Chapter 10

Introduction to quantum mechanics

David Morin, morin@physics.harvard.edu

This chapter gives a brief introduction to quantum mechanics. Quantum mechanics can be thought of roughly as the study of physics on very small length scales, although there are also certain macroscopic systems it directly applies to. The descriptor "quantum" arises because in contrast with classical mechanics, certain quantities take on only discrete values. However, some quantities still take on continuous values, as we'll see.

In quantum mechanics, particles have wavelike properties, and a particular wave equation, the *Schrodinger equation*, governs how these waves behave. The Schrodinger equation is different in a few ways from the other wave equations we've seen in this book. But these differences won't keep us from applying all of our usual strategies for solving a wave equation and dealing with the resulting solutions.

In some respect, quantum mechanics is just another example of a system governed by a wave equation. In fact, we will find below that some quantum mechanical systems have *exact* analogies to systems we've already studied in this book. So the results can be carried over, with no modifications whatsoever needed. However, although it is fairly straightforward to deal with the actual waves, there are many things about quantum mechanics that are a combination of subtle, perplexing, and bizarre. To name a few: the measurement problem, hidden variables along with Bell's theorem, and wave-particle duality. You'll learn all about these in an actual course on quantum mechanics.

Even though there are many things that are highly confusing about quantum mechanics, the nice thing is that it's relatively easy to apply quantum mechanics to a physical system to figure out how it behaves. There is fortunately no need to understand all of the subtleties about quantum mechanics in order to use it. Of course, in most cases this isn't the best strategy to take; it's usually not a good idea to blindly forge ahead with something if you don't understand what you're actually working with. But this lack of understanding can be forgiven in the case of quantum mechanics, because no one really understands it. (Well, maybe a couple people do, but they're few and far between.) If the world waited to use quantum mechanics until it understood it, then we'd be stuck back in the 1920's. The bottom line is that quantum mechanics can be used to make predictions that are consistent with experiment. It hasn't failed us yet. So it would be foolish not to use it.

The main purpose of this chapter is to demonstrate how similar certain results in quantum mechanics are to earlier results we've derived in the book. You actually know a good

deal of quantum mechanics already, whether you realize it or not.

The outline of this chapter is as follows. In Section 10.1 we give a brief history of the development of quantum mechanics. In Section 10.2 we write down, after some motivation, the *Schrodinger wave equation*, both the time-dependent and time-independent forms. In Section 10.3 we discuss a number of examples. The most important thing to take away from this section is that all of the examples we discuss have *exact* analogies in the string/spring systems earlier in the book. So we technically won't have to solve anything new here. All the work has been done before. The only thing new that we'll have to do is interpret the old results. In Section 10.4 we discuss the *uncertainty principle*. As in Section 10.3, we'll find that we already did the necessary work earlier in the book. The uncertainty principle turns out to be a direct consequence of a result from Fourier analysis. But the interpretation of this result as an uncertainty principle has profound implications in quantum mechanics.

10.1 A brief history

Before discussing the Schrodinger wave equation, let's take a brief (and by no means comprehensive) look at the historical timeline of how quantum mechanics came about. The actual history is of course never as clean as an outline like this suggests, but we can at least get a general idea of how things proceeded.

1900 (Planck): Max Planck proposed that light with frequency ν is emitted in quantized lumps of energy that come in integral multiples of the quantity,

$$\boxed{E = h\nu = \hbar\omega} \tag{1}$$

where $h \approx 6.63 \cdot 10^{-34}\,\text{J}\cdot\text{s}$ is *Planck's constant*, and $\hbar \equiv h/2\pi = 1.06 \cdot 10^{-34}\,\text{J}\cdot\text{s}$.

The frequency ν of light is generally very large (on the order of $10^{15}\,\text{s}^{-1}$ for the visible spectrum), but the smallness of h wins out, so the $h\nu$ unit of energy is very small (at least on an everyday energy scale). The energy is therefore essentially continuous for most purposes. However, a puzzle in late 19th-century physics was the *blackbody radiation* problem. In a nutshell, the issue was that the classical (continuous) theory of light predicted that certain objects would radiate an infinite amount of energy, which of course can't be correct. Planck's hypothesis of quantized radiation not only got rid of the problem of the infinity, but also correctly predicted the shape of the power curve as a function of temperature.

The results that we derived for electromagnetic waves in Chapter 8 are still true. In particular, the energy flux is given by the Poynting vector in Eq. 8.47. And $E = pc$ for a light. Planck's hypothesis simply adds the information of how many lumps of energy a wave contains. Although strictly speaking, Planck initially thought that the quantization was only a function of the emission process and not inherent to the light itself.

1905 (Einstein): Albert Einstein stated that the quantization was in fact inherent to the light, and that the lumps can be interpreted as particles, which we now call "photons." This proposal was a result of his work on the *photoelectric effect*, which deals with the absorption of light and the emission of elections from a material.

We know from Chapter 8 that $E = pc$ for a light wave. (This relation also follows from Einstein's 1905 work on relativity, where he showed that $E = pc$ for any massless particle, an example of which is a photon.) And we also know that $\omega = ck$ for a light wave. So Planck's $E = \hbar\omega$ relation becomes

$$E = \hbar\omega \implies pc = \hbar(ck) \implies \boxed{p = \hbar k} \tag{2}$$

This result relates the momentum of a photon to the wavenumber of the wave it is associated with.

1913 (BOHR): Niels Bohr stated that electrons in atoms have wavelike properties. This correctly explained a few things about hydrogen, in particular the quantized energy levels that were known.

1924 (DE BROGLIE): Louis de Broglie proposed that *all* particles are associated with waves, where the frequency and wavenumber of the wave are given by the same relations we found above for photons, namely $E = \hbar\omega$ and $p = \hbar k$. The larger E and p are, the larger ω and k are. Even for small E and p that are typical of a photon, ω and k are very large because $\hbar$ is so small. So any everyday-sized particle with large (in comparison) energy and momentum values will have extremely large ω and k values. This (among other reasons) makes it virtually impossible to observe the wave nature of macroscopic amounts of matter.

This proposal (that $E = \hbar\omega$ and $p = \hbar k$ also hold for massive particles) was a big step, because many things that are true for photons are *not* true for massive (and nonrelativistic) particles. For example, $E = pc$ (and hence $\omega = ck$) holds only for massless particles (we'll see below how ω and k are related for massive particles). But the proposal was a reasonable one to try. And it turned out to be correct, in view of the fact that the resulting predictions agree with experiments.

The fact that any particle has a wave associated with it leads to the so-called *wave-particle duality*. Are things particles, or waves, or both? Well, it depends what you're doing with them. Sometimes things behave like waves, sometimes they behave like particles. A vaguely true statement is that things behave like waves until a measurement takes place, at which point they behave like particles. However, approximately one million things are left unaddressed in that sentence. The wave-particle duality is one of the things that few people, if any, understand about quantum mechanics.

1925 (HEISENBERG): Werner Heisenberg formulated a version of quantum mechanics that made use of *matrix mechanics*. We won't deal with this matrix formulation (it's rather difficult), but instead with the following wave formulation due to Schrodinger (this is a waves book, after all).

1926 (SCHRODINGER): Erwin Schrodinger formulated a version of quantum mechanics that was based on waves. He wrote down a wave equation (the so-called *Schrodinger equation*) that governs how the waves evolve in space and time. We'll deal with this equation in depth below. Even though the equation is correct, the correct interpretation of what the wave actually meant was still missing. Initially Schrodinger thought (incorrectly) that the wave represented the charge density.

1926 (BORN): Max Born correctly interpreted Schrodinger's wave as a probability amplitude. By "amplitude" we mean that the wave must be squared to obtain the desired probability. More precisely, since the wave (as we'll see) is in general complex, we need to square its absolute value. This yields the probability of finding a particle at a given location (assuming that the wave is written as a function of x).

