment is doomed to failure. Now, if we combine equations (2.9) and (2.10) by multiplying them, we find that the experiment's success will require

$$(\Delta x)_m (\Delta p)_m \ll 2\pi \tag{2.11}$$

The exact meaning of the "much less than"symbol in (2.11) is ambiguous. Roughly it came about because we insisted that we not have any photons passing into detector B. If, for example, we let the combination $k(\Delta x)_m$ in equation (2.9) be equal to $\frac{\sqrt{2}}{4}\pi = 1.1$, we can show that the interference effects are completely destroyed, and half the photons will go into each detector, rather than all into A. So we want inequality (2.9) to be quite a bit smaller, perhaps as small as 0.5 or even less.

Now, if we *could* do the experiment described, we really *would* be able to detect which way the photon went *and* prove that it went both ways. Perhaps not surprisingly, the experiment fails, and the reason is that Eq. (2.11) simply cannot be satisfied. It is *impossible* to specify the position and momentum of a mirror, even theoretically, with arbitrary precision. The reason is that quantum mechanics applies not only to light, but also to mirrors as well. Mirrors must satisfy the uncertainty relationship (2.8), as well as photons. Indeed, as far as we know, (2.8) applies to electrons, protons, neutrons, atoms, molecules, mirrors, and even planets. Quantum mechanics is *universal*. All of physics must be rewritten to incorporate quantum mechanics. Everything, and not just photons, acts like waves (at least sometimes), and our goal will be to come up with a wave theory that applies not just to light, but to everything.

Although it is possible (at least in principle) to satisfy one of the two relationships (2.9) or (2.10). it is impossible to satisfy both. If we satisfy (2.9), then interference phenomena will occur, and all (or the vast majority) of the photons will fall into detector A, but we will be incapable of measuring which of the two paths the photon took. If we satisfy (2.10), then we will successfully measure which way the photon went, but the uncertainty in the position of the mirror will destroy the interference. In essence, the process of measuring where the photon went affects the photon. Sometimes it is stated that quantum mechanics simply states that measuring systems disturbs them, changes them, but quantum mechanics is far more profound than this simple statement.

That other particles besides light have wave-like properties was first proposed by deBroglie in 1924, and confirmed in the case of electrons by Davisson and Germer in 1928. In 1930, it was demonstrated for atoms and molecules, and since then for protons and neutrons. It is now believed that everything has both particle and wave properties, though in some cases (gravity, for example), this has not been experimentally demonstrated.

The deBroglie hypothesis was that Eq. (2.8) applies to electrons, and shortly thereafter it was similarly speculated that Eq. (2.3) applies as well. We will simply assume that these two relations apply to *all* particles.

B. The Schrödinger Equation

In late 1925, Erwin Schrödinger was giving a talk about the deBroglie hypothesis to a group of colleagues, when Debye suggested that if you are going to use wave relations to describe electrons, you probably should develop a wave equation, something akin to Maxwell's equations, to describe that electron. This goal was achieved by Schrödinger, and we attempt here to 'derive' Schrödinger's equation. To obtain this equation, we will have to make a number of assumptions and guesses. In the end, what assumptions we make are not really important, what is important is the result, and we can only ask ourselves whether the result is consistent with what is observed in the world around us, or if it is contradicted by it. Hence we won't worry too much about the fine mathematical points of our derivation.

We start by assuming that an electron (even a single electron) in one-dimension is described by a wave function $\Psi(x,t)$. Furthermore, we will assume, as Schrödinger did, that it is a *complex* wave function. In electricity and magnetism, the introduction of complex electric and magnetic fields is a mathematical convenience, but in quantum mechanics, it will turn out to be a necessity. We will assume that $\Psi(x,t)$ has a single component, unlike the electric or magnetic field, which as vector fields have three components, and also that in free space (no forces or interactions) waves similar to (2.5) will be solutions of our equations. In other words, we are looking for equations which are satisfied by waves of the form

