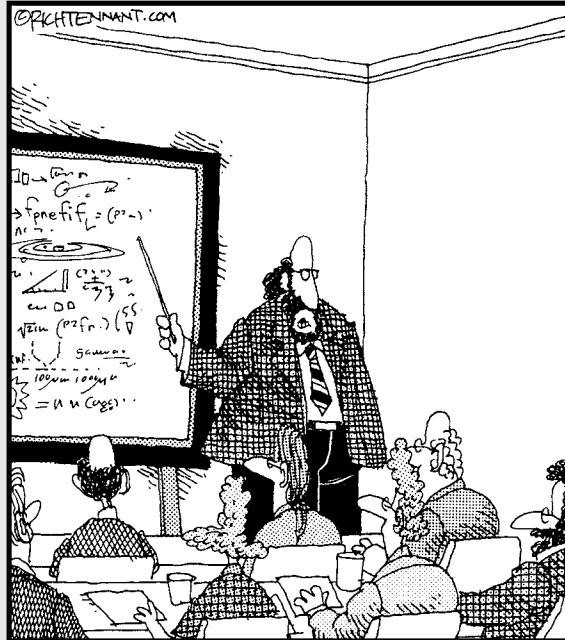


# Part II

## Bound and Undetermined: Handling Particles in Bound States

The 5<sup>th</sup> Wave

By Rich Tennant



"Along with 'Antimatter,' and 'Dark Matter,' we've recently discovered the existence of 'Doesn't Matter,' which appears to have no effect on the universe whatsoever."

### *In this part . . .*

**T**his part is where you get the lowdown on one of quantum physics' favorite topics: solving the energy levels and wave functions for particles trapped in various bound states. For example, you may have a particle trapped in a square well, which is much like having a pea in a box. Or you may have a particle in harmonic oscillation. Quantum physics is expert at handling those kinds of situations.

## Chapter 3

# Getting Stuck in Energy Wells

### *In This Chapter*

- ▶ Understanding potential wells
- ▶ Working with infinite square wells
- ▶ Determining energy levels
- ▶ Trapping particles with potential barriers
- ▶ Handling free particles

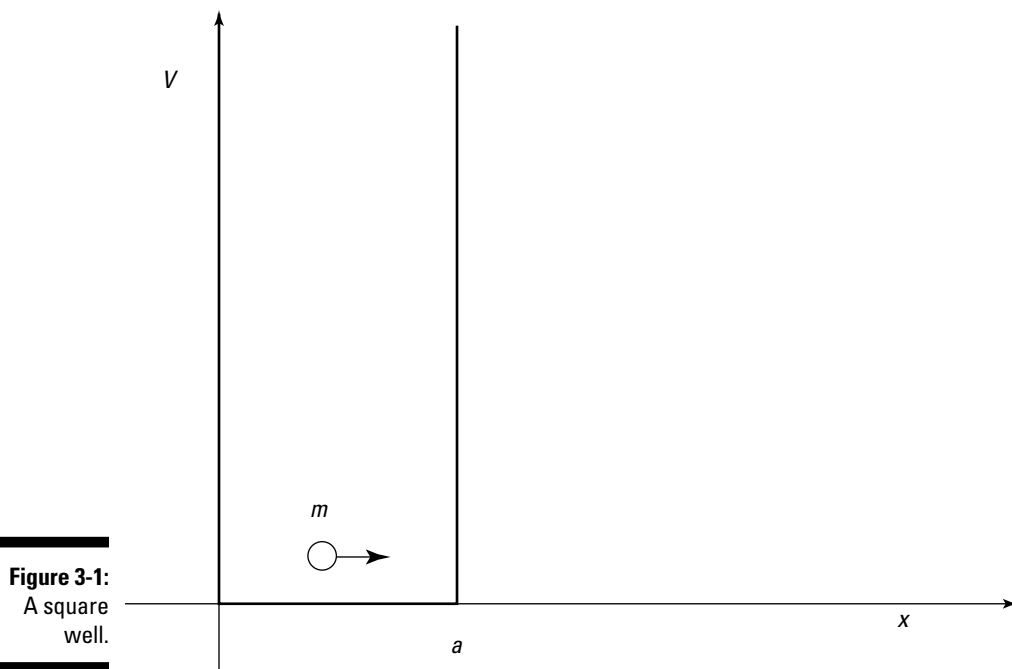
**W**hat's that, Lassie? Stuck in an energy well? Go get help! In this chapter, you get to see quantum physics at work, solving problems in one dimension. You see particles trapped in potential wells and solve for the allowable energy states using quantum physics. That goes against the grain in classical physics, which doesn't restrict trapped particles to any particular energy spectrum. But as you know, when the world gets microscopic, quantum physics takes over.

The equation of the moment is the Schrödinger equation (derived in Chapter 2), which lets you solve for the wave function,  $\psi(x)$ , and the energy levels,  $E$ :

$$\frac{-\hbar^2}{2m}\nabla^2\psi(r)+V(r)\psi(r)=E\psi(r)$$

## *Looking into a Square Well*

A *square well* is a potential (that is, a potential energy well) that forms a square shape, as you can see in Figure 3-1.



The potential, or  $V(x)$ , goes to infinity at  $x < 0$  and  $x > a$  (where  $x$  is distance), like this:

- ✓  $V(x) = \infty$ , where  $x < 0$
- ✓  $V(x) = 0$ , where  $0 \leq x \leq a$
- ✓  $V(x) = \infty$ , where  $x > a$

Using square wells, you can trap particles. If you put a particle into a square well with a limited amount of energy, it'll be trapped because it can't overcome the infinite potential at either side of the square well. Therefore, the particle has to move inside the square well.

So does the particle just sort of roll around on the bottom of the square well? Not exactly. The particle is in a bound state, and its wave function depends on its energy. The wave function isn't complicated:

$$\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x \quad n = 1, 2, 3 \dots$$

So you have the allowed wave functions for the states  $n = 1, 2, 3$ , and so on. The energy of the allowable bound states are given by the following equation:

$$E = \frac{\hbar^2 \pi^2}{2ma^2} n^2 \quad n = 1, 2, 3 \dots$$

The rest of this chapter shows you how to solve problems like this one.

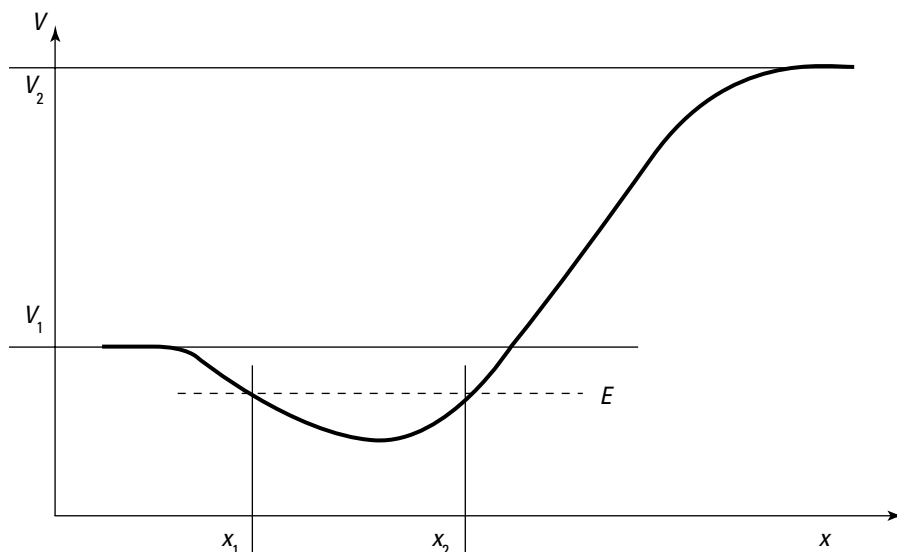
## Trapping Particles in Potential Wells

Take a look at the potential in Figure 3-2. Notice the dip, or *well*, in the potential, which means that particles can be trapped in it if they don't have too much energy.

The particle's kinetic energy summed with its potential energy is a constant, equal to its total energy:

$$\frac{p^2}{2m} + V = E$$

If its total energy is less than  $V_1$ , the particle will be trapped in the potential well, you see in Figure 3-2; to get out of the well, the particle's kinetic energy would have to become negative to satisfy the equation, which is impossible.



**Figure 3-2:**  
A potential  
well.

In this section, you take a look at the various possible states that a particle with energy  $E$  can take in the potential given by Figure 3-2. Quantum-mechanically speaking, those states are of two kinds — bound and unbound. This section looks at them in overview.

## Binding particles in potential wells

*Bound states* happen when the particle isn't free to travel to infinity — it's as simple as that. In other words, the particle is confined to the potential well.

A particle traveling in the potential well you see in Figure 3-2 is bound if its energy,  $E$ , is less than both  $V_1$  and  $V_2$ . In that case, the particle moves (in a classical approximation) between  $x_1$  and  $x_2$ . A particle trapped in such a well is represented by a wave function, and you can solve the Schrödinger equation for the allowed wave functions and the allowed energy states. You need to use two boundary conditions (the Schrödinger equation is a second-order differential equation) to solve the problem completely.



Bound states are *discrete* — that is, they form an energy spectrum of discrete energy levels. The Schrödinger equation gives you those states. In addition, in one-dimensional problems, the energy levels of a bound state are not degenerate — that is, no two energy levels are the same in the entire energy spectrum.

## Escaping from potential wells

If a particle's energy,  $E$ , is greater than the potential  $V_1$  in Figure 3-2, the particle can escape from the potential well. There are two possible cases:  $V_1 < E < V_2$  and  $E > V_2$ . This section looks at them separately.

### Case 1: Energy between the two potentials ( $V_1 < E < V_2$ )

If  $V_1 < E < V_2$ , the particle in the potential well has enough energy to overcome the barrier on the left but not on the right. The particle is thus free to move to negative infinity, so its allowed  $x$  region is between  $-\infty$  and  $x_1$ .

Here, the allowed energy values are continuous, not discrete, because the particle isn't completely bound. The energy eigenvalues are not degenerate — that is, no two energy eigenvalues are the same (see Chapter 2 for more on eigenvalues).