This probability isn't a consequence of ignorance, as is the case with virtually every other example of probability you're familiar with. For example, in a coin toss, if you know everything about the initial motion of the coin (velocity, angular velocity), along with all external influences (air currents, nature of the floor it lands on, etc.), then you can predict which side will land facing up. Quantum mechanical probabilities aren't like this. They aren't a consequence of missing information. The probabilities are *truly* random, and there is no further information (so-called "hidden variables") that will make things unrandom. The topic of hidden variables includes various theorems (such as Bell's theorem) and experimental results that you will learn about in a quantum mechanics course.

1926 (DIRAC): Paul Dirac showed that Heisenberg's and Schrodinger's versions of quantum mechanics were equivalent, in that they could both be derived from a more general version of quantum mechanics.

10.2 The Schrodinger equation

In this section we'll give a "derivation" of the Schrodinger equation. Our starting point will be the classical nonrelativistic expression for the energy of a particle, which is the sum of the kinetic and potential energies. We'll assume as usual that the potential is a function of only x. We have

$$E = K + V = \frac{1}{2}mv^2 + V(x) = \frac{p^2}{2m} + V(x). \tag{3}$$

We'll now invoke de Broglie's claim that all particles can be represented as waves with frequency ω and wavenumber k, and that $E = \hbar\omega$ and $p = \hbar k$. This turns the expression for the energy into

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x). \tag{4}$$

A wave with frequency ω and wavenumber k can be written as usual as $\psi(x,t) = Ae^{i(kx-\omega t)}$ (the convention is to put a minus sign in front of the ωt). In 3-D we would have $\psi(\mathbf{r},t) = Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$, but let's just deal with 1-D. We now note that

$$\begin{aligned} \frac{\partial\psi}{\partial t} &= -i\omega\psi \quad\Longrightarrow\quad \omega\psi = i\frac{\partial\psi}{\partial t}\,, \qquad \text{and} \\ \frac{\partial^2\psi}{\partial x^2} &= -k^2\psi \quad\Longrightarrow\quad k^2\psi = -\frac{\partial^2\psi}{\partial x^2}\,. \end{aligned} \tag{5}$$

If we multiply the energy equation in Eq. (4) by ψ, and then plug in these relations, we obtain

$$\hbar(\omega\psi) = \frac{\hbar^2}{2m}(k^2\psi) + V(x)\psi \quad\Longrightarrow\quad \boxed{i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\cdot\frac{\partial^2\psi}{\partial x^2} + V\psi} \tag{6}$$

This is the *time-dependent Schrodinger equation.* If we put the x and t arguments back in, the equation takes the form,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\cdot\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t). \tag{7}$$

In 3-D, the x dependence turns into dependence on all three coordinates (x,y,z), and the $\partial^2\psi/\partial x^2$ term becomes $\nabla^2\psi$ (the sum of the second derivatives). Remember that Born's (correct) interpretation of $\psi(x)$ is that $|\psi(x)|^2$ gives the probability of finding the particle at position x.

Having successfully produced the time-dependent Schrodinger equation, we should ask: Did the above reasoning actually *prove* that the Schrodinger equation is valid? No, it didn't, for three reasons.

1. The reasoning is based on de Broglie's assumption that there is a wave associated with every particle, and also on the assumption that the ω and k of the wave are related to E and p via Planck's constant in Eqs. (1) and (2). We had to accept these assumptions on faith.

2. Said in a different way, it is impossible to actually prove anything in physics. All we can do is make an educated guess at a theory, and then do experiments to try to show

that the theory is consistent with the real world. The more experiments we do, the more comfortable we are that the theory is a good one. But we can never be absolutely sure that we have the correct theory. In fact, odds are that it's simply the limiting case of a more correct theory.

3. The Schrodinger equation actually isn't valid, so there's certainly no way that we proved it. Consistent with the above point concerning limiting cases, the quantum theory based on Schrodinger's equation is just a limiting theory of a more correct one, which happens to be quantum field theory (which unifies quantum mechanics with special relativity). This is turn must be a limiting theory of yet another more correct one, because it doesn't incorporate gravity. Eventually there will be one theory that covers everything (although this point can be debated), but we're definitely not there yet.

Due to the "i" that appears in Eq. (6), $\psi(x)$ is complex. And in contrast with waves in classical mechanics, the entire complex function now matters in quantum mechanics. We won't be taking the real part in the end. Up to this point in the book, the use of complex functions was simply a matter of convenience, because it is easier to work with exponentials than trig functions. Only the real part mattered (or imaginary part – take your pick, but not both). But in quantum mechanics the whole complex wavefunction is relevant. However, the theory is structured in such a way that anything you might want to measure (position, momentum, energy, etc.) will always turn out to be a real quantity. This is a necessary feature of any valid theory, of course, because you're not going to go out and measure a distance of $2 + 5i$ meters, or pay an electrical bill of $17 + 6i$ kilowatt hours.

As mentioned in the introduction to this chapter, there is an endless number of difficult questions about quantum mechanics that can be discussed. But in this short introduction to the subject, let's just accept Schrodinger's equation as valid, and see where it takes us.

Solving the equation

If we put aside the profound implications of the Schrodinger equation and regard it as simply a mathematical equation, then it's just another wave equation. We already know the solution, of course, because we used the function $\psi(x,t) = Ae^{i(kx-\omega t)}$ to produce Eqs. (5) and (6) in the first place. But let's pretend that we don't know this, and let's solve the Schrodinger equation as if we were given it out of the blue.

As always, we'll guess an exponential solution. If we first look at exponential behavior in the time coordinate, our guess is $\psi(x,t) = e^{-i\omega t}f(x)$ (the minus sign here is convention). Plugging this into Eq. (7) and canceling the $e^{-i\omega t}$ yields

$$\hbar\omega f(x) = -\frac{\hbar^2}{2m}\frac{\partial^2 f(x)}{\partial x^2} + V(x)f(x). \tag{8}$$

But from Eq. (1), we have $\hbar\omega = E$. And we'll now replace $f(x)$ with $\psi(x)$. This might cause a little confusion, since we've already used ψ to denote the entire wavefunction $\psi(x,t)$. However, it is general convention to also use the letter ψ to denote the spatial part. So we now have

$$\boxed{E\,\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x)} \tag{9}$$

This is called the *time-independent Schrodinger equation*. This equation is more restrictive than the original time-*dependent* Schrodinger equation, because it assumes that the particle/wave has a definite energy (that is, a definite ω). In general, a particle can be in a state that is the superposition of states with various definite energies, just like the motion of a

string can be the superposition of various normal modes with definite ω's. The same reasoning applies here as with all the other waves we've discussed: From Fourier analysis and from the linearity of the Schrodinger equation, we can build up any general wavefunction from ones with specific energies. Because of this, it suffices to consider the time-independent Schrodinger equation. The solutions for that equation form a basis for all possible solutions.[1]

Continuing with our standard strategy of guessing exponentials, we'll let $\psi(x) = Ae^{ikx}$. Plugging this into Eq. (9) and canceling the e^{ikx} gives (going back to the $\hbar\omega$ instead of E)

$$\hbar\omega = -\frac{\hbar^2}{2m}(-k^2) + V(x) \quad \Longrightarrow \quad \hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x). \tag{10}$$

This is simply Eq. (4), so we've ended up back where we started, as expected. However, our goal here was to show how the Schrodinger equation can be solved from scratch, without knowing where it came from.

Eq. (10) is (sort of) a dispersion relation. If $V(x)$ is a constant C in a given region, then the relation between ω and k (namely $\omega = \hbar k^2/2m + C$) is independent of x, so we have a nice sinusoidal wavefunction (or exponential, if k is imaginary). However, if $V(x)$ isn't constant, then the wavefunction isn't characterized by a unique wavenumber. So a function of the form e^{ikx} doesn't work as a solution for $\psi(x)$. (A Fourier superposition can certainly work, since any function can be expressed that way, but a single e^{ikx} by itself doesn't work.) This is similar to the case where the density of a string isn't constant. We don't obtain sinusoidal waves there either.

10.3 Examples

In order to solve for the wavefunction $\psi(x)$ in the time-independent Schrodinger equation in Eq. (9), we need to be given the potential energy $V(x)$. So let's now do some examples with particular functions $V(x)$.