$$\Psi(x,t) = N\exp\left[i(kx-\omega t)\right] \tag{2.12}$$

There is no particular reason to think this will work for arbitrary k or ω. In fact, we know that for non-relativistic particles of mass m, we expect there to be a relationship between the momentum p and the energy E given by

$$E = \frac{p^2}{2m} \tag{2.13}$$

Now, we would like to somehow relate equations (2.13) and (2.12) with the quantum mechanical relations (2.3) and (2.6). We want these in the form of a wave relationship; that is, we want expressions involving things like derivatives of the wave (2.12). Noting that when you take the derivative of (2.12) with respect to x, you get a factor of ik, it is easy to see that

$$p\Psi(x,t) = \hbar k\Psi(x,t) = \frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t) \tag{2.14}$$

It is tempting to naively “cancel” the wave function from both sides of this equation, and write something like

$$p \to \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{2.15}$$

I have written this with an arrow, rather than an equals sign, because I want to make clear that this should not be viewed as an equality, but rather as a transformation. When we move from the classical to the quantum mechanical, we replace the classical momentum with the momentum operator, the expression on the right. If we perform this replacement twice, it is easy to see that

$$p^2\Psi(x,t) = (\hbar k)^2\Psi(x,t) = \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2\Psi(x,t) = -\hbar^2\frac{\partial^2}{\partial x^2}\Psi(x,t) \tag{2.16}$$

In a similar manner, we can convert energy into a time derivative by using (2.3). We find

$$E\Psi(x,t) = \hbar\omega\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{2.17}$$

which suggests that when we “quantize” a theory, we make the similar substitution

$$E \to i\hbar\frac{\partial}{\partial t} \tag{2.18}$$

We now use (2.13), a classical equation, to relate (2.16) and (2.17) and produce a full wave equation.

$$E\Psi(x,t) = \frac{p^2}{2m}\Psi(x,t),$$

$$i\hbar\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t), \tag{2.19}$$

This, then, is Schrödinger's one-dimensional equation for a free non-relativistic particle. To clarify the steps we went through in deriving it, it is helpful to put them in the proper order, rather than the hodgepodge derivation we just completed. These steps are

(1) Start with an equation for the energy in terms of the momentum and position[4]
(2) Multiply it on the right side by the wave function ψ
(3) Replace the momentum by the differential operator (2.15)
(4) Replace the energy by the differential operator (2.18)

For example, let us apply these steps for a non-free particle, one that is acted on by a force. We need to start with an expression for the energy. Most forces can be written as the derivative of some potential function; that is, in one dimension,

$$F(x,t) = -\frac{\partial}{\partial x} V(x,t) \tag{2.20}$$

Then the potential just contributes to the energy, and the total energy is

$$E = \frac{p^2}{2m} + V(x,t) \tag{2.21}$$

Following our prescription, we multiply this on the right by the wave function

$$E\Psi(x,t) = \frac{p^2}{2m}\Psi(x,t) + V(x,t)\Psi(x,t) \tag{2.22}$$

We then replace E and p by differential operators (2.15) and (2.18) to give us

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x,t)\Psi(x,t) \tag{2.23}$$

and we have Schrödinger's equation, now with a potential.

What do we do if we are in more than one dimension? Well, we simply start with the three-dimensional formula for energy

$$E = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r},t) = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(\mathbf{r},t) \tag{2.24}$$

We now multiply by the wave function on the right, which, not surprisingly, now will be a function of all three space variables. What we do with the three momentum expressions is not specified by (2.15), but it isn't hard to guess that the correct procedure is to replace

$$p_x \to \frac{\hbar}{i}\frac{\partial}{\partial x}, \qquad p_y \to \frac{\hbar}{i}\frac{\partial}{\partial y}, \qquad p_z \to \frac{\hbar}{i}\frac{\partial}{\partial z}. \tag{2.25}$$

or, more succinctly,

$$\mathbf{p} \to \frac{\hbar}{i}\nabla \tag{2.26}$$

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[4] In the example done already, only the momentum appeared, but in more general cases the position will also appear. The important thing to note is that time derivatives do *not* appear; the velocity must be first rewritten in terms of the momentum. As we will see later, time may also occasionally appear.