The Schrödinger equation is a second-order differential equation, so it has two linearly independent solutions; however, in this case, only one of those solutions is physical and doesn't diverge.

The wave equation in this case turns out to oscillate for  $x < x_2$  and to decay rapidly for  $x > x_2$ .

***Case 2: Energy greater than the higher potential ( $E > V_2$ )***

If  $E > V_2$ , the particle isn't bound at all and is free to travel from negative infinity to positive infinity.

The energy spectrum is continuous and the wave function turns out to be a sum of a function moving to the right and one moving to the left. The energy levels of the allowed spectrum are therefore doubly degenerate.

That's all the overview you need — time to start solving the Schrödinger equation for various different potentials, starting with the easiest of all: infinite square wells.

## ***Trapping Particles in Infinite Square Potential Wells***

Infinite square wells, in which the walls go to infinity, are a favorite in physics problems. You explore the quantum physics take on these problems in this section.

### ***Finding a wave-function equation***

Take a look at the infinite square well that appears back in Figure 3-1. Here's what that square well looks like:

- ✓  $V(x) = \infty$ , where  $x < 0$
- ✓  $V(x) = 0$ , where  $0 \leq x \leq a$
- ✓  $V(x) = \infty$ , where  $x > a$

The Schrödinger equation looks like this in three dimensions:

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r) = E \psi(r)$$

Writing out the Schrödinger equation gives you the following:

$$\frac{-\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(r) + V(r) \psi(r) = E \psi(r)$$

You're interested in only one dimension —  $x$  (distance) — in this chapter, so the Schrödinger equation looks like

$$\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x)$$

Because  $V(x) = 0$  inside the well, the equation becomes

$$\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E \psi(x)$$

And in problems of this sort, the equation is usually written as

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

where  $k^2 = \frac{2mE}{\hbar^2}$  ( $k$  is the wave number).

So now you have a second-order differential equation to solve for the wave function of a particle trapped in an infinite square well.

You get two independent solutions because this equation is a second-order differential equation:

$$\psi_1(x) = A \sin(kx)$$

$$\psi_2(x) = B \cos(kx)$$



$A$  and  $B$  are constants that are yet to be determined.

The general solution of  $\frac{d^2}{dx^2} \psi(x) + k^2 \psi(x) = 0$  is the sum of  $\psi_1(x)$  and  $\psi_2(x)$ :

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

## Determining the energy levels

The equation  $\psi(x) = A \sin(kx) + B \cos(kx)$  tells you that you have to use the boundary conditions to find the constants  $A$  and  $B$  (the preceding section explains how to derive the equation). What are the boundary conditions? The wave function must disappear at the boundaries of an infinite square well, so

$$\psi(0) = 0$$

$$\psi(a) = 0$$



The fact that  $\psi(0) = 0$  tells you right away that B must be zero because  $\cos(0) = 1$ . And the fact that  $\psi(a) = 0$  tells you that  $\psi(a) = A \sin(ka) = 0$ . Because sine is zero when its argument is a multiple of  $\pi$ , this means that

$$ka = n\pi \quad n = 1, 2, 3 \dots$$

Note that although  $n = 0$  is technically a solution, it yields  $\psi(x) = 0$  for all  $x$ , which is not normalizable, so it's not a physical solution — the physical solutions begin with  $n = 1$ .

This equation can also be written as

$$k = \frac{n\pi}{a} \quad n = 1, 2, 3 \dots$$

And because  $k^2 = 2mE/\hbar^2$ , you have the following equation, where  $n = 1, 2, 3, \dots$  — those are the allowed energy states. These are quantized states, corresponding to the quantum numbers 1, 2, 3, and so on:

$$\frac{2mE}{\hbar^2} = \frac{n^2 \pi^2}{a^2}$$

$$E = \frac{n^2 \hbar^2 \pi^2}{2ma^2}$$

Note that the first physical state corresponds to  $n = 1$ , which gives you this next equation:

$$E = \frac{\hbar^2 \pi^2}{2ma^2}$$

This is the lowest physical state that the particles can occupy. Just for kicks, put some numbers into this, assuming that you have an electron, mass  $9.11 \times 10^{-31}$  kilograms, confined to an infinite square well of width of the order of the *Bohr radius* (the average radius of an electron's orbit in a hydrogen atom); let's say  $a = 3.00 \times 10^{-10}$  meters.

$E = \frac{\hbar^2 \pi^2}{2ma^2}$  gives you this energy for the ground state:

$$\frac{(1.05 \times 10^{-34})^2}{2(9.11 \times 10^{-31})} \frac{(3.14)^2}{(3.00 \times 10^{-10})^2} = 6.69 \times 10^{-18} \text{ Joules}$$

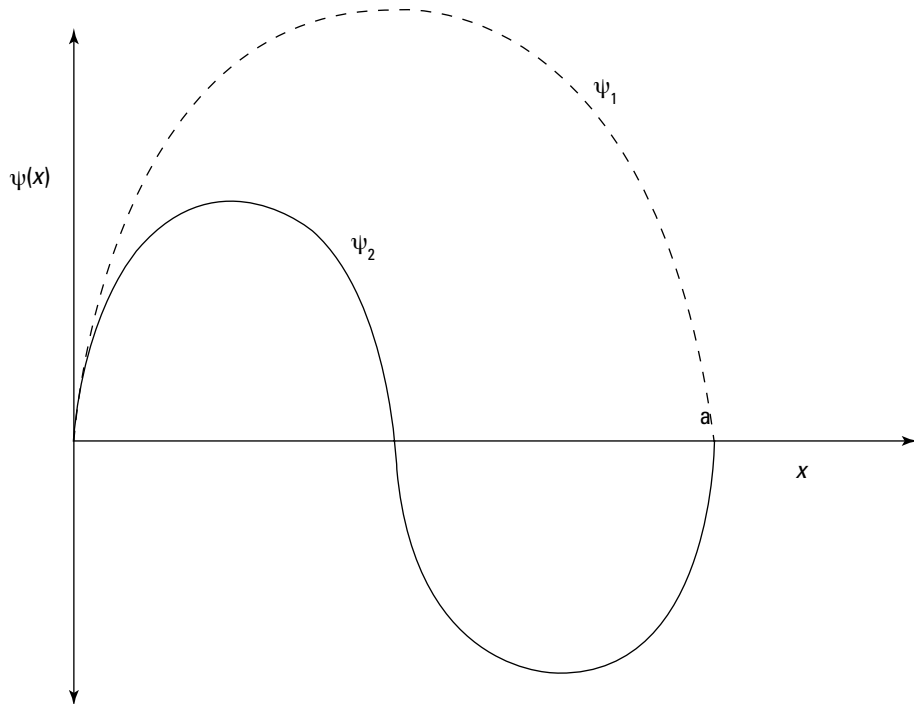
That's a very small amount, about 4.2 electron volts (eV — the amount of energy one electron gains falling through 1 volt). Even so, it's already on the order of the energy of the ground state of an electron in the ground state of a hydrogen atom (13.6 eV), so you can say you're certainly in the right quantum physics ballpark now.

## *Normalizing the wave function*

Okay, you have this for the wave equation for a particle in an infinite square well:

$$\psi(a) = A \sin\left(\frac{n\pi x}{a}\right)$$

The wave function is a sine wave, going to zero at  $x = 0$  and  $x = a$ . You can see the first two wave functions plotted in Figure 3-3.



**Figure 3-3:**  
Wave  
functions  
in a square  
well.

Normalizing the wave function lets you solve for the unknown constant A. In a *normalized* function, the probability of finding the particle between  $x$  and  $dx$ ,  $|\psi(x)|^2 dx$ , adds up to 1 when you integrate over the whole square well,  $x = 0$  to  $x = a$ :

$$1 = \int_0^a |\psi(x)|^2 dx$$

Substituting for  $\psi(x)$  gives you the following:

$$1 = |A|^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx$$

Here's what the integral in this equation equals:

$$\int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = a/2$$

So from the previous equation,  $1 = |A|^2 (a/2)$ . Solve for A:

$$A = \left(\frac{2}{a}\right)^{1/2}$$

Therefore, here's the normalized wave equation with the value of A plugged in:

$$\psi(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) \quad n = 1, 2, 3 \dots$$

And that's the normalized wave function for a particle in an infinite square well.

## ***Adding time dependence to wave functions***

Now how about seeing how the wave function for a particle in an infinite square well evolves with time? The Schrödinger equation looks like this:

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r) = E \psi(r)$$

You can also write the Schrödinger equation this way, where  $H$  is the Hermitian Hamiltonian operator:

$$H\psi(r) = E\psi(r)$$

That's actually the *time-independent* Schrödinger equation. The *time-dependent* Schrödinger equation looks like this:

$$i\hbar \frac{\partial}{\partial t} \psi(r, t) = H\psi(r, t)$$

Combining the preceding three equations gives you the following, which is another form of the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r, t) + V(r, t) \psi(r, t)$$

And because you're dealing with only one dimension,  $x$ , this equation becomes

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

This is simpler than it looks, however, because the potential doesn't change with time. In fact, because  $E$  is constant, you can rewrite the equation as

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = E\psi(x, t)$$

That equation makes life a lot simpler — it's easy to solve the time-dependent Schrödinger equation if you're dealing with a constant potential. In this case, the solution is

$$\psi(x, t) = \psi(x) e^{-iEt/\hbar}$$



Neat. When the potential doesn't vary with time, the solution to the time-dependent Schrödinger equation simply becomes  $\psi(x)$ , the spatial part, multiplied by  $e^{-iEt/\hbar}$ , the time-dependent part.

So when you add in the time-dependent part to the time-independent wave function, you get the time-dependent wave function, which looks like this:

$$\psi(x, t) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) e^{-iEt/\hbar} \quad n = 1, 2, 3 \dots$$

The energy of the  $n$ th quantum state is

$$E = \frac{n^2 \hbar^2 \pi^2}{2ma^2} \quad n = 1, 2, 3 \dots$$

Therefore, the result is

$$\psi(x, t) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) \exp\left(-\frac{in^2 \hbar^2 \pi^2 t}{2ma^2}\right) \quad n = 1, 2, 3 \dots$$

where  $\exp(x) = e^x$ .