10.3.1 Constant potential

The simplest example is where we have a constant potential, $V(x) = V_0$ in a given region. Plugging $\psi(x) = Ae^{ikx}$ into Eq. (9) then gives

$$E = \frac{\hbar^2 k^2}{2m} + V_0 \quad \Longrightarrow \quad k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}\,. \tag{11}$$

(We've taken the positive square root here. We'll throw in the minus sign by hand to obtain the other solution, in the discussion below.) k is a constant, and its real/imaginary nature depends on the relation between E and V_0. If $E > V_0$, then k is real, so we have oscillatory solutions,

$$\psi(x) = Ae^{ikx} + Be^{-ikx}. \tag{12}$$

But if $E < V_0$, then k is imaginary, so we have exponentially growing or decaying solutions. If we let $\kappa \equiv |k| = \sqrt{2m(V_0 - E)}/\hbar$, then $\psi(x)$ takes the form,

$$\psi(x) = Ae^{\kappa x} + Ba^{-\kappa x}. \tag{13}$$

We see that it is possible for $\psi(x)$ to be nonzero in a region where $E < V_0$. Since $\psi(x)$ is the probability amplitude, this implies that it is possible to have a particle with $E < V_0$.

[1] The "time-dependent" and "time-independent" qualifiers are a bit of a pain to keep saying, so we usually just say "the Schrodinger equation," and it's generally clear from the context which one we mean.

This isn't possible classically, and it is one of the many ways in which quantum mechanics diverges from classical mechanics. We'll talk more about this when we discuss the finite square well in Section 10.3.3.

If $E = V_0$, then this is the one case where the strategy of guessing an exponential function doesn't work. But if we go back to Eq. (9) we see that $E = V_0$ implies $\partial^2\psi/\partial x^2 = 0$, which in turn implies that ψ is a linear function,

$$\psi(x) = Ax + B. \tag{14}$$

In all of these cases, the full wavefunction (including the time dependence) for a particle with a specific value of E is given by

$$\boxed{\psi(x,t) = e^{-i\omega t}\psi(x) = e^{-iEt/\hbar}\psi(x)} \tag{15}$$

Again, we're using the letter ψ to stand for two different functions here, but the meaning of each is clear from the number of arguments. Any general wavefunction is built up from a superposition of the states in Eq. (15) with different values of E, just as the general motion of a string is built of from various normal modes with different frequencies ω. The fact that a particle can be in a superposition of states with different energies is another instance where quantum mechanics diverges from classical mechanics. (Of course, it's easy for classical *waves* to be in a superposition of normal modes with different energies, by Fourier analysis.)

The above $E > V_0$ and $E < V_0$ cases correspond, respectively, to being above or below the cutoff frequency in the string/spring system we discussed in Section 6.2.2. We have an oscillatory solution if E (or ω) is above a particular value, and an exponential solution if E (or ω) is below a particular value. The two setups (quantum mechanical with constant V_0, and string/spring with springs present everywhere) are exactly analogous to each other. The spatial parts of the solutions are exactly the same (well, before taking the real part in the string/spring case). The frequencies, however, are different, because the dispersion relations are different ($\hbar\omega = \hbar^2k^2/2m + V_0$ and $\omega^2 = c^2k^2 + \omega_s^2$, respectively). But this affects only the rate of oscillation, and not the shape of the function.

The above results hold for any particular region where $V(x)$ is constant. What if the region extends from, say, $x = 0$ to $x = +\infty$? If $E > V_0$, the oscillatory solutions are fine, even though they're not normalizable. That is, the integral of $|\psi|^2$ is infinite (at least for any nonzero coefficient in ψ; if the coefficient were zero, then we wouldn't have a particle). So we can't make the total probability equal to 1. However, this is fine. The interpretation is that we simply have a stream of particles extending to infinity. We shouldn't be too worried about this divergence, because when dealing with traveling waves on a string (for example, when discussing reflection and transmission coefficients) we assumed that the sinusiodal waves extended to $\pm\infty$, which of course is impossible in reality.

If $E < V_0$, then the fact that $x = +\infty$ is in the given region implies that the coefficient A in Eq. (13) must be zero, because otherwise ψ would diverge as $x \to \infty$. So we are left with only the $Ba^{-\kappa x}$ term. (It's one thing to have the integral of $|\psi|^2$ diverge, as it did in the previous paragraph. It's another thing to have the integral diverge and be dominated by values at large x. There is then zero probability of finding the particle at a finite value of x.) If the region where $E < V_0$ is actually the entire x axis, from $-\infty$ to ∞, then the B coefficient in Eq. (13) must also be zero. So $\psi(x) = 0$ for all x. In other words, there is no allowed wavefunction. It is impossible to have a particle with $E < V_0$ everywhere.

10.3.2 Infinite square well

Consider the potential energy,

$$V(x) = \begin{cases} 0 & (0 \le x \le L) \\ \infty & (x < 0 \ \text{ or } \ x > L). \end{cases} \tag{16}$$

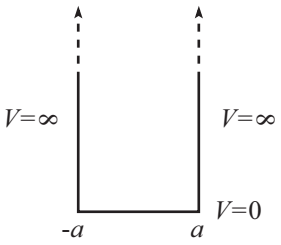

Figure 1

This is called an "infinite square well," and it is shown in Fig. 1. The "square" part of the name comes from the right-angled corners and not from the actual shape, since it's a very (infinitely) tall rectangle. This setup is also called a "particle in a box" (a 1-D box), because the particle can freely move around inside a given region, but has zero probability of leaving the region, just like a box. So $\psi(x) = 0$ outside the box.

The particle does indeed have zero chance of being found outside the region $0 \le x \le L$. Intuitively, this is reasonable, because the particle would have to climb the infinitely high potential cliff at the side of the box. Mathematically, this can be derived rigorously, and we'll do this below when we discuss the finite square well.

We'll assume $E > 0$, because the $E < 0$ case makes $E < V_0$ everywhere, which isn't possible, as we mentioned above. Inside the well, we have $V(x) = 0$, so this is a special case of the constant potential discussed above. We therefore have the oscillatory solution in Eq. (12) (since $E > 0$), which we will find more convenient here to write in terms of trig functions,

$$\psi(x) = A\cos kx + B\sin kx, \qquad \text{where} \quad E = \frac{\hbar^2 k^2}{2m} \implies k = \frac{\sqrt{2mE}}{\hbar}. \tag{17}$$

The coefficients A and B may be complex.

We now claim that ψ must be continuous at the boundaries at $x = 0$ and $x = L$. When dealing with, say, waves on a string, it was obvious that the function $\psi(x)$ representing the transverse position must be continuous, because otherwise the string would have a break in it. But it isn't so obvious with the quantum-mechanical ψ. There doesn't seem to be anything horribly wrong with having a discontinuous probability distribution, since probability isn't an actual object. However, it is indeed true that the probability distribution is continuous in this case (and in any other case that isn't pathological). For now, let's just assume that this is true, but we'll justify it below when we discuss the finite square well.

Since $\psi(x) = 0$ outside the box, continuity of $\psi(x)$ at $x = 0$ quickly gives $A\cos(0) + B\sin(0) = 0 \implies A = 0$. Continuity at $x = L$ then gives $B\sin kL = 0 \implies kL = n\pi$, where n is an integer. So $k = n\pi/L$, and the solution for $\psi(x)$ is $\psi(x) = B\sin(n\pi x/L)$. The full solution including the time dependence is given by Eq. (15) as

$$\boxed{\psi(x,t) = Be^{-iEt/\hbar}\sin\left(\frac{n\pi x}{L}\right)} \qquad \text{where} \quad \boxed{E = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}} \tag{18}$$

We see that the energies are quantized (that is, they can take on only discrete values) and indexed by the integer n. The string setup that is analogous to the infinite square well is a string with fixed ends, which we discussed in Chapter 4 (see Section 4.5.2). In both of these setups, the boundary conditions yield the same result that an integral number of half wavelengths fit into the region. So the k values take the same form, $k = n\pi/L$.