It is then only a minute's work to find that Schrödinger's equation for a particle in 3D takes the form

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r},t)\Psi(\mathbf{r},t). \tag{2.27}$$

Other possibilities come to mind; for example, what if we have more than one particle? Can we deal with the possibility of having an unknown number of particles? What if the particles are relativistic? What if there are non-conservative forces, like magnetism? Is it possible that the wave function has multiple components, much as the electric and magnetic fields do? All of these are issues that we will deal with in time, but for now we will treat (2.23) and (2.27) as Schrödinger's equation in 1D and 3D. They will provide ample examples of interesting and sometimes difficult problems to solve, but for now, let us set these aside and ask a bit about the interpretation of the wave function Ψ.

Before we move on, one minor comment is in order. Equations (2.23) and (2.27) are *complex* equations, because they explicitly contain the imaginary number *i*. Even if we made the wave function Ψ real at the initial time $t = 0$, it is easy to show that Schrödinger's equation demands that it become complex (not real) at other times. Hence complex numbers are a necessity, not merely a convenience.

C. The Meaning of the Wave Function

We have derived a wave equation (actually, at least two different ones) for the wave function ψ, but we never said what ψ is. In contrast, for example, in electromagnetism, we can define the electric field $\mathbf{E}(\mathbf{r},t)$ as the force on a small test charge divided by that charge. Is there a similar interpretation of Ψ?

The answer is no. There is no known method to actually measure the wave function. Or, at least, there is no known way to measure the wave function without changing it in the very act of measuring it. It can be shown that if we could somehow actually measure the wave function *directly*, we would be able to produce all kinds of miracles, such as communicating faster than light. But as far as we can tell, quantum mechanics does not allow one to measure the wave function itself.

What you can measure is the location of a particle. However, as I attempted to illustrate with all my gedanken experiments in section A, the wave function must often be more than one place at a time, even though the position of the particle must only be one place. This leads to confusion about what the wave function represents. If you look at equation (2.8), it seems reasonable to interpret the square of the amplitude of the wave function with the probability of finding the particle there. For example, in one dimension, we assume the probability density to take the form

$$\rho(x,t)=\left|\Psi(x,t)\right|^2=\Psi^*(x,t)\Psi(x,t) \tag{2.28}$$

This has units of inverse length, since probability is dimensionless and we are in one dimension. In particular, if we have a region $[a,b]$ in which we are going to look for the particle, the probability of finding the particle's position *x* in this region will be given by

$$P\left(a < x < b\right) = \int_a^b \left|\Psi\left(x,t\right)\right|^2 dx = \int_a^b \Psi^*\left(x,t\right)\Psi\left(x,t\right)dx \tag{2.29}$$

In particular, if we have one particle, and we look everywhere for it, the particle must be somewhere, so the probability of finding it somewhere must be 1, so we have

$$1 = \int_{-\infty}^{\infty} \left|\Psi\left(x,t\right)\right|^2 dx = \int_{-\infty}^{\infty} \Psi^*\left(x,t\right)\Psi\left(x,t\right)dx \tag{2.30}$$

Because the probability density is found by squaring the amplitude of the wave function, the wave function is sometimes called the *probability amplitude*.

In three dimensions, similar statements apply. The probability density (now with units of inverse length cubed) is found by squaring the amplitude.

$$\rho\left(\mathbf{r},t\right) = \left|\Psi\left(\mathbf{r},t\right)\right|^2 = \Psi^*\left(\mathbf{r},t\right)\Psi\left(\mathbf{r},t\right) \tag{2.31}$$

The probability of finding a particle in a region V of space is given by

$$P\left(\mathbf{r} \in V\right) = \iiint\limits_V \left|\Psi\left(\mathbf{r},t\right)\right|^2 d^3\mathbf{r} = \iiint\limits_V \Psi^*\left(\mathbf{r},t\right)\Psi\left(\mathbf{r},t\right)d^3\mathbf{r} \tag{2.32}$$