## *Shifting to symmetric square well potentials*

The standard infinite square well looks like this:

- ✓  $V(x) = \infty$ , where  $x < 0$
- ✓  $V(x) = 0$ , where  $0 \leq x \leq a$
- ✓  $V(x) = \infty$ , where  $x > a$

But what if you want to shift things so that the square well is symmetric around the origin instead? That is, you move the square well so that it extends from  $-a/2$  to  $a/2$ ? Here's what the new infinite square well looks like in this case:

- ✓  $V(x) = \infty$ , where  $x < -a/2$
- ✓  $V(x) = 0$ , where  $-a/2 \leq x \leq a/2$
- ✓  $V(x) = \infty$ , where  $x > a/2$

You can translate from this new square well to the old one by adding  $a/2$  to  $x$ , which means that you can write the wave function for the new square well in this equation like the following:

$$\psi(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right) \quad n = 1, 2, 3 \dots$$

Doing a little trig gives you the following equations:

$$\psi(x) = \left(\frac{2}{a}\right)^{1/2} \cos\left(\frac{n\pi x}{a}\right) \quad n = 1, 3, 5 \dots$$

$$\psi(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) \quad n = 2, 4, 6 \dots$$

So as you can see, the result is a mix of sines and cosines. The bound states are these, in increasing quantum order:

$$\psi_1(x) = \left(\frac{2}{a}\right)^{1/2} \cos\left(\frac{\pi x}{a}\right)$$

$$\psi_2(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{2\pi x}{a}\right)$$

$$\psi_3(x) = \left(\frac{2}{a}\right)^{1/2} \cos\left(\frac{3\pi x}{a}\right)$$

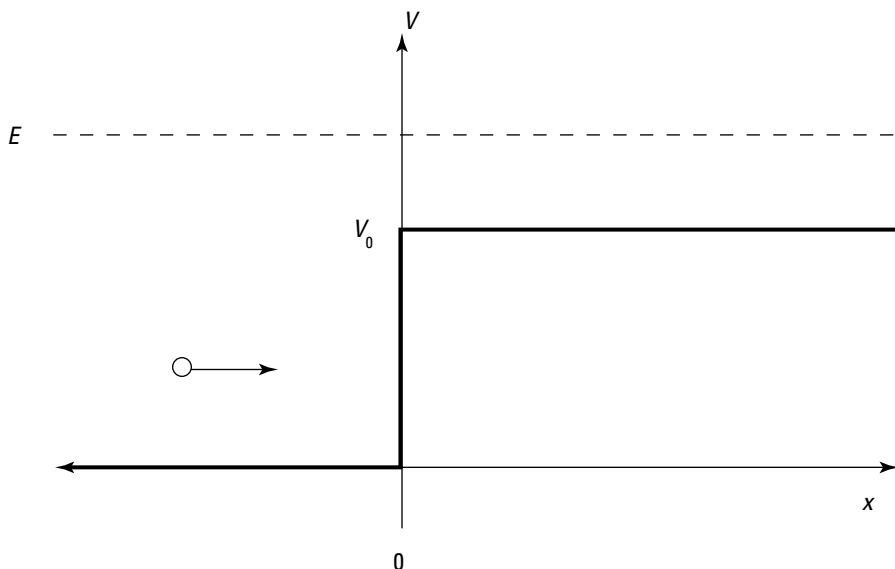
$$\psi_4(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{4\pi x}{a}\right)$$

And so on.

Note that the cosines are symmetric around the origin:  $\psi(x) = \psi(-x)$ . The sines are anti-symmetric:  $-\psi(x) = \psi(-x)$ .

## Limited Potential: Taking a Look at Particles and Potential Steps

Truly infinite potentials (which I discuss in the previous sections) are hard to come by. In this section, you look at some real-world examples, where the potential is set to some finite  $V_0$ , not infinity. For example, take a look at the situation in Figure 3-4. There, a particle is traveling toward a potential step. Currently, the particle is in a region where  $V = 0$ , but it'll soon be in the region  $V = V_0$ .



**Figure 3-4:**  
A potential  
step,  $E > V_0$ .

There are two cases to look at here in terms of  $E$ , the energy of the particle:

- ✓  $E > V_0$ : Classically, when  $E > V_0$ , you expect the particle to be able to continue on to the region  $x > 0$ .
- ✓  $E < V_0$ : When  $E < V_0$ , you'd expect the particle to bounce back and not be able to get to the region  $x > 0$  at all.

In this section, you start by taking a look at the case where the particle's energy,  $E$ , is greater than the potential  $V_0$ , as shown in Figure 3-4; then you take a look at the case where  $E < V_0$ .

## *Assuming the particle has plenty of energy*

Start with the case where the particle's energy,  $E$ , is greater than the potential  $V_0$ . From a quantum physics point of view, here's what the Schrödinger equation would look like:

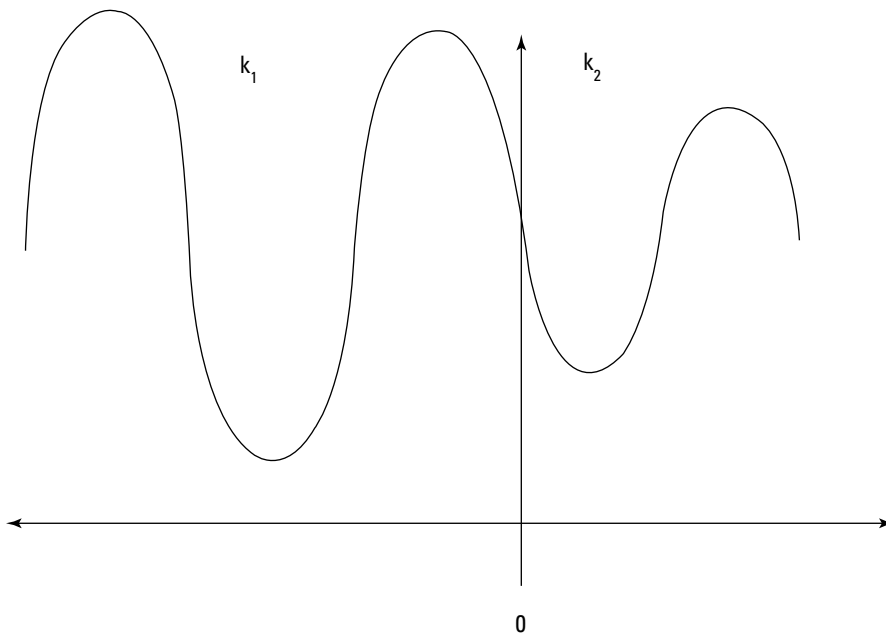
- ✓ **For the region  $x < 0$ :**  $\frac{d^2\psi_1}{dx^2}(x) + k_1^2\psi_1(x) = 0$

Here,  $k_1^2 = 2mE/\hbar^2$ .

✓ For the region  $x > 0$ :  $\frac{d^2\psi_2}{dx^2}(x) + k_2^2\psi_2(x) = 0$

In this equation,  $k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$ .

In other words,  $k$  is going to vary by region, as you see in Figure 3-5.



**Figure 3-5:**  
The value of  
 $k$  by region,  
where  
 $E > V_0$ .

Treating the first equation as a second-order differential equation, you can see that the most general solution is the following:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, \text{ where } x < 0$$

And for the region  $x > 0$ , solving the second equation gives you this:

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}, \text{ where } x > 0$$

Note that  $e^{ikx}$  represents plane waves traveling in the  $+x$  direction, and  $e^{-ikx}$  represents plane waves traveling in the  $-x$  direction.



What this solution means is that waves can hit the potential step from the left and be either transmitted or reflected. Given that way of looking at the problem, you may note that the wave can be reflected only going to the right, not to the left, so  $D$  must equal zero. That makes the wave equation become the following:

✓ Where  $x < 0$ :  $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$

✓ Where  $x > 0$ :  $\psi_2(x) = Ce^{ik_2x}$

The term  $Ae^{ik_1x}$  represents the incident wave,  $Be^{-ik_1x}$  is the reflected wave, and  $Ce^{ik_2x}$  is the transmitted wave.

### Calculating the probability of reflection or transmission

You can calculate the probability that the particle will be reflected or transmitted through the potential step by calculating the *reflection* and *transmission coefficients*. These are defined in terms of something called the *current density*  $J(x)$ ; this is given in terms of the wave function by

$$J(x) = \frac{i\hbar}{2m} \left[ \psi(x) \frac{d\psi^*(x)}{dx} - \psi^*(x) \frac{d\psi(x)}{dx} \right]$$

If  $J_r$  is the reflected current density, and  $J_i$  is the incident current density, then  $R$ , the reflection coefficient is

$$R = \frac{J_r}{J_i}$$

$T$ , the transmission coefficient, is

$$T = \frac{J_t}{J_i}$$

You now have to calculate  $J_r$ ,  $J_t$  and  $J_i$ . Actually, that's not so hard — start with  $J_i$ . Because the incident part of the wave is  $\psi_i(x) = Ae^{ik_1x}$ , the incident current density is

$$J_i = \frac{i\hbar}{2m} \left[ \psi_i(x) \frac{d\psi_i^*(x)}{dx} - \psi_i^*(x) \frac{d\psi_i(x)}{dx} \right]$$

And this just equals  $\frac{\hbar k_1}{m} |A|^2$ .  $J_r$  and  $J_t$  work in the same way:

$$J_r = \frac{\hbar k_1}{m} |B|^2$$

$$J_t = \frac{\hbar k_2}{m} |C|^2$$

So you have this for the reflection coefficient:

$$R = \frac{J_r}{J_i} = \frac{|B|^2}{|A|^2}$$

T, the transmission coefficient, is

$$T = \frac{J_t}{J_i} = \frac{k_2|C|^2}{k_1|A|^2}$$

### *Finding A, B, and C*

So how do you figure out the constants A, B, and C? You do that as you figure out the coefficients with the infinite square well potential — with boundary conditions (see the earlier section “Trapping Particles in Infinite Square Well Potentials”). However, here, you can’t necessarily say that  $\psi(x)$  goes to zero, because the potential is no longer infinite. Instead, the boundary conditions are that  $\psi(x)$  and  $d\psi(x)/dx$  are continuous across the potential step’s boundary. In other words,

$$\psi_1(0) = \psi_2(0)$$

$$\frac{d\psi_1}{dx}(0) = \frac{d\psi_2}{dx}(0)$$

You know the following:

$$\text{Where } x < 0: \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\text{Where } x > 0: \psi_2(x) = Ce^{ik_2x}$$

Therefore, plugging these two equations into  $\psi_1(0) = \psi_2(0)$  gives you  $A + B = C$ .