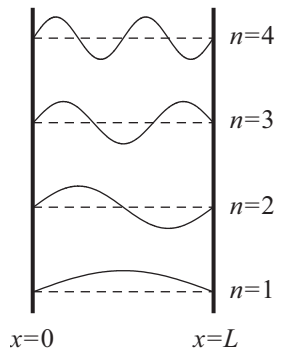

Figure 2

The dispersion relation, however, is different. It was simply $\omega = ck$ for waves on a string, whereas it is $\hbar\omega = \hbar^2 k^2/2m$ for the $V(x) = 0$ region of the infinite well. But as in the above case of the constant potential, this difference affects only the rate at which the waves oscillate in time. It does't affect the spatial shape, which is determined by the wavenumber k. The wavefunctions for the lowest four energies are shown in Fig. 2 (the vertical separation between the curves is meaningless). These look exactly like the normal modes in the "both ends fixed" case in Fig. 24 in Chapter 4.

The corresponding energies are shown in Fig. 3. Since $E \propto \omega = (\hbar^2/2m)k^2 \propto n^2$, the gap between the energies grows as n increases. Note that the energies in the case of a string are also proportional to n^2, because although $\omega = ck \propto n$, the energy is proportional to ω^2 (because the time derivative in Eq. (4.50) brings down a factor of ω). So Figs. 2 and 3 both apply to both systems. The difference between the systems is that a string has $\omega \propto \sqrt{E}$, where as the quantum mechanical system has $\omega \propto E$.

There is no $n = 0$ state, because from Eq. (18) this would make ψ be identically zero. That wouldn't be much of a state, because the probability would be zero everywhere. The lack of a $n = 0$ state is consistent with the uncertainty principle (see Section 10.4 below), because such a state would have $\Delta x \Delta p = 0$ (since $\Delta x < L$, and $\Delta p = 0$ because $n = 0 \Longrightarrow k = 0 \Longrightarrow p = \hbar k = 0$), which would violate the principle.

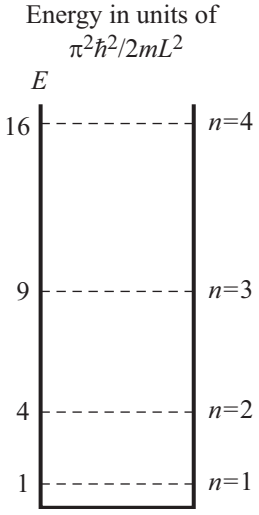

Figure 3

10.3.3 Finite square well

Things get more complicated if we have a finite potential well. For future convenience, we'll let $x = 0$ be located at the center of the well. If we label the ends as $\pm a$, then $V(x)$ is given by

$$V(x) = \begin{cases} 0 & (|x| \le a) \\ V_0 & (|x| > a). \end{cases} \tag{19}$$

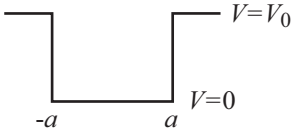

Figure 4

This is shown in Fig. 4. Given V_0, there are two basic possibilities for the energy E:

- $E > V_0$ (unbound state): From Eq. (11), the wavenumber k takes the general form of $\sqrt{2m(E - V(x))}/\hbar$. This equals $\sqrt{2mE}/\hbar$ inside the well and $\sqrt{2m(E - V_0)}/\hbar$ outside. k is therefore real everywhere, so $\psi(x)$ is an oscillatory function both inside and outside the well. k is larger inside the well, so the wavelength is shorter there. A possible wavefunction might look something like the one in Fig. 5. It is customary to draw the $\psi(x)$ function on top of the E line, although this technically has no meaning because ψ and E have different units.

  The wavefunction extends infinitely on both direction, so the particle can be anywhere. Hence the name "unbound state." We've drawn an even-function standing wave in Fig. 5, although in general we're concerned with traveling waves for unbound states. These are obtained from superpositions of the standing waves, with a phase thrown in the time dependence. For traveling waves, the relative sizes of $\psi(x)$ in the different regions depend on the specifics of how the problem is set up.

- $0 < E < V_0$ (bound state): The wavenumber k still equals $\sqrt{2mE}/\hbar$ inside the well and $\sqrt{2m(E - V_0)}/\hbar$ outside, but now that latter value is imaginary. So ψ is an oscillatory function inside the well, but an exponential function outside. Furthermore, it must be an exponentially *decaying* function outside, because otherwise it would diverge at $x = \pm\infty$. Since the particle has an exponentially small probability of being found far away from the well, we call this a "bound state." We'll talk more below about the strange fact that the probability is nonzero in the region outside the well, where $E < V(x)$.

  There is also the third case were $E = V_0$, but this can be obtained as the limit of the other two cases (more easily as the limit of the bound-state case). The fourth case, $E < 0$, isn't allowed, as we discussed at the end of Section 10.3.1.

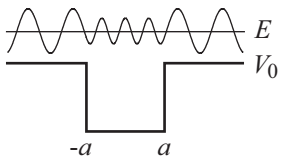

Figure 5

In both of these cases, the complete solution for $\psi(x)$ involves solving the boundary conditions at $x = \pm a$. The procedure is the same for both cases, but let's concentrate on the bound-state case here. The boundary conditions are given by the following theorem.

Theorem 10.1 *If $V(x)$ is everywhere finite (which is the case for the finite square well), then both $\psi(x)$ and $\psi'(x)$ are everywhere continuous.*

Proof: If we solve for ψ'' in Eq. (9), we see that ψ'' is always finite (because $V(x)$ is always finite). This implies two things. First, it implies that ψ' must be continuous, because if ψ' were discontinuous at a given point, then its derivative ψ'' would be infinite there (because ψ' would make a finite jump over zero distance). So half of the theorem is proved.

Second, the finiteness of ψ'' implies that ψ' must also be finite everywhere, because if ψ' were infinite at a given point (excluding $x = \pm\infty$), then its derivative ψ'' would also be infinite there (because ψ' would make an infinite jump over a finite distance).

Now, since ψ' is finite everywhere, we can repeat the same reasoning with ψ' and ψ that we used with ψ'' and ψ' in the first paragraph above: Since ψ' is always finite, we know that ψ must be continuous. So the other half of the theorem is also proved. ■

Having proved this theorem, let's outline the general strategy for solving for ψ in the $E < V_0$ case. The actual task of going through the calculation is left for Problem 10.2. The calculation is made much easier with the help of Problem 10.1 which states that only even and odd functions need to be considered.

If we let $k \equiv i\kappa$ outside the well, then we have $\kappa = \sqrt{2m(V_0 - E)}/\hbar$, which is real and positive since $E < V_0$. The general forms of the wavefunctions in the left, middle, and right regions are

$$\begin{aligned} x < -a: &\qquad \psi_1(x) = A_1 e^{\kappa x} + B_1 e^{-\kappa x}, \\ -a < x < a: &\qquad \psi_2(x) = A_2 e^{ikx} + B_2 e^{-ikx}, \\ x > a: &\qquad \psi_3(x) = A_3 e^{\kappa x} + B_3 e^{-\kappa x}, \end{aligned} \tag{20}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}, \qquad \text{and} \qquad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{21}$$

We've given only the x dependence in these wavefunctions. To obtain the full wavefunction $\psi(x,t)$, all of these waves are multiplied by the *same* function of t, namely $e^{-i\omega t} = e^{-iEt/\hbar}$.

We now need to solve for various quantities. How many unknowns do we have, and how many equations/facts do we have? We have seven unknowns: A_1, A_2, A_3, B_1, B_2, B_3, and E (which appears in k and κ). And we have seven facts:

- Four boundary conditions at $x = \pm a$, namely continuity of ψ and ψ' at both points.
- Two boundary conditions at $x = \pm\infty$, namely $\psi = 0$ in both cases.
- One normalization condition, namely $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$.