If we integrate over all of space, the probability is one

$$1 = \iiint \left|\Psi\left(\mathbf{r},t\right)\right|^2 d^3\mathbf{r} = \iiint \Psi^*\left(\mathbf{r},t\right)\Psi\left(\mathbf{r},t\right)d^3\mathbf{r} \tag{2.33}$$

The interpretation of the wave function as a probability density is so distasteful to many physicists that many eschew this formulation of quantum mechanics entirely. For example, in Bohmian quantum mechanics, the wave function is called a pilot wave, a non-detectable function which nonetheless guides the motions of actual particles. In the many worlds interpretation, no interpretation at all is given to the wave function (it is what it is), and probabilities do not appear in the theory at all, or at best are derived as a limiting case. And according to Ballentine, our textbook for this course, quantum mechanics should not be written in terms of the wave function itself, but rather in terms of the density matrix. However, throughout most of these notes I will treat the wave function as if it is real and use the traditional Copenhagen interpretation of quantum mechanics.

A few comments are in order. In classical mechanics, a particle is described at any time completely by giving its position x and its velocity v, the time derivative of the position. It is not sufficient to give only the position, since its subsequent motion will depend on the initial velocity. In quantum mechanics, the particle is completely described ONLY by the initial wave function $\Psi\left(x,t=0\right)$. This is because Schrödinger's equation, (2.23) or (2.27), are first order in time. Given the wave function at $t = 0$, we can determine from these equations the first time derivative of the wave function, and therefore can determine the wave function a moment later. Repeating the process, we could actually numerically integrate Schrödinger's equation and determine the wave function at arbitrary time (in some cases, this can actually be practical). Hence the wave function of the particle is completely described at any time by the wave function alone; we don't need its time derivative.

Another minor concern has to do with the normalization condition (2.30) or (2.33). If we start with an arbitrary wave function at $t = 0$, and let it evolve using

Schrödinger's equation, how do we make sure that these equations are satisfied at subsequent times? The answer is that both versions of Schrödinger's equation automatically assure "conservation of probability", so to speak, and therefore no additional work is required to maintain the normalization conditions.

A more difficult problem, and one we will not entirely resolve, has to do with measurement. If a particle is described by a spread-out wave function, and we measure its position, what happens? If we measure the same particle repeatedly, will the particle jump from place to place erratically between measurements? The answer to the latter turns out to be no. If you measure a particle, no matter how spread out, and discover that it is at a point x, and then immediately measure the position again, it will still be at x. Of course, the particle may move *between* measurements, given enough time, so you may have to repeat the experiment pretty quickly (photons, for example, move at the speed of light). This implies that the process of *measuring* the wave function results in a *change* of the wave function. This process is described in chapter 3 of these notes, assuming I get that far in typing them up.

One last comment has to do with the phase of the wave function. Suppose we take an arbitrary complex wave function ψ and multiply it, for example, by a factor of two. The wave function will still satisfy Schrödinger's equation, but will no longer satisfy the normalization conditions, so it cannot describe anything realistic. In contrast, suppose instead that we multiply the wave function by an arbitrary phase; that is, by a complex number of magnitude one, so we have

$$\Psi(\mathbf{r},t) \to \Psi'(\mathbf{r},t) = e^{i\theta}\Psi(\mathbf{r},t) \tag{2.34}$$

where θ is an arbitrary real number. Then the probability density will remain unchanged

$$\begin{aligned}\rho'(\mathbf{r},t) &= \left|\Psi'(\mathbf{r},t)\right|^2 = \left|e^{i\theta}\Psi(\mathbf{r},t)\right|^2 = e^{-i\theta}\Psi^*(\mathbf{r},t)e^{i\theta}\Psi(\mathbf{r},t) = \Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t) \\ &= \rho(\mathbf{r},t)\end{aligned} \tag{2.35}$$

In other words, if we detect the position of the particle, it will have the exact same probability distribution. It is also easy to see that if $\Psi(\mathbf{r},t)$ satisfies Schrödinger's equation (2.27), so also will $\Psi'(\mathbf{r},t)$. Hence the two wave functions $\Psi(\mathbf{r},t)$ and $\Psi'(\mathbf{r},t)$ are physically indistinguishable, and we can treat them as identical. In some formulations of quantum mechanics, they are identical; we will treat them as if they are different in principle but identical experimentally.