And plugging them into  $\frac{d\psi_1}{dx}(0) = \frac{d\psi_2}{dx}(0)$  gives you

$$k_1A - k_1B = k_2C$$

Solving for B in terms of A gives you this result:

$$B = \frac{k_1 - k_2}{k_1 + k_2} A$$

Solving for C in terms of A gives you

$$C = \frac{2k_1}{k_1 + k_2} A$$

You can then calculate A from the normalization condition of the wave function:

$$1 = \int |\psi(x)|^2 dx$$

But you don't actually need A, because it drops out of the ratios for the reflection and transmission coefficients, R and T. In particular,

$$R = \frac{|B|^2}{|A|^2}$$

$$T = \frac{k_2 |C|^2}{k_1 |A|^2}$$

Therefore,

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

$$T = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

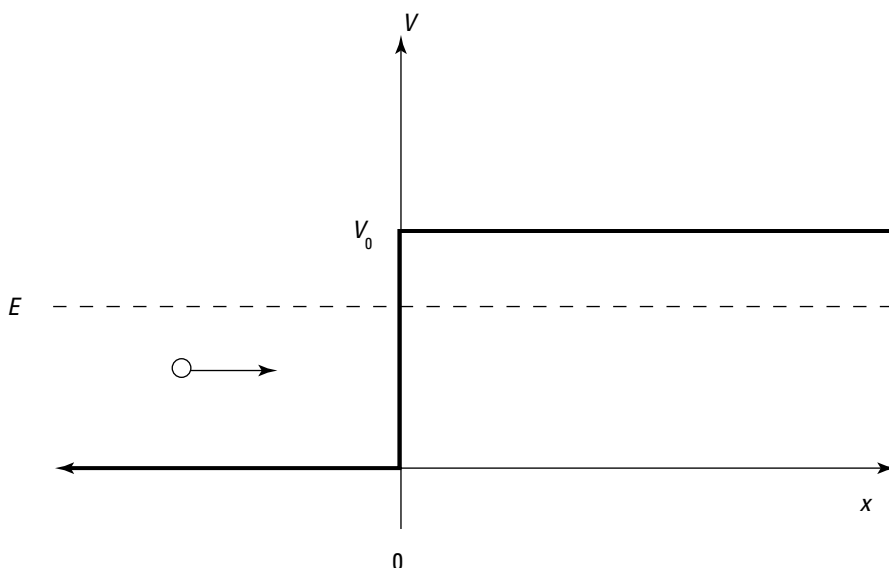
That's an interesting result, and it disagrees with classical physics, which says that there should be no particle reflection at all. As you can see, if  $k_1 \neq k_2$ , then there will indeed be particle reflection.

Note that as  $k_1$  goes to  $k_2$ , R goes to 0 and T goes to 1, which is what you'd expect.

So already you have a result that differs from the classical — the particle can be reflected at the potential step. That's the wave-like behavior of the particle coming into play again.

## *Assuming the particle doesn't have enough energy*

Okay, now try the case where  $E < V_0$  when there's a potential step, as shown in Figure 3-6. In this case, the particle doesn't have enough energy to make it into the region  $x > 0$ , according to classical physics. See what quantum physics has to say about it.



**Figure 3-6:**  
A potential  
step,  $E < V_0$ .

Tackle the region  $x < 0$  first. There, the Schrödinger equation would look like this:

$$\frac{d^2 \psi_1}{dx^2}(x) + k_1^2 \psi_1(x) = 0$$

where  $k_1^2 = 2mE/\hbar^2$ .

You know the solution to this from the previous discussion on potential steps (see “Limited Potential: Taking a Look at Particles and Potential Steps”):

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad x < 0$$

Okay, but what about the region  $x > 0$ ? That's a different story. Here's the Schrödinger equation:

$$\frac{d^2\psi_2(x)}{dx^2} + k^2\psi_2(x) = 0 \quad (\text{where } x > 0)$$

$$\text{where } k^2 = \frac{2m(E - V_0)}{\hbar^2}.$$

But hang on;  $E - V_0$  is less than zero, which would make  $k$  imaginary, which is impossible physically. So change the sign in the Schrödinger equation from plus to minus:

$$\frac{d^2\psi_2(x)}{dx^2} - k^2\psi_2(x) = 0 \quad x > 0$$

And use the following for  $k_2$  (note that this is positive if  $E < V_0$ ):

$$k_2^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

Okay, so now you have to solve the differential

$$\frac{d^2\psi_2(x)}{dx^2} + k^2\psi_2(x) = 0 \quad (\text{where } x > 0). \text{ There are two linearly independent solutions:}$$

$$\psi(x) = Ce^{-k_2x}$$

$$\psi(x) = De^{k_2x}$$

And the general solution to  $\frac{d^2\psi_2(x)}{dx^2} + k^2\psi_2(x) = 0$  (where  $x > 0$ ) is

$$\psi_2(x) = Ce^{-k_2x} + De^{k_2x} \quad x > 0$$

However, wave functions must be finite everywhere, and the second term is clearly not finite as  $x$  goes to infinity, so  $D$  must equal zero (note that if  $x$  goes to negative infinity, the first term also diverges, but because the potential step is limited to  $x > 0$ , that isn't a problem). Therefore, here's the solution for  $x > 0$ :

$$\psi_2(x) = Ce^{-k_2x} \quad x > 0$$

So your wave functions for the two regions are

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad x < 0$$

$$\psi_2(x) = Ce^{-k_2x} \quad x > 0$$

Putting this in terms of the incident, reflected, and transmitted wave functions,  $\psi_i(x)$ ,  $\psi_r(x)$ , and  $\psi_t(x)$ , you have the following:

$$\psi_i(x) = Ae^{ik_1x}$$

$$\psi_r(x) = Be^{-ik_1x}$$

$$\psi_t(x) = Ce^{-k_2x}$$

### ***Finding transmission and reflection coefficients***

Now you can figure out the reflection and transmission coefficients, R and T (as you do for the case  $E > V_0$  in the earlier section “Assuming the particle has plenty of energy”):

$$R = \frac{J_r}{J_i}$$

$$T = \frac{J_t}{J_i}$$

Actually, this is very easy in this case; take a look at  $J_t$ :

$$J_t = \frac{i\hbar}{2m} \left[ \psi_t(x) \frac{d\psi_t^*(x)}{dx} - \psi_t^*(x) \frac{d\psi_t(x)}{dx} \right]$$

But because  $\psi_t(x) = Ce^{-k_2x}$ ,  $\psi_t(x)$  is completely real, which means that in this case, the following is true:

$$J_t = \frac{i\hbar}{2m} \left[ \psi_t(x) \frac{d\psi_t(x)}{dx} - \psi_t(x) \frac{d\psi_t(x)}{dx} \right]$$

And this equation, of course, is equal to zero.

So  $J_t = 0$ ; therefore,  $T = 0$ . If  $T = 0$ , then R must equal 1. That means that you have a complete reflection, just as in the classical solution.

### ***The nonzero solution: Finding a particle in $x > 0$***

Despite the complete reflection, there's a difference between the mathematical and classical solution: There actually is a nonzero chance of finding the

particle in the region  $x > 0$ . To see that, take a look at the probability density for  $x > 0$ , which is

$$P(x) = |\psi_t(x)|^2$$

Plugging in for the wave function  $\psi_t(x)$  gives you

$$P(x) = |\psi_t(x)|^2 = |C|^2 e^{-2k_2 x}$$

You can use the continuity conditions to solve for  $C$  in terms of  $A$ :

$$\psi_1(0) = \psi_2(0)$$

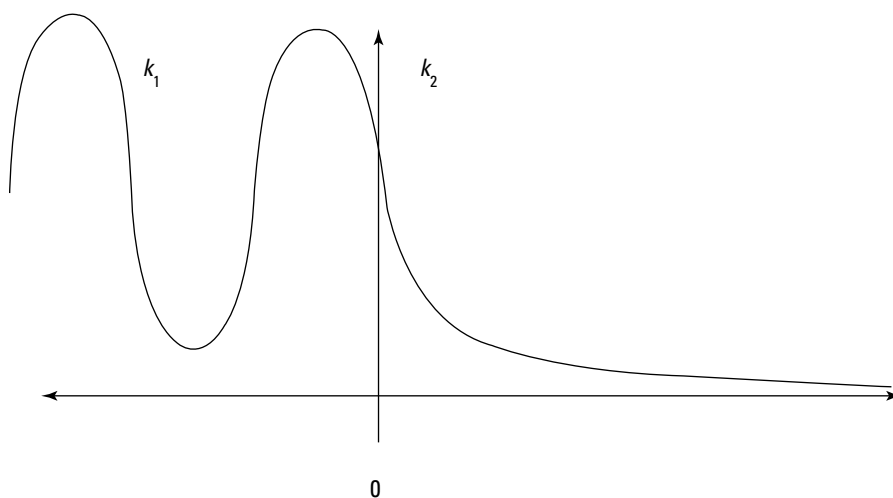
$$\frac{d\psi_1}{dx}(0) = \frac{d\psi_2}{dx}(0)$$

Using the continuity conditions gives you the following:

$$P(x) = |C|^2 e^{-2k_2 x} = \frac{4k_1^2 |A|^2 e^{-2k_2 x}}{k_1^2 + k_2^2}$$

This does fall quickly to zero as  $x$  gets large, but near  $x = 0$ , it has a nonzero value.

You can see what the probability density looks like for the  $E < V_0$  case of a potential step in Figure 3-7.