As we mentioned at the end of Section 10.3.1, the boundary conditions at $\pm\infty$ quickly tell us that B_1 and A_3 equal zero. Also, in most cases we're not concerned with the overall normalization constant (the usual goal is to find E), so we can ignore the normalization condition and just find all the other constants in terms of, say, A_1. So were're down to four equations (the four boundary conditions at $x = \pm a$), and four unknowns (A_2, B_2, B_3, and E). Furthermore, the even/odd trick discussed in Problem 10.1 cuts things down by a factor of 2, so we're down to two equations and two unknowns (the energy E, along with one of the coefficients), which is quite manageable. The details are left for Problem 10.2, but let's get a rough idea here of what the wavefunctions look like.

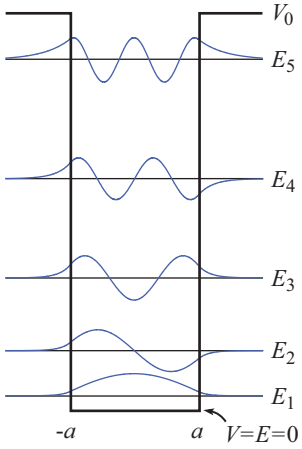

Figure 6

It turns out that the energies and states are again discrete and can be labeled by an integer n, just as in the infinite-well case. However, the energies don't take the simple form in Eq. (18), although they approximately do if the well is deep. Fig. 6 shows the five states for a well of a particular depth V_0. We've drawn each wave relative to the line that represents the energy E_n. Both ψ and ψ' are continuous at $x = \pm a$, and ψ goes to 0 at $x = \pm\infty$. We've chosen the various parameters (one of which is the depth) so that there are exactly five states (see Problem 10.2 for the details on this). The deeper the well, the more states there are.

Consistent with Eq. (20), ψ is indeed oscillatory inside the well (that is, the curvature is toward the x axis), and exponential decaying outside the well (the curvature is away from the x axis). As E increases, Eq. (21) tells us that k increases (so the wiggles inside the well have shorter wavelengths), and also that κ decreases (so the exponential decay is slower). These facts are evident in Fig. 6. The exact details of the waves depend on various parameters, but the number of bumps equals n.

Explanation of the quantized energy levels

The most important thing to note about these states is that they are *discrete*. In the infinite-well case, this discreteness was clear because an integral number of half wavelengths needed to fit into the well (because $\psi = 0$ at the boundaries). The discreteness isn't so obvious in the finite-well case (because $\psi \neq 0$ at the boundaries), but it is still reasonably easy to see. There are two ways to understand it. First, the not-so-enlightening way is to note that we initially had 7 equation and 7 unknowns. So all the unknowns, including E, are determined. There may be different discrete solutions, but at least we know that we can't just pick a random value for E and expect it to work.

Second, the more physical and enlightening way is the following. If we choose a random value of E, it probably won't yield an allowable function ψ, and here's why. Pick an arbitrary value of the coefficient A_1 in Eq. (20), and set $B_1 = 0$. So we have an exponentially decaying function in the left region, which behaves properly at $x = -\infty$. Since E determines κ, we know everything about the $A_1 e^{\kappa x}$ function.

Now pick a point x_0 in the left region, and imagine marching rightward on the x axis. We claim that all of the subsequent values of ψ are completely determined, all the way up to $x = +\infty$. This is clear in the left region, because we know what the function is. But it is also true in the middle and right regions, because we know the values of ψ, ψ', and ψ'' at any given point, so we can recursively find these three values at the "next" point as we march along. More precisely: (a) from the definition of the derivative, the values of ψ and ψ' at a given point yield the value of ψ at the next point, (b) likewise, the values of ψ' and ψ'' at a given point yield the value of ψ' at the next point, and (c) finally, the value of ψ at a given point yields the value of ψ'' at that point, via the Schrodinger equation, Eq. (9). So we can recursively march all the way up to $x = +\infty$, and the entire function is determined. There is no freedom whatsoever in what the function turns out to be.

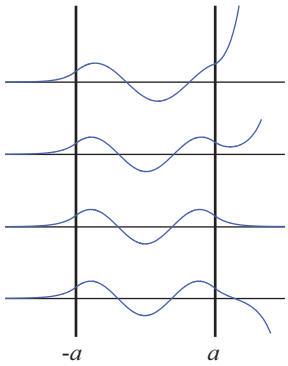

Figure 7

A particular choice of E and A_1 might yield the first (top) function shown in Fig. 7. It has the correct exponential and oscillatory nature in the left and middle regions, respectively. But in the right region it apparently has an exponentially growing piece. Because it diverges at $x = +\infty$, this function isn't an allowable one. So it is impossible for the energy to take on the value that we chose.

We can try to remedy the divergence at $x = +\infty$ by increasing the value of E. This will make ψ oscillate quicker inside the well, so that it encounters the $x = a$ boundary with a negative slope. We then might end up with the second function shown in Fig. 7. We still have the divergence at $x = +\infty$, so again we have an invalid ψ. If we increase E a little more, by precisely the right amount, then we'll end up with the third function shown in Fig.

7. The growing exponential term is now absent from the right region, so we have success. This function is allowable, as is the associated energy.

If we increase E a little more, then we'll end up with something like the fourth (bottom) function in Fig. 7. This function diverges, but now in the negative direction. So we're back to an invalid ψ. If we continue to increase E, then eventually we'll end up with the situation where there is now (approximately) one additional half oscillation, and the function again decays to zero at $x = +\infty$. And so on and so forth with additional half-oscillations, although eventually E will become larger than V_0, in which case we won't have a bound state anymore. (We can also decrease E from the value in the top plot in Fig. 7. We will encounter ψ's with two bumps and then one bump. The latter will have the lowest possible energy.) This reasoning makes it clear why only discrete values of E are allowed. Only special values of E make the coefficient A_3 in Eq. (20) be zero. Other values of E produce an exponentially growing piece in the right region, resulting in a non-normalizable wavefunction.

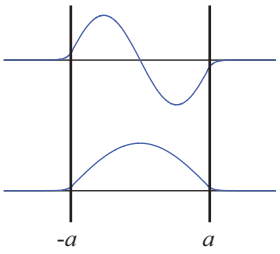

Figure 8

The terminology for this bound-state setup is that the particle is "trapped" in the well. However, we have discovered the strange fact that the particle has a nonzero probability of being found outside the well where $E < V_0$, because ψ is nonzero there. Strange, but true. Classically, it is impossible for a particle to have $E < V$. But classical mechanics isn't correct. It usually is, but not always. And this is one of the places where it fails.

What happens if $V_0 \to \infty$, so that the finite well approaches an infinite well? κ equals $\sqrt{2m(V_0 - E)}/\hbar$, so it approaches ∞ as $V_0 \to \infty$. The exponential decay outside the well is therefore infinitely quick. In the case of a very large by finite V_0, Fig. 8 shows what the first two states look like. As V_0 increases further, the region of the exponential decay gets smaller and smaller. Eventually you can't tell the difference between the plots in Fig. 8 and the bottom two plots in Fig. 2 for the infinite well. Technically the decay for the finite well always extends to $x = \pm\infty$, because the exponential function never actually equals zero. But it's essentially zero after a very short distance.

We see that as $V_0 \to \infty$, ψ approaches a function that is still continuous, but has a discontinuity in its first derivative. So if we consider the infinite well in Section 10.3.2 to be the limit of a finite well as $V_0 \to \infty$ (which is the most reasonable way to consider it), then the present discussion justifies our assumption in Section 10.3.2 that ψ was continuous. And furthermore it justifies why we didn't also assume that ψ' was continuous.

As with the infinite square well, the finite square well also has a direct analogy with a setup involving a string. Recall the discussion of the string/spring system in Section 6.2.2, involving evanescent waves and a low-frequency cutoff. Consider the system shown in Fig. 9, where the springs extend to $x = \pm\infty$. From Section 6.2.2, we know that if the frequency is below the cutoff frequency, then we have a sinusoidal wave in the middle region, but an evanescent wave (that is, an exponentially decaying wave) in the side regions. This is exactly what we have in the quantum-mechanical finite-well setup. In both setups the most general forms of the waves (as functions of x) in the different regions are given by Eq. (20) (but we need to take the real part in the string/spring case). And the boundary conditions are the same: continuity of ψ and ψ' at the boundaries, and $\psi = 0$ at $x = \pm\infty$. If you've solved for one $\psi(x)$, you've solved for the other.