D. The Fourier Transform of the Wave Function

Suppose at a given time the wave function in one dimension takes the form $\Psi(x,t_0)=\psi(x)$. Consider now the Fourier Transform, as given by equations (1.77).

$$\tilde{\psi}(k)=\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}\psi(x)e^{-ikx} \tag{2.36a}$$

$$\psi(x)=\int_{-\infty}^{\infty}\frac{dk}{\sqrt{2\pi}}\tilde{\psi}(k)e^{ikx} \tag{2.36b}$$

For example, suppose that our wave function takes the form $\psi(x)\sim e^{ik_0x}$. Then the Fourier transform will look like $\tilde{\psi}(k)\sim\delta(k-k_0)$, so the Fourier transform will be concentrated at $k = k_0$. Furthermore, the momentum, according to eq. (2.6), will be $\hbar k_0$. Put simply, when the Fourier transform of the wave function is concentrated at a particular value of k, the momentum is simply $\hbar$ times that value of k.

Now, when the particle is spread out in x, we interpreted the wave function as a probability distribution for the position x. How do we interpret the Fourier transform wave function $\tilde{\psi}(k)$, when it is spread out in k? Probably not surprisingly, the answer is that it represents a probability distribution for the momentum p. From (2.36b), we see that if $\tilde{\psi}(k)$ is spread out in k, then the wave function $\psi(x)$ is simply a linear combination of many different waves of the form e^{ikx}. The square of the amplitude of the Fourier transform tells you the probability density that the momentum is around that value. If you integrate over different k values, you can find out the probability that the momentum lies in a given range. One way to write this is

$$P(\hbar k_A < p < \hbar k_B)=\int_{k_A}^{k_B}dk\left|\tilde{\psi}(k)\right|^2 \tag{2.37}$$

Before accepting this equation as valid, the first thing we should check is that the interpretation of this as a probability makes sense. We should demand that the probability of the particle having *some* momentum is equal to 1, so we find

$$P(-\infty < p < \infty)=\int_{-\infty}^{\infty}dk\left|\tilde{\psi}(k)\right|^2=\int_{-\infty}^{\infty}dx\left|\psi(x)\right|^2=1, \tag{2.38}$$

where we have used (1.78) together with the normalization constraint (2.30) to complete the proof.

Indeed, as we look at the wave function and its Fourier transform, there is a kind of complementary relationship between the two. Given either, we can find the other using (2.36). One describes the particle in terms of position, the other in terms of momentum. *Both* (in general) will represent only a probability distribution for the position or momentum. *Either* is a complete description of the particle. There is no particular reason to think of $\psi(x)$ as the actual wave function, and $\tilde{\psi}(k)$ as simply something mathematically related to it. Indeed, in the next chapter we will modify our notation so that we can refer to the wave function without specifying which of these two functions we are referring to.

E. Expectation Values and Uncertainties

As we have already said, when you measure the position or momentum of a particle, you cannot generally predict exactly what position or momentum it will have. Instead, we get a *distribution*, a sort of list of probabilities. Although it is most descriptive to give a complete list of the possible probabilities, which for position means knowing $\left|\psi(x)\right|^2$, sometimes it is sufficient to ask what the average outcome will be if we perform a measurement.