**Figure 3-7:**  
The value of  
 $k$  by region,  
 $E < V_0$ .

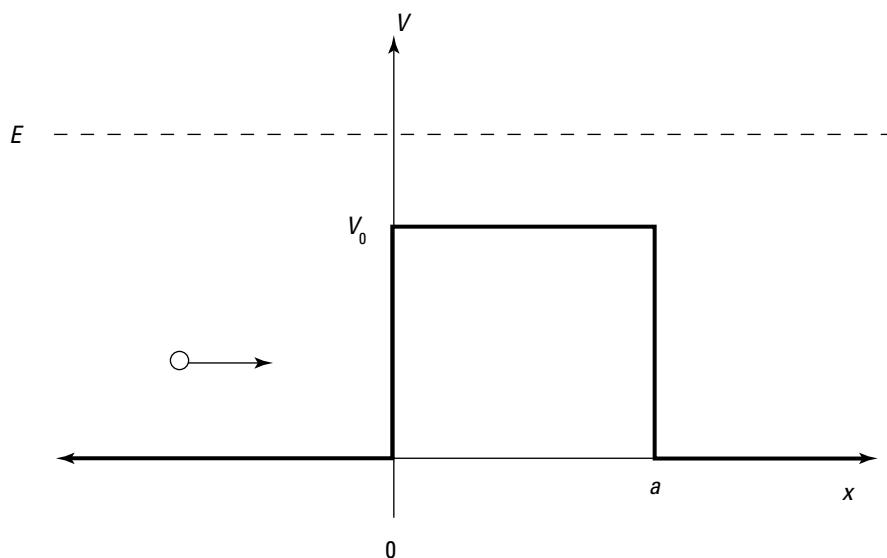
Okay, you've taken care of infinite square wells and potential steps. Now what about the case where the potential step doesn't extend out to infinity but is itself bounded? That brings you to *potential barriers*, which I discuss in the next section.

## Hitting the Wall: Particles and Potential Barriers

What if the particle could work its way through a potential step — that is, the step was of limited extent? Then you'd have a potential barrier, which is set up something like this:

- ✓  $V(x) = 0$ , where  $x < 0$
- ✓  $V(x) = V_0$ , where  $0 \leq x \leq a$
- ✓  $V(x) = 0$ , where  $x > a$

You can see what this potential looks like in Figure 3-8.



**Figure 3-8:**  
A potential  
barrier  
 $E > V_0$ .



In solving the Schrödinger equation for a potential barrier, you have to consider two cases, corresponding to whether the particle has more or less energy than the potential barrier. In other words, if  $E$  is the energy of the incident particle, the two cases to consider are  $E > V_0$  and  $E < V_0$ . This section starts with  $E > V_0$ .

## Getting through potential barriers when $E > V_0$

In the case where  $E > V_0$ , the particle has enough energy to pass through the potential barrier and end up in the  $x > a$  region. This is what the Schrödinger equation looks like:

✓ For the region  $x < 0$ :  $\frac{d^2\psi_1}{dx^2}(x) + k_1^2\psi_1(x) = 0$

where  $k_1^2 = 2mE/\hbar^2$

✓ For the region  $0 \leq x \leq a$ :  $\frac{d^2\psi_2}{dx^2}(x) + k_2^2\psi_2(x) = 0$

where  $k_2^2 = 2m(E - V_0)/\hbar^2$

✓ For the region  $x > a$ :  $\frac{d^2\psi_3}{dx^2}(x) + k_1^2\psi_3(x) = 0$

where  $k_1^2 = 2mE/\hbar^2$

The solutions for  $\psi_1(x)$ ,  $\psi_2(x)$ , and  $\psi_3(x)$  are the following:

✓ Where  $x < 0$ :  $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$

✓ Where  $0 \leq x \leq a$ :  $\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$

✓ Where  $x > a$ :  $\psi_3(x) = Ee^{ik_1x} + Fe^{-ik_1x}$

In fact, because there's no leftward traveling wave in the  $x > a$  region,  $F = 0$ , so  $\psi_3(x) = Ee^{ik_1x}$ .

So how do you determine A, B, C, D, and E? You use the continuity conditions, which work out here to be the following:

$$\begin{aligned}\psi_1(0) &= \psi_2(0) \\ \frac{d\psi_1}{dx}(0) &= \frac{d\psi_2}{dx}(0) \\ \psi_2(a) &= \psi_3(a) \\ \frac{d\psi_2}{dx}(a) &= \frac{d\psi_3}{dx}(a)\end{aligned}$$

Okay, from these equations, you get the following:

- ✓  $A + B = C + D$
- ✓  $ik_1(A - B) = ik_2(C - D)$
- ✓  $Ce^{ik_2a} + De^{-ik_2a} = Ee^{ik_1a}$
- ✓  $ik_2Ce^{ik_2a} - ik_2De^{-ik_2a} = ik_1Ee^{ik_1a}$

So putting all of these equations together, you get this for the coefficient E in terms of A:

$$E = 4k_1k_2Ae^{-ik_1a} \left[ 4k_1k_2 \cos(k_2a) - 2i(k_1^2 + k_2^2) \sin(k_2a) \right]^{-1}$$

Wow. So what's the transmission coefficient, T? Well, T is

$$T = \frac{|E|^2}{|A|^2}$$

And this works out to be

$$T = \left[ 1 + \frac{1}{4} \left( \frac{k_1^2 - k_2^2}{k_1k_2} \right)^2 \sin^2(k_2a) \right]^{-1}$$

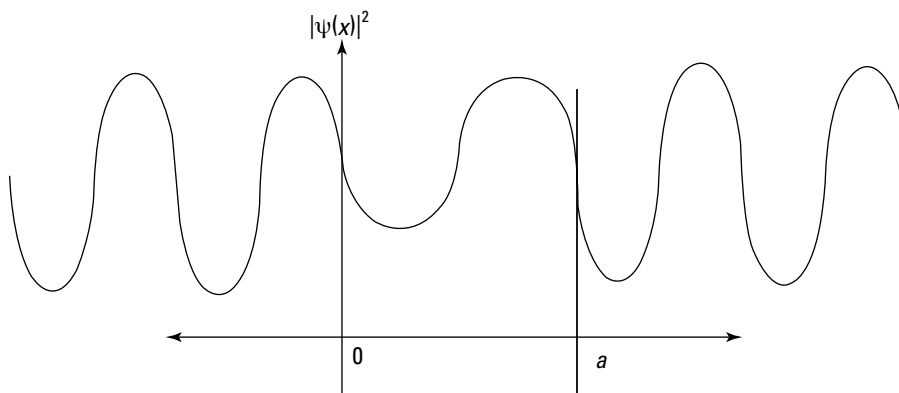
Whew! Note that as  $k_1$  goes to  $k_2$ , T goes to 1, which is what you'd expect.

So how about  $R$ , the reflection coefficient? I'll spare you the algebra; here's what  $R$  equals:

$$R = \frac{(k_2^2 - k_1^2) \sin^2(k_2 a)}{4k_1^2 k_2^2 + (k_1^2 - k_2^2)^2 \sin^2(k_2 a)}$$

You can see what the  $E > V_0$  probability density,  $|\psi(x)|^2$ , looks like for the potential barrier in Figure 3-9.

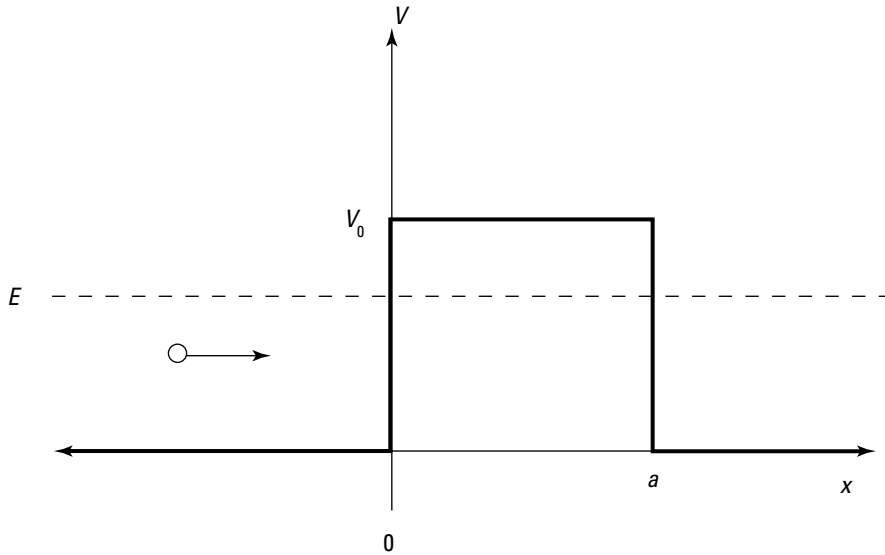
**Figure 3-9:**  
 $|\psi(x)|^2$  for  
a potential  
barrier  
 $E > V_0$ .



That completes the potential barrier when  $E > V_0$ .

## *Getting through potential barriers, even when $E < V_0$*

What happens if the particle doesn't have as much energy as the potential of the barrier? In other words, you're now facing the situation you see in Figure 3-10.



**Figure 3-10:**  
A potential  
barrier  
 $E < V_0$ .

Now the Schrödinger equation looks like this:

✓ For the region  $x < 0$ :  $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$

✓ For the region  $0 \leq x \leq a$ :  $\frac{d^2\psi_2}{dx^2}(x) + k^2\psi_2(x) = 0$

where  $k^2 = \frac{2m(E - V_0)}{\hbar^2}$ .

But now  $E - V_0$  is less than 0, which would make  $k$  imaginary. And that's impossible physically. So change the sign in the Schrödinger equation from plus to minus:

$$\frac{d^2\psi_2(x)}{dx^2} - k_2^2\psi_2(x) = 0$$

And use this for  $k_2$ :  $k_2^2 = \frac{2m(V_0 - E)}{\hbar^2}$ .

✓ For the region  $x > a$ :  $\frac{d^2\psi_3(x)}{dx^2} + k_1^2\psi_3(x) = 0$

where  $k_1^2 = \frac{2mE}{\hbar^2}$ .