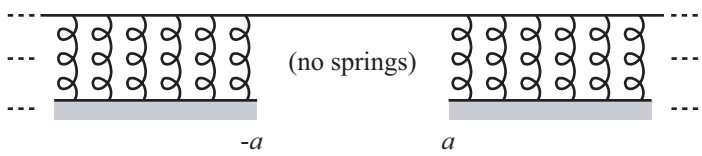

Figure 9

However, as with the other examples we've studied, the dispersion relation in the string/spring system is different from the relation in the quantum-mechanical system. In particular, in the quantum case, the wave equations and dispersion relations inside and outside the well are

$$\begin{aligned} \text{Inside}: \quad & i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\cdot\frac{\partial^2\psi}{\partial x^2} \implies \hbar\omega = \frac{\hbar^2k^2}{2m}, \\ \text{Outside}: \quad & i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\cdot\frac{\partial^2\psi}{\partial x^2} + V_0\psi \implies \hbar\omega = \frac{\hbar^2k^2}{2m} + V_0. \end{aligned} \tag{22}$$

And for the string/spring system we have

$$\begin{aligned} \text{Middle}: \quad & \frac{\partial^2\psi}{\partial t^2} = c^2\frac{\partial^2\psi}{\partial x^2} \implies \omega^2 = c^2k^2, \\ \text{Sides}: \quad & \frac{\partial^2\psi}{\partial t^2} = c^2\frac{\partial^2\psi}{\partial x^2} + \omega_s^2\psi \implies \omega^2 = c^2k^2 + \omega_s^2. \end{aligned} \tag{23}$$

But the differences in these equations don't affect the shape of the waves, because the shape is determined by the wavenumbers k and κ, where κ is the exponential decay constant. ω is irrelevant for the shape; it determines only how fast the wave oscillates in time. κ is given by $\kappa = \sqrt{2m(V_0 - \hbar\omega)}/\hbar$ in the quantum case, and $\sqrt{(\omega_s^2 - \omega^2)}/c$ in the string/spring case. So in both cases, k and κ are related by an equation of the form, $k^2 + \kappa^2 = A$, where A is a constant that equals $2mV_0/\hbar^2$ in the quantum case, and ω_s^2/c^2 in the string/spring case. Note that ω doesn't appear in A in either case. When you solve Problem 10.2, you will see that the shape of the wave is determined by the boundary conditions, along with the $k^2 + \kappa^2 = A$ equation. So the shape is indeed independent of ω.

10.3.4 Tunneling

Consider the string/spring system that is the "opposite" of the system shown in Fig. 9. So we now have springs in the middle region, and a normal string in the outer regions, as shown in Fig. 10.

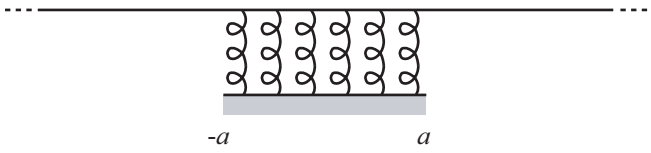

Figure 10

If a rightward-traveling wave comes in from the left, and if the frequency ω is less than the cutoff frequency ω_s, then we will have an evanescent wave in the middle region. And we will also have rightward-traveling wave in the right region (but no leftward-traveling wave, because we're not sending anything in from the right). So the waves in the three regions take the general form,

$$\begin{aligned} x < -a: \quad & \psi_1(x) = A_1e^{ikx} + B_1e^{-ikx}, \\ -a < x < a: \quad & \psi_2(x) = A_2e^{\kappa x} + B_2e^{-\kappa x}, \\ x > a: \quad & \psi_3(x) = A_3e^{ikx}. \end{aligned} \tag{24}$$

We've given only the x dependence here. All of these waves are multiplied by the same function of t, namely $e^{-i\omega t}$. The ratio B_1/A_1 is the reflection coefficient, and the ratio A_3/A_1

is the transmission coefficient. Note that we can have both the exponentially growing and decaying terms in the middle region, because the boundary conditions at $\pm\infty$ don't apply.

The frequency ω can take on any value. It need not take on certain discrete values as it did in the "opposite" string/spring system analogous to the finite well above. There are two ways of seeing why this is true. First, it makes physical sense, because you are free to wiggle the string at whatever ω you want, when creating the incoming wave, $A_1 e^{i(kx-\omega t)}$.[2]

Second, it makes mathematical sense if we count the number of unknowns and equations. In the finite-well case, we had seven unknowns: A_1, A_2, A_3, B_1, B_2, B_3, and E (or equivalently ω); see Eqs. (20) and (21). And we had seven equations: Six boundary conditions and the normalization condition. So we could solve for everything. In the present case, we have six unknowns: A_1, A_2, A_3, B_1, B_2, and ω (which determines k and κ). And we have four equations: two boundary conditions at each of $x = \pm a$ (there are no boundary conditions at $x = \pm\infty$). Since we have two more unknowns than equations, there will be two unknowns that we can't solve for. We can take these to be A_1 and ω. In other words, we are free to give the incoming wave whatever amplitude and frequency we want it to have, which makes sense.

We can therefore solve for the reflection and transmission coefficients, B_1/A_1 and A_3/A_1 in terms of ω (and any other parameters in the setup). The calculation is rather messy, so we won't do it here (see Problem [to be added]). The situation isn't symmetric, since we're throwing things in from the left, so we can't make easy use of the even/odd trick from Problem 10.1.

The important point to note is that the coefficient A_3 is *not* equal to zero. This is believable, because the string in the middle region will move at least a little, so the right end of it will wiggle the string in the right region, creating a rightward-traveling $A_3 e^{i(kx-\omega t)}$ wave. Intuitively, if the springs are weak, or if the width $2a$ of the middle region is small, then virtually all of the wave will make it through, so $A_3 \approx A_1$. In the other extreme, if the springs are stiff, or if the width $2a$ of the middle region is large, then A_3 will be small, but it will always be nonzero. Increasing the stiffness of the springs and/or increasing a should make A_3 smaller, but it should just be a matter of degree, and A_3 should asymptotically approach zero. There isn't any reason why A_3 should suddenly exactly equal zero.

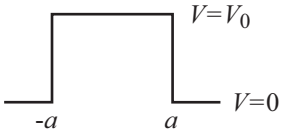

Figure 11

Let's now consider the analogous quantum system shown in Fig. 11. $V(x)$ equals zero except for the $-a < x < a$ region where it equals V_0. If we send a particle (or technically a stream of particles) in from the left, and if the energy is less than the height V_0 of the bump, then we have exactly the same situation as with the string/spring system. We have sinusoidal waves in the outer regions, and an evanescent wave in the middle region. The wavefunctions are again given by Eq. (24). The boundary conditions are also the same, so the resulting wavefunctions are exactly the same. (As with the finite-well case, the dispersion relations, and hence the ω's, are different, but this doesn't affect the shape of the waves.) So we again reach the conclusion that A_3 is nonzero.

However, while this conclusion is quite intuitive in the string/spring setup, it is quite bizarre and highly counterintuitive in the quantum-mechanical setup. Classically, if a particle has $E < V_0$, then it has zero chance of making it over the potential-energy bump. If a stream of particles comes in from the left, all of them are reflected, and none of them make it through. But not so in quantum mechanics. Since A_3 is nonzero, there is a nonzero probability that a particle can make it through. This phenomenon is known as *tunneling*. With macroscopic particles, the probability is prohibitively small. If you roll a ball toward

[2] We can't use the same reasoning in the case of the finite well, because there would be a kink in the string where you grab it (in the middle region). In the present setup, it doesn't matter if there's a kink very far to the left. (If we wiggled the string in the finite-well case very far to the left, then the evanescent wave generated would die out well before the middle region. So essentially no sinusoidal wave would be generated.)

a hill, and if it doesn't reach the top, then you will (essentially) never see it appear on the other side of the hill and roll down. But on the atomic level there are countless examples and applications of tunneling, including alpha decay, flash memory, and scanning tunneling microscopes.