The *expectation value* $\bar{a}$ of some quantity *a* is the average of what you would get if you performed many measurements. If there are only discrete values of *a* that can occur, the expectation would take the form

$$\bar{a} = \sum_a aP(a) \tag{2.39}$$

where $P(a)$ is the probability of some outcome *a* occurring, and the sum is taken over all values of *a* that might occur.[5] This sum is simply converted into an integral (and the probability replaced by the probability density) when the variable *a* is continuous, so we have

$$\bar{a} = \int a\rho(a)\,da \tag{2.40}$$

Let us apply this to the position and the momentum of a single particle in one dimension. The probability density for the particle to have position *x* is $\left|\psi(x)\right|^2$, while for momentum the probability density for the particle to have momentum $\hbar k$ is $\left|\tilde{\psi}(k)\right|^2$, so we have

$$\bar{x} = \int x\left|\psi(x)\right|^2 dx \tag{2.41a}$$

$$\bar{p} = \int \hbar k\left|\tilde{\psi}(k)\right|^2 dk \tag{2.41b}$$

Of course, even though this is the average value, the value you get on any given measurement will tend to be difference. It is possible to define variances Δx and Δp as the root-mean-square difference between the expectation value and the value you get on particular measurements. Mathematically, these are given by

$$(\Delta x)^2 = \int (x-\bar{x})^2\left|\psi(x)\right|^2 dx \tag{2.42a}$$

$$(\Delta p)^2 = \int (\hbar k-\bar{p})^2\left|\tilde{\psi}(k)\right|^2 dk \tag{2.42b}$$

It is these two quantities that satisfy the famous Heisenberg uncertainty principle, eq. (2.8), which we will prove in a later chapter:

$$(\Delta x)(\Delta p) \geq \tfrac{1}{2}\hbar \tag{2.43}$$

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[5] Note that in this sum, there is no harm in including values which actually cannot occur, since they will have probability zero.

The uncertainty principle goes a long way towards understanding how quantum mechanics can solve classical conundrums. Consider, for example, the hydrogen atom, which consists of a heavy proton (which we treat as stationary) and a light electron in orbit around it. Classically, the energy of the hydrogen atom is given by

$$E = \frac{\mathbf{p}^2}{2m} - \frac{ke^2}{r}, \tag{2.44}$$

where r is the separation of the electron from the proton, $\mathbf{p}$ is the momentum of the electron, and m is its mass.[6] This is a problem, because the electron can be as close to the atom as it wants to, while keeping its momentum small, and hence the energy can be infinitely negative. Before the advent of quantum mechanics, it was not understood why the electron would not simply spiral into the proton, emitting electromagnetic energy. Quantum mechanically, however, it is *impossible* to both specify the position of the particle precisely and simultaneously limit the momentum. Suppose, for example, we want the electron to be "near" the proton. We want $r = 0$, but we cannot demand this precisely, because the electron is a wave function. Instead we ask the electron to be within about a distance a of the proton. We might therefore approximate

$$r \approx \Delta x \approx a \tag{2.45}$$

We'd also like to get the momentum as low as possible, but because of (2.43), we can't actually force it to be quite zero. Instead, we approximate

$$p \approx \Delta p \approx \frac{\hbar}{2\Delta x} = \frac{\hbar}{2a} \tag{2.46}$$

Plugging (2.45) and (2.46) into (2.44), we find that the energy is given by

$$E \approx \frac{\hbar^2}{8ma^2} - \frac{ke^2}{a} \tag{2.47}$$

We now see how quantum mechanics solves the problem. If we make the electron get too close to the proton, the kinetic energy term (the first term) will become very large, and we will end up with a positive energy. We can find the best possible size for the separation by finding where the derivative of (2.47) vanishes, which turns out to be

$$a \approx \frac{\hbar^2}{4mke^2} \tag{2.48}$$

Plugging this back into (2.47) yields an approximate energy

$$E \approx -2mk^2e^4/\hbar^2 \tag{2.49}$$

This answer turns out to be too large by precisely a factor of four. Part of this can be attributed to the fact that we used an uncertainty relation in one dimension, when we are really working in three; the remaining (smaller) error is simply due to the fact that we worked with an approximation, so we shouldn't *expect* to get the answer exactly right.

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[6] The exact form of the Coulomb interaction, the last term in (2.44), will depend on our choice of units. In this class we will always use SI units, so e is the charge on the proton and k is Coulomb's constant.