All this means that the solutions for  $\psi_1(x)$ ,  $\psi_2(x)$ , and  $\psi_3(x)$  are the following:

✓ Where  $x < 0$ :  $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$

✓ Where  $0 \leq x \leq a$ :  $\psi_2(x) = Ce^{k_2x} + De^{-k_2x}$

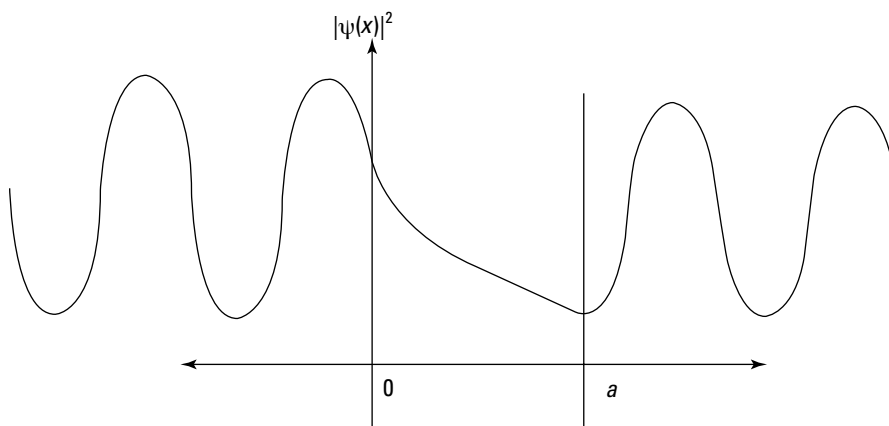
✓ Where  $x > a$ :  $\psi_3(x) = Ee^{ik_1x} + Fe^{-ik_1x}$

In fact, there's no leftward traveling wave in the region  $x > a$ ;  $F = 0$ , so  $\psi_3(x)$  is  $\psi_3(x) = Ee^{ik_1x}$ .

This situation is similar to the case where  $E > V_0$ , except for the region  $0 \leq x \leq a$ . The wave function oscillates in the regions where it has positive energy,  $x < 0$  and  $x > a$ , but is a decaying exponential in the region  $0 \leq x \leq a$ .

You can see what the probability density,  $|\psi(x)|^2$ , looks like in Figure 3-11.

**Figure 3-11:**  
 $|\psi(x)|^2$  for  
a potential  
barrier  
 $E < V_0$ .



### *Finding the reflection and transmission coefficients*

How about the reflection and transmission coefficients,  $R$  and  $T$ ? Here's what they equal:

$$R = \frac{|B|^2}{|A|^2}$$

$$T = \frac{|E|^2}{|A|^2}$$

As you may expect, you use the continuity conditions to determine A, B, and E:

$$\checkmark \psi_1(0) = \psi_2(0)$$

$$\checkmark \frac{d\psi_1}{dx}(0) = \frac{d\psi_2}{dx}(0)$$

$$\checkmark \psi_2(a) = \psi_3(a)$$

$$\checkmark \frac{d\psi_2}{dx}(a) = \frac{d\psi_3}{dx}(a)$$

A fair bit of algebra and trig is involved in solving for R and T; here's what R and T turn out to be:

$$R = \frac{4k_1^2 k_2^2}{(k_1^2 + k_2^2) \sinh(k_2 a)}$$

$$T = \left[ \cosh^2(k_2 a) + \left( \frac{k_1^2 + k_2^2}{2k_1^2 k_2^2} \right)^2 \sinh^2(k_2 a) \right]^{-1}$$

Despite the equation's complexity, it's amazing that the expression for T can be nonzero. Classically, particles can't enter the forbidden zone  $0 \leq x \leq a$  because  $E < V_0$ , where  $V_0$  is the potential in that region; they just don't have enough energy to make it into that area.

### ***Tunneling through***

Quantum mechanically, the phenomenon where particles can get through regions that they're classically forbidden to enter is called *tunneling*. Tunneling is possible because in quantum mechanics, particles show wave properties.

Tunneling is one of the most exciting results of quantum physics — it means that particles can actually get through classically forbidden regions because of the spread in their wave functions. This is, of course, a microscopic effect — don't try to walk through any closed doors — but it's a significant one. Among other effects, tunneling makes transistors and integrated circuits possible.

You can calculate the transmission coefficient, which tells you the probability that a particle gets through, given a certain incident intensity, when tunneling is involved. Doing so is relatively easy in the preceding section

because the barrier that the particle has to get through is a square barrier. But in general, calculating the transmission coefficient isn't so easy. Read on.

### ***Getting the transmission with the WKB approximation***

The way you generally calculate the transmission coefficient is to break up the potential you're working with into a succession of square barriers and to sum them. That's called the *Wentzel-Kramers-Brillouin* (WKB) approximation — treating a general potential,  $V(x)$ , as a sum of square potential barriers.

The result of the WKB approximation is that the transmission coefficient for an arbitrary potential,  $V(x)$ , for a particle of mass  $m$  and energy  $E$  is given by this expression (that is, as long as  $V(x)$  is a smooth, slowly varying function):

$$T \sim \exp \left[ - \left( \frac{2}{\hbar} \right) \int_{x_1}^{x_2} \left( 2m(V(x) - E) \right)^{1/2} dx \right]$$

So now you can amaze your friends by calculating the probability that a particle will tunnel through an arbitrary potential. It's the stuff science fiction is made of — well, on the microscopic scale, anyway.

## ***Particles Unbound: Solving the Schrödinger Equation for Free Particles***

What about particles outside any square well — that is, free particles? There are plenty of particles that act freely in the universe, and quantum physics has something to say about them.

Here's the Schrödinger equation:

$$\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x)$$

What if the particle were a free particle, with  $V(x) = 0$ ? In that case, you'd have the following equation:

$$\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) - E\psi(x) = 0$$

And you can rewrite this as

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

where the wave number,  $k$ , is  $k^2 = \frac{2mE}{\hbar^2}$ .

You can write the general solution to this Schrödinger equation as

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

If you add time-dependence to the equation, you get this time-dependent wave function:

$$\psi(x, t) = A \exp\left(ikx - \frac{iEt}{\hbar}\right) + B \exp\left(-ikx - \frac{iEt}{\hbar}\right)$$

That's a solution to the Schrödinger equation, but it turns out to be unphysical. To see this, note that for either term in the equation, you can't normalize the probability density,  $|\psi(x)|^2$  (see the earlier section titled "Normalizing the wave function" for more on normalizing):

$$|\psi(x)|^2 = |A|^2 \text{ or } |B|^2$$

What's going on here? The probability density for the position of the particle is uniform throughout all  $x$ ! In other words, you can't pin down the particle at all.

This is a result of the form of the time-dependent wave function, which uses an exact value for the wave number,  $k$  — and  $p = \hbar k$  and  $E = \hbar k^2/2m$ . So what that equation says is that you know  $E$  and  $p$  exactly. And if you know  $p$  and  $E$  exactly, that causes a large uncertainty in  $x$  and  $t$  — in fact,  $x$  and  $t$  are completely uncertain. That doesn't correspond to physical reality.

For that matter, the wave function  $\psi(x)$ , as it stands, isn't something you can normalize. Trying to normalize the first term, for example, gives you this integral:

$$\int_{-\infty}^{+\infty} \psi(x) \psi^*(x) dx$$

And for the first term of  $\psi(x, t)$ , this is

$$\int_{-\infty}^{+\infty} \psi(x) \psi^*(x) dx = |A|^2 \int_{-\infty}^{+\infty} dx \rightarrow \infty$$



And the same is true of the second term in  $\psi(x, t)$ .

So what do you do here to get a physical particle? The next section explains.

## Getting a physical particle with a wave packet



If you have a number of solutions to the Schrödinger equation, any linear combination of those solutions is also a solution. So that's the key to getting a physical particle: You add various wave functions together so that you get a *wave packet*, which is a collection of wave functions of the form  $e^{i(kx - Et/\hbar)}$  such that the wave functions interfere constructively at one location and interfere destructively (go to zero) at all other locations:

$$\psi(x, t) = \sum_{n=1}^{\infty} \phi_n e^{i(kx - Et/\hbar)}$$

This is usually written as a continuous integral:

$$\psi(x, t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} \phi(k, t) e^{i(kx - Et/\hbar)} dk$$

What is  $\phi(k, t)$ ? It's the amplitude of each component wave function, and you can find  $\phi(k, t)$  from the Fourier transform of the equation:

$$\phi(p, t) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \psi(x, t) e^{-i(kx - Et/\hbar)} dx$$

Because  $k = p/\hbar$ , you can also write the wave packet equations like this, in terms of  $p$ , not  $k$ :

$$\psi(x, t) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \phi(p, t) e^{i(px - Et/\hbar)} dp$$

$$\phi(p, t) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \psi(x, t) e^{-i(px - Et/\hbar)} dx$$

Well, you may be asking yourself just what's going on here. It looks like  $\psi(x, t)$  is defined in terms of  $\phi(p, t)$ , but  $\phi(p, t)$  is defined in terms of  $\psi(x, t)$ . That looks pretty circular.

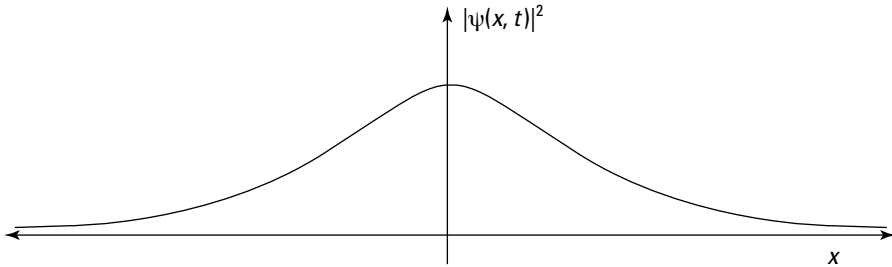
The answer is that the two previous equations aren't definitions of  $\psi(x, t)$  or  $\phi(p, t)$ ; they're just equations relating the two. You're free to choose your own wave packet shape yourself — for example, you may specify the shape

of  $\phi(p, t)$ , and  $\psi(x, t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} \phi(k, t) e^{i(kx - Et/\hbar)} dk$  would let you find  $\psi(x, t)$ .