10.4 Uncertainty principle

The *uncertainty principle* (often prefixed with "Heisenberg," after the physicist who first formulated it) makes a statement about the uncertainties in the position and momentum of a particle. There are actually many different uncertainty principles, applying to many different pairs (always pairs) of variables, but the most common one involves the position and momentum. This uncertainty principle says that the product of the uncertainties in x and p can never be smaller than a certain value. More precisely,

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}} \tag{25}$$

This tells us that if we know one of x or p very well, then we must be rather unsure of the other.

REMARK: Although we won't be concerned here with the precise definition of the uncertainties, Δx and Δp, we'll give the official definition for completeness. The uncertainty in a variable is defined to be the *standard deviation* of the variable, which in turn is defined by (with an "overline" denoting the average)

$$\Delta x = \sqrt{\overline{(x - \overline{x})^2}} \tag{26}$$

In words: to find Δx, you first calculate the average value, $\overline{x}$. Then you calculate the average value of the squares of the distances from $\overline{x}$. And then you take the square root of the result. In general, the probability distributions for x and p are continuous ones, so the averages in Eq. (26) involve calculating some integrals. But to illustrate the procedure, let's look at the simpler case of a discrete distribution. Let's say we have three equally possible values of x: 1, 2, and 6. Then the average value is $\overline{x} = 3$, and the squares of the differences from $\overline{x}$ are $(1-3)^2 = 4$, $(2-3)^2 = 1$, and $(6-3)^2 = 9$. The average value of these squares is $14/3$, and the square root of this is $\sqrt{14/3} \Longrightarrow \Delta x \approx 2.16$. But as we mentioned, the precise definition of the uncertainties won't be important here. For the present purposes, we can just take the uncertainty to be the rough spread of the bump of the probability distribution of x or p. ♣

The quickest way to rigorously prove the uncertainty principle makes use of what are called quantum-mechanical *operators*, which you will learn about when you take an actual course on quantum mechanics. But if you want to understand physically what's going on with the uncertainty principle, the best way is to invoke a few results from Chapter 3 on Fourier analysis. It turns out that the uncertainly principle is simply a fancy way of interpreting a certain fact from Fourier analysis.

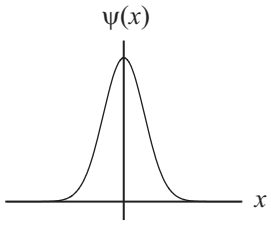

Figure 12

Consider the wavefunction $\psi(x)$ shown in Fig. 12. This represents a particle that is localized to within roughly the spread of the bump. Our Fourier result in Eq. (3.43) says that we can write (we'll use the letter ϕ here instead of C)

$$\psi(x) = \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk, \qquad \text{where} \quad \phi(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx. \tag{27}$$

$\phi(k)$ is the Fourier transform of $\psi(x)$, and it tells us how much of $\psi(x)$ is made up of the function e^{ikx} with a particular value of k.

Eq. (27) is a mathematical statement that need not have anything to do with physics. But now let's introduce some physics. We know from de Broglie's proposal in Section 10.1 that the function e^{ikx} corresponds to a momentum of $p = \hbar k$. Therefore, since $\phi(k)$ tells us how much of $\psi(x)$ is made up of the function e^{ikx} with a particular value of k, we see that $\phi(k)$ (or technically $|\phi(k)|^2$, once it is normalized to 1) gives the probability that the particle has a momentum of $p = \hbar k$.

Recall now from Section 3.4.1 that if a Gaussian function $\psi(x)$ is narrow, then the (also Gaussian) function $\phi(k)$ is wide, and vice versa. This opposing behavior of the widths is also true in general for the other pairs of non-Gaussian functions we dealt with (exponential/Lorentzian, square-wave/sinc). If a function is narrow (wide), then its Fourier transform is wide (narrow). This can be proved rigorously, but due to all the examples we gave in Chapter 3, we'll just accept it as true here.

Therefore, since $\phi(k)$ is the Fourier transform of $\psi(x)$, we see that if we're very sure about the position (so $\psi(x)$ is narrow), then we're very unsure about the momentum (because $\phi(k)$ is wide). Basically, if we want to construct a thin spike, then we need to use many different e^{ikx} functions to build it up.

If you do things rigorously, you will obtain the $\hbar/2$ term on the righthand side of Eq. (25). But even from our above qualitative argument, this term is believable, because we saw in Section 3.4 that the product of the rough widths of a plot and its Fourier transform is always of order 1. That is, $\Delta x \Delta k \approx 1$. And since $p = \hbar k$, we obtain $\Delta x \Delta p \approx \hbar$. So the exact result of $\Delta x \Delta p \geq \hbar/2$ is plausible. It turns out that if x (and hence also p) is a Gaussian function, then the lower bound of $\hbar/2$ is achieved. But for any other function, $\Delta x \Delta p$ is strictly larger than $\hbar/2$.

A common physical interpretation of the uncertainty principle is the following. If you want to measure the position of a particle, the most reasonable way to do this is to look at it. This involves shining photons and observing the ones that bounce off in your direction. Since photons carry momentum (which is given by $p = E/c = h\nu/c$), they will transfer some random fraction of this momentum to the particle when they hit it. You will therefore be uncertain of the particle's resulting momentum. Furthermore, if you want to narrow down the position, you will need to use a shorter wavelength of light, because it is impossible to resolve the position of a particle to more accuracy than the order of the wavelength of the light you're using. (Trying to do so would be like trying accurately measure the width of a penny by using a ruler whose smallest markings are inches.) Therefore, if you want to decrease Δx, then you need to decrease the wavelength λ, which means increasing the frequency ν (since $\nu = c/\lambda$), which means increasing the photon's momentum (since $p = E/c = h\nu/c$). This then increases Δp. So a small Δx implies a large Δp, consistent with the uncertainty principle.

However, although this physical reasoning makes the uncertainty principle a little more believable, it can be slightly misleading, because you might think that it is possible to conjure up a clever way of measuring a position that doesn't use light and doesn't disturb the particle. The uncertainty principle states that this isn't possible. It states that no matter how clever you are, you won't be able to beat the $\Delta x \Delta p \geq \hbar/2$ lower bound. The uncertainty principle isn't a measurement-specific result. Rather, it is a mathematical consequence of the wave nature of matter with a little Fourier analysis thrown in.

10.5 Problems

10.1. **Even and odd functions** $*$

Show that if the potential energy is an even function of x (that is, $V(-x) = V(x)$), then when solving the time-independent Schrodinger equation, it suffices to consider even and odd functions ψ (that is, ones for which $\psi(-x) = \psi(x)$ or $\psi(-x) = -\psi(x)$). By "suffices," we mean that any solution can be written as a linear combination of even and/or odd solutions. *Hint:* Replace x with $-x$ in the Schrodinger equation.

10.2. **Finite square well** $**$

Consider the finite square well discussed in Section 10.3.3 and shown in Fig. 4. From Problem 10.1 we know that we need only consider even and odd functions for ψ. Let's consider the even functions here (Exercise [to be added] covers the odd functions).

(a) If $\psi(x)$ is even, write down the most general possible form of the functions $\psi_2(x)$ and $\psi_3(x)$ in Eq. (20).

(b) Apply the boundary conditions at a, and show that $(ka)\tan(ka) = \kappa a$. We could cancel a factor of a here, but it's easier to work with the dimensionless quantities, ka and κa.

(c) From the definitions of k and κ in Eq. (21), it quickly follows that $(ka)^2 + (\kappa a)^2 = 2mV_0a^2/\hbar^2$. Show graphically how to obtain the solutions for k and κ (and hence E) by drawing the appropriate curves in the κa vs. ka plane and finding their intersections.