## Going through a Gaussian example

Here's an example in which you get concrete, selecting an actual wave packet shape. Choose a so-called Gaussian wave packet, which you can see in Figure 3-12 — localized in one place, zero in the others.

**Figure 3-12:**  
A Gaussian  
wave  
packet.



The amplitude  $\phi(k)$  you may choose for this wave packet is

$$\phi(k) = A \exp \left[ \frac{-a^2 (k - k_0)^2}{4} \right]$$

You start by normalizing  $\phi(k)$  to determine what A is. Here's how that works:

$$1 = \int_{-\infty}^{+\infty} |\phi(k)|^2 dk$$

Substituting in  $\phi(k)$  gives you this equation:

$$1 = |A|^2 \int_{-\infty}^{+\infty} \exp \left[ \frac{-a^2}{2} (k - k_0)^2 \right] dk$$

Doing the integral (that means looking it up in math tables) gives you the following:

$$1 = |A|^2 \left[ \frac{2\pi}{a^2} \right]^{1/2}$$

Therefore,  $A = \left[ \frac{a^2}{2\pi} \right]^{1/4}$ .

So here's your wave function:

$$\psi(x) = \frac{1}{(2\pi)^{1/2}} \left[ \frac{a^2}{2\pi} \right]^{1/4} \int_{-\infty}^{+\infty} \exp \left[ \frac{-a^2 (k - k_0)^2}{4} \right] e^{ikx} dk$$

This little gem of an integral can be evaluated to give you the following:

$$\psi(x) = \left[ \frac{2}{\pi a^2} \right]^{1/4} \exp \left[ \frac{-x^2}{a^2} \right] e^{ik_0 x}$$

So that's the wave function for this Gaussian wave packet (**Note:** The  $\exp[-x^2/a^2]$  is the Gaussian part that gives the wave packet the distinctive shape that you see in Figure 3-12) — and it's already normalized.

Now you can use this wave packet function to determine the probability that the particle will be in, say, the region  $0 \leq x \leq a/2$ . The probability is

$$\int_0^{a/2} |\psi(x)|^2 dx$$

In this case, the integral is

$$\left[ \frac{2}{\pi a^2} \right]^{1/2} \int_0^{a/2} \exp \left( \frac{-2x^2}{a^2} \right) dx$$

And this works out to be

$$\left[ \frac{2}{\pi a^2} \right]^{1/2} \int_0^{a/2} \exp \left( \frac{-2x^2}{a^2} \right) dx = 1/3$$

So the probability that the particle will be in the region  $0 \leq x \leq a/2$  is  $1/3$ . Cool!



## Chapter 4

# Back and Forth with Harmonic Oscillators

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### *In This Chapter*

- ▶ Hamiltonians: Looking at total energy
  - ▶ Solving for energy states with creation and annihilation operators
  - ▶ Understanding the matrix version of harmonic oscillator operators
  - ▶ Writing computer code to solve the Schrödinger equation
- 

**H**armonic oscillators are physics setups with periodic motion, such as things bouncing on springs or tick-tocking on pendulums. You're probably already familiar with harmonic oscillator problems in the macroscopic arena, but now you're going microscopic. There are many, many physical cases that can be approximated by harmonic oscillators, such as atoms in a crystal structure.

In this chapter, you see both exact solutions to harmonic oscillator problems as well as computational methods for solving them. Knowing how to solve the Schrödinger equation using computers is a useful skill for any quantum physics expert.

## *Grappling with the Harmonic Oscillator Hamiltonians*

Okay, time to start talking Hamiltonians (and I'm not referring to fans of the U.S. Founding Father Alexander Hamilton). The Hamiltonian will let you find the energy levels of a system.

## *Going classical with harmonic oscillation*

In classical terms, the force on an object in harmonic oscillation is the following (this is Hooke's law):

$$F = -kx$$

In this equation,  $k$  is the spring constant, measured in Newtons/meter, and  $x$  is displacement. The key point here is that the restoring force on whatever is in harmonic motion is proportional to its displacement. In other words, the farther you stretch a spring, the harder it'll pull back.

Because  $F = ma$ , where  $m$  is the mass of the particle in harmonic motion and  $a$  is its instantaneous acceleration, you can substitute for  $F$  and write this equation as

$$ma + kx = 0$$

Here's the equation for instantaneous acceleration, where  $x$  is displacement and  $t$  is time:

$$a = \frac{d^2x}{dt^2}$$

So substituting for  $a$ , you can rewrite the force equation as

$$ma + kx = m \frac{d^2x}{dt^2} + kx = 0$$

Dividing by the mass of the particle gives you the following:

$$\frac{d^2x}{dt^2} + \frac{kx}{m} = \frac{0}{m}$$

If you take  $k/m = \omega^2$  (where  $\omega$  is the angular frequency), this becomes

$$\frac{d^2x}{dt^2} + \omega^2 x = 0$$

You can solve this equation for  $x$ , where  $A$  and  $B$  are constants:

$$x = A \sin \omega t + B \cos \omega t$$

Therefore, the solution is an oscillating one because it involves sines and cosines, which represent periodic waveforms.

## *Understanding total energy in quantum oscillation*

Now look at harmonic oscillators in quantum physics terms. The *Hamiltonian* ( $H$ ) is the sum of kinetic and potential energies — the total energy of the system:

$$H = KE + PE$$

For a harmonic oscillator, here's what these energies are equal to:

- ✓ The kinetic energy at any one moment is the following, where  $p$  is the particle's momentum and  $m$  is its mass:

$$KE = \frac{p^2}{2m}$$

- ✓ The particle's potential energy is equal to the following, where  $k$  is the spring constant and  $x$  is displacement:

$$PE = \frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 x^2$$

(**Note:** The  $k$  is replaced because  $\omega^2 = k/m$ .)

Therefore, in quantum physics terms, you can write the Hamiltonian as  $H = KE + PE$ , or

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 X^2$$

where  $P$  and  $X$  are the momentum and position operators.

You can apply the Hamiltonian operator to various eigenstates (see Chapter 2 for more on eigenstates),  $|\psi\rangle$ , of the harmonic oscillator to get the total energy,  $E$ , of those eigenstates:

$$H|\psi\rangle = \frac{P^2}{2m}|\psi\rangle + \frac{1}{2} m\omega^2 X^2|\psi\rangle = E|\psi\rangle$$

The problem now becomes one of finding the eigenstates and eigenvalues. However, this doesn't turn out to be an easy task. Unlike the potentials  $V(x)$  covered in Chapter 3,  $V(x)$  for a harmonic oscillator is more complex, depending as it does on  $x^2$ .

So you have to be clever. The way you solve harmonic oscillator problems in quantum physics is with operator algebra — that is, you introduce a new set of operators. And they're coming up now.

## Creation and Annihilation: Introducing the Harmonic Oscillator Operators



Creation and annihilation may sound like big make-or-break the universe kinds of ideas, but they play a starring role in the quantum world when you're working with harmonic oscillators. You use the creation and annihilation operators to solve harmonic oscillator problems because doing so is a clever way of handling the tougher Hamiltonian equation (see the preceding section). Here's what these two new operators do:

- ✓ **Creation operator:** The creation operator raises the energy level of an eigenstate by one level, so if the harmonic oscillator is in the fourth energy level, the creation operator raises it to the fifth level.
- ✓ **Annihilation operator:** The annihilation operator does the reverse, lowering eigenstates one level.

These operators make it easier to solve for the energy spectrum without a lot of work solving for the actual eigenstates. In other words, you can understand the whole energy spectrum by looking at the energy difference between eigenstates.

## Mind your $p$ 's and $q$ 's: Getting the energy state equations

Here's how people usually solve for the energy spectrum. First, you introduce two new operators,  $p$  and  $q$ , which are dimensionless; they relate to the  $P$  (momentum) and  $X$  (position) operators this way:

$$\begin{aligned} \checkmark \quad p &= P / (m\hbar\omega)^{1/2} \\ \checkmark \quad q &= X (m\omega/\hbar)^{1/2} \end{aligned}$$



You use these two new operators,  $p$  and  $q$ , as the basis of the annihilation operator,  $a$ , and the creation operator,  $a^\dagger$ :

$$\checkmark \quad a = \frac{1}{\sqrt{2}}(q + ip)$$

$$\checkmark \quad a^\dagger = \frac{1}{\sqrt{2}}(q - ip)$$

Now you can write the harmonic oscillator Hamiltonian like this, in terms of  $a$  and  $a^\dagger$ :

$$H = \hbar\omega \left( a^\dagger a + \frac{1}{2} \right)$$

As for creating new operators here, the quantum physicists went crazy, even giving a name to  $a^\dagger a$ : the  $N$  or *number operator*. So here's how you can write the Hamiltonian:

$$H = \hbar\omega \left( N + \frac{1}{2} \right)$$

The  $N$  operator returns the *number* of the energy level of the harmonic oscillator. If you denote the eigenstates of  $N$  as  $|n\rangle$ , you get this, where  $n$  is the number of the  $n$ th state:

$$N|n\rangle = n|n\rangle$$

Because  $H = \hbar\omega(N + 1/2)$ , and because  $H|n\rangle = E_n|n\rangle$ , then by comparing the previous two equations, you have

$$E_n = \left( n + \frac{1}{2} \right) \hbar\omega \quad n = 0, 1, 2, \dots$$

Amazingly, that gives you the energy eigenvalues of the  $n$ th state of a quantum mechanical harmonic oscillator. So here are the energy states:

$\checkmark$  The ground state energy corresponds to  $n = 0$ :

$$E_0 = \frac{1}{2} \hbar\omega$$

✓ The first excited state is

$$E_1 = \frac{3}{2}\hbar\omega$$

✓ The second excited state has an energy of

$$E_2 = \frac{5}{2}\hbar\omega$$

And so on. That is, the energy levels are discrete and *nondegenerate* (not shared by any two states). Thus, the energy spectrum is made up of equidistant bands.