10.6 Solutions

10.1. **Even and odd functions**

Assume that $\psi(x)$ is a solution to the time-independent Schrodinger equation,

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x). \tag{28}$$

If we replace x with $-x$ (or if that seems like a fishy step, you can define $z \equiv -x$, and then later on relabel the letter z with the letter x), then we have

$$E\psi(-x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial(-x)^2} + V(-x)\psi(-x). \tag{29}$$

Using the given fact that $V(-x) = V(x)$, along with $(-x)^2 = x^2$, we obtain

$$E\psi(-x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial x^2} + V(x)\psi(-x). \tag{30}$$

This tells us that if $\psi(x)$ is a solution to the Schrodinger equation with potential $V(x)$ and total energy E, then $\psi(-x)$ is also a solution with the *same* $V(x)$ and E. And since the Schrodinger equation is linear, this means that any linear combination of the functions $\psi(x)$ and $\psi(-x)$ is also a solution for the same $V(x)$ and E. In particular, the combinations,

$$\psi_{\text{even}}(x) = \frac{1}{2}\Big(\psi(x) + \psi(-x)\Big) \qquad \text{and} \qquad \psi_{\text{odd}}(x) = \frac{1}{2}\Big(\psi(x) - \psi(-x)\Big) \tag{31}$$

are solutions. But these two function are even and odd, as you can verify by replacing x with $-x$. And since $\psi(x) = \big(\psi_{\text{even}}(x) + \psi_{\text{odd}}(x)\big)/2$, any solution with a particular energy can be written as a linear combination of the even and odd solutions with that energy. It turns out that in many cases there is only one solution with a given energy, so it is either even or odd (so one of the functions in Eq. (31) is identically zero).

10.2. **Finite square well**

(a) Since $\psi_2(x)$ is even, only the $\cos kx$ parts of the exponentials in Eq. (20) survive. So $\psi_2(x) = A\cos kx$. In the righthand region, the boundary condition at infinity tells us that the $e^{\kappa x}$ term can't exist, so $\psi_3(x) = Be^{-\kappa x}$. And then in the lefthand region we have $\psi_1(x) = Be^{\kappa x}$, but this ends up giving redundant information.

(b) k and κ are unknowns, but they aren't independent, because E determines both of them through Eq. (21). ψ_1 and ψ_2 therefore contain three unknowns, namely A, B, and E. And we have three equations, namely the two boundary conditions at $x = a$ (the boundary conditions at $x = -a$ are redundant, given that we are using an even function by construction), and the normalization condition. However, since our goal is to find only k and κ (and from these, E), we won't need to use the normalization condition.

The boundary conditions at $x = a$ (continuity of the wavefunction and its slope) are

$$\begin{aligned} \psi_2(a) &= \psi_3(a) \implies A\cos ka = Be^{-\kappa a}, \\ \psi_2'(a) &= \psi_3'(a) \implies -kA\sin ka = -\kappa Be^{-\kappa a}. \end{aligned} \tag{32}$$

Dividing these gives

$$k\tan ka = \kappa \implies (ka)\tan(ka) = \kappa a, \tag{33}$$

as desired.

(c) If we square and add the relations in Eq. (21), the E's cancel, and we end up with (after multiplying through by a^2)

$$(ka)^2 + (\kappa a)^2 = 2mV_0a^2/\hbar^2. \tag{34}$$

Eqs. (33) and (34) are two equations in two unknowns, k and κ (or equivalently ka and κa). They can't be solved analytically, so if we want to obtain precise values we have to solve them numerically (after being given the values of a, m, V_0, and $\hbar$). However, to get a general idea of what the solutions look like, it is far more instructive to solve the equations graphically than numerically. Our goal is to find the specific pairs of k and κ values that simultaneously satisfy Eqs. (33) and (34). These pairs can be found by drawing the curves represented by Eqs. (33) and (34) in the κa vs. ka plane and finding their intersections. (We're working with ka and κa because these quantities are dimensionless.) These two curves are shown in Fig. 13. Eq. (33) is a series of $(ka)\tan(ka)$ curves, and Eq. (34) is a circle. The intersections are shown by the dots. The (k, κ) pairs associated with these dots give the desired solutions.

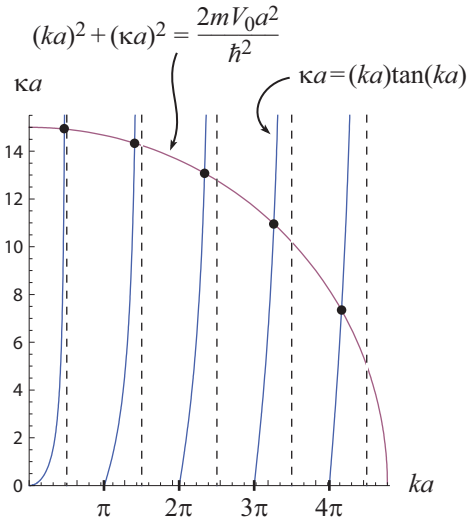

Figure 13

For a given value of a, the $(ka)\tan(ka)$ curves are located at fixed positions, but the size of the circle depends on the value of $mV_0a^2/\hbar^2$. And the size of the circle determines how many solutions there are. Let's look at the cases of very small and very large circles. Given the values of m, a, and $\hbar$, this is equivalent to looking at the cases of very small V_0 and very large V_0.

SMALL V_0 (SHALLOW WELL): There is always at least one even solution, no matter how small V_0 is, because the circle always intersects at least the first of the $(ka)\tan(ka)$ curves, even if the radius is very small. (The same can't be said for the odd states, as you will see in Exercise [to be added].) In the small-V_0 limit, the circle is close to the origin, so ka and κa are small (more precisely, these dimensionless quantities are much smaller than 1). We can therefore use $\tan(ka) \approx ka$ to write Eq. (33) as $k^2a^2 \approx \kappa a$. This says that κa is a second-order small quantity, much smaller that ka. (In other words, the slope of the $(ka)\tan(ka)$ curve equals zero at the origin.) The $(\kappa a)^2$ term in Eq. (34) is therefore negligible, so our solution for k and κ is $k \approx \sqrt{2mV_0/\hbar^2}$ and $\kappa \approx 0$.

The plot of the wave looks something like the function shown in Fig. 14. Since $\kappa \approx 0$, the exponential part of the function hardly decays, so it's almost a straight line. Also, $ka \approx \sqrt{2mV_0a^2/\hbar^2}$, which is the radius of the circle in Fig. 13, which we are assuming is small. Therefore, since $2ka$ is the phase change inside the well, the wave has hardly any net curvature in the middle region, so it's roughly a straight line there too. So we end up with a nearly straight line, with a slight negative curvature in the middle,

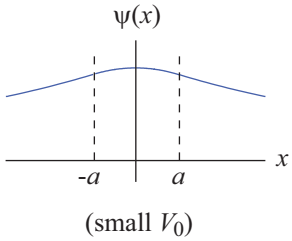

Figure 14

and a slight positive curvature on the sides. Note that since $\kappa \to 0$, virtually all of the area under the curve (or technically under the $|\psi|^2$ curve) lies *outside* the well. So the particle has essentially zero probability of actually being found inside the well. This is consistent with the fact that the energy E is very small (because it is squeezed between 0 and the very small V_0), which means that the wavefunction should be nearly the same as the wavefunction for a very small E that is barely larger than V_0. But in that case we have a free particle which can be anywhere from $-\infty$ to ∞.

LARGE V_0 (DEEP WELL): If V_0 is large, then the circle in Fig. 13 is very large, so there are many solutions for k and κ. This makes sense, because the well is very deep, so it should roughly approximate an infinite square well, which we know from Section 10.3.2 has an infinite number of possible states. From Fig. 13, a large V_0 (and hence a large circle) implies that the solutions for ka are roughly equal to $\pi/2$, $3\pi/2$, $5\pi/2$, etc. (except for the solutions near the right end of the circle), because the $(ka)\tan(ka)$ curves asymptotically approach the vertical dotted lines in the figure, which are located at the odd multiples of $\pi/2$. This means that the total phase of the cosine in the well is approximately $k(2a) = \pi$, 3π, 5π, etc. So the number of wavelengths that fit into the well is approximately 1/2, 3/2, 5/2, etc. This makes sense, because we approximately have an infinite well, and from Fig. 3 you can see that these are the numbers of wavelengths that fit into an infinite well for the even functions (the ones with odd values of n).