## Finding the Eigenstates

When you have the eigenstates (see Chapter 2 to find out all about eigenstates), you can determine the allowable states of a system and the relative probability that the system will be in any of those states.

The commutator of operators A, B is  $[A, B] = AB - BA$ , so note that the commutator of  $a$  and  $a^\dagger$  is the following:

$$[a, a^\dagger] = \frac{1}{2}[q + ip, q - ip]$$

This is equal to the following:

$$[a, a^\dagger] = \frac{1}{2}[q + ip, q - ip] = -i[q, p]$$

This equation breaks down to  $[a, a^\dagger] = 1$ . And putting together this equation with  $H = \hbar\omega\left(N + \frac{1}{2}\right)$ , you get  $[a, H] = \hbar\omega a$  and  $[a^\dagger, H] = -\hbar\omega a^\dagger$ .

***Finding the energy of  $a|n\rangle$*** 

Okay, with the commutator relations, you're ready to go. The first question is if the energy of state  $|n\rangle$  is  $E_n$ , what is the energy of the state  $a|n\rangle$ ? Well, to find this rearrange the commutator  $[a, H] = \hbar\omega a$  to get  $Ha = aH - \hbar\omega a$ . Then use this to write the action of  $\hbar$  on  $a|n\rangle$  like this:

$$\begin{aligned} H(a|n\rangle) &= (aH - \hbar\omega a)|n\rangle \\ &= (E_n - \hbar\omega)(a|n\rangle) \end{aligned}$$

So  $a|n\rangle$  is also an eigenstate of the harmonic oscillator, with energy  $E_n - \hbar\omega$ , not  $E_n$ . That's why  $a$  is called the annihilation or lowering operator: It lowers the energy level of a harmonic oscillator eigenstate by one level.

***Finding the energy of  $a^\dagger|n\rangle$*** 

So what's the energy level of  $a^\dagger|n\rangle$ ? You can write that can like this:

$$\begin{aligned} H(a^\dagger|n\rangle) &= (a^\dagger H + \hbar\omega a^\dagger)|n\rangle \\ &= (E_n + \hbar\omega)(a^\dagger|n\rangle) \end{aligned}$$

All this means that  $a^\dagger|n\rangle$  is an eigenstate of the harmonic oscillator, with energy  $E_n + \hbar\omega$ , not just  $E_n$  — that is, the  $a^\dagger$  operator raises the energy level of an eigenstate of the harmonic oscillator by one level.

***Using  $a$  and  $a^\dagger$  directly***

If you've been following along from the preceding section, you know that  $H(a|n\rangle) = (E_n - \hbar\omega)(a|n\rangle)$  and  $H(a^\dagger|n\rangle) = (E_n + \hbar\omega)(a^\dagger|n\rangle)$ . You can derive the following from these equations:

$$\checkmark a|n\rangle = C|n-1\rangle$$

$$\checkmark a^\dagger|n\rangle = D|n+1\rangle$$

C and D are positive constants, but what do they equal? The states  $|n-1\rangle$  and  $|n+1\rangle$  have to be *normalized*, which means that  $\langle n-1|n-1\rangle = \langle n+1|n+1\rangle = 1$ . So take a look at the quantity using the C operator:

$$(\langle n|a^\dagger)(a|n\rangle) = C^2 \langle n-1|n-1\rangle$$

And because  $|n-1\rangle$  is normalized,  $\langle n-1|n-1\rangle = 1$ :

$$(\langle n|a^\dagger)(a|n\rangle) = C^2$$

$$\langle n|a^\dagger a|n\rangle = C^2$$

But you also know that  $a^\dagger a = N$ , the energy level operator, so you get the following equation:

$$\langle n|N|n\rangle = C^2$$

$N|n\rangle = n|n\rangle$ , where  $n$  is the energy level, so

$$n\langle n|n\rangle = C^2$$

However,  $\langle n|n\rangle = 1$ , so

$$n = C^2$$

$$n^{1/2} = C$$

This finally tells you, from  $a|n\rangle = C|n-1\rangle$ , that

$$a|n\rangle = n^{1/2} |n-1\rangle$$

That's cool — now you know how to use the lowering operator,  $a$ , on eigenstates of the harmonic oscillator.

What about the raising operator,  $a^\dagger$ ? First we rearrange the commutator  $[a^\dagger, H] = -\hbar\omega a^\dagger$ , to get

$$Ha^\dagger = a^\dagger H + \hbar\omega a$$

Then you follow the same course of reasoning you take with the  $a$  operator to show the following:

$$a^\dagger|n\rangle = (n+1)^{1/2} |n+1\rangle$$

So at this point, you know what the energy eigenvalues are and how the raising and lowering operators affect the harmonic oscillator eigenstates. You've made quite a lot of progress, using the  $a$  and  $a^\dagger$  operators instead of trying to solve the Schrödinger equation.

## *Finding the harmonic oscillator energy eigenstates*

The charm of using the operators  $a$  and  $a^\dagger$  is that given the ground state,  $|0\rangle$ , those operators let you find all successive energy states. If you want to find an excited state of a harmonic oscillator, you can start with the ground state,  $|0\rangle$ , and apply the raising operator,  $a^\dagger$ . For example, you can do this:

$$\checkmark \quad |1\rangle = a^\dagger |0\rangle = |1\rangle$$

$$\checkmark \quad |2\rangle = \frac{1}{\sqrt{2}} a^\dagger |1\rangle = \frac{1}{\sqrt{2!}} (a^\dagger)^2 |0\rangle$$

$$\checkmark \quad |3\rangle = \frac{1}{\sqrt{3}} a^\dagger |2\rangle = \frac{1}{\sqrt{3!}} (a^\dagger)^3 |0\rangle$$

$$\checkmark \quad |4\rangle = \frac{1}{\sqrt{4}} a^\dagger |3\rangle = \frac{1}{\sqrt{4!}} (a^\dagger)^4 |0\rangle$$

And so on. In general, you have this relation:

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle$$

### *Working in position space*

Okay,  $|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle$  is fine as far as it goes — but just what is  $|0\rangle$ ? Can't you get a spatial eigenstate of this eigenvector? Something like  $\psi_0(x)$ , not just  $|0\rangle$ ? Yes, you can. In other words, you want to find  $\langle x|0\rangle = \psi_0(x)$ . So you need the representations of  $a$  and  $a^\dagger$  in position space.

The  $p$  operator is defined as

$$p = \frac{P}{(\hbar\omega)^{1/2}}$$

Because  $P = -i\hbar \frac{d}{dx}$ , you can write

$$p = \frac{-i\hbar}{(m\hbar\omega)^{1/2}} \frac{d}{dx} = -i \left( \frac{\hbar}{m\omega} \right)^{1/2} \frac{d}{dx}$$

And writing  $x_0 = (\hbar/m\omega)^{1/2}$ , this becomes

$$p = \frac{-i\hbar}{(m\hbar\omega)^{1/2}} \frac{d}{dx} = -ix_0 \frac{d}{dx}$$

Okay, what about the  $a$  operator? You know that

$$a = \frac{1}{\sqrt{2}}(q + ip)$$

And that

$$q = X \left( \frac{m\omega}{\hbar} \right)^{1/2} = X/x_0$$

Therefore,

$$a = \frac{1}{\sqrt{2}} \left( \frac{X}{x_0} + x_0 \frac{d}{dx} \right)$$

You can also write this equation as

$$a = \frac{1}{x_0\sqrt{2}} \left( X + x_0^2 \frac{d}{dx} \right)$$

Okay, so that's  $a$  in the position representation. What's  $a^\dagger$ ? That turns out to be this:

$$a^\dagger = \frac{1}{x_0\sqrt{2}} \left( X - x_0^2 \frac{d}{dx} \right)$$

Now's the time to be clever. You want to solve for  $|0\rangle$  in the position space, or  $\langle x|0\rangle$ . Here's the clever part — when you use the lowering operator,  $a$ , on  $|0\rangle$ , you have to get 0 because there's no lower state than the ground state, so  $a|0\rangle = 0$ . And applying the  $\langle x|$  bra gives you  $\langle x|a|0\rangle = 0$ .

That's clever because it's going to give you a homogeneous differential equation (that is, one that equals zero). First, you substitute for  $a$ :

$$\langle x|a|0\rangle = 0$$

$$\frac{1}{x_0\sqrt{2}} \langle x| \left( X + x_0^2 \frac{d}{dx} \right) |0\rangle = 0$$

Then you use  $\langle x|0\rangle = \psi_0(x)$ :

$$\frac{1}{x_0\sqrt{2}} \left( X + x_0^2 \frac{d}{dx} \right) \psi_0(x) = 0$$

$$\frac{1}{x_0\sqrt{2}} \left( x\psi_0(x) + x_0^2 \frac{d\psi_0(x)}{dx} \right) = 0$$

Multiplying both sides by  $x_0\sqrt{2}$  gives you the following

$$x\psi_0(x) + x_0^2 \frac{d\psi_0(x)}{dx} = 0$$

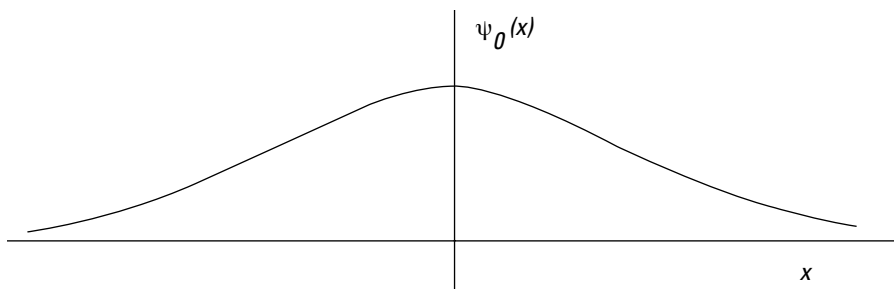
$$\frac{d\psi_0(x)}{dx} = \frac{-x\psi_0(x)}{x_0^2}$$

The solution to this compact differential equation is

$$\psi_0(x) = A \exp\left(-\frac{x^2}{2x_0^2}\right)$$

That's a gaussian function, so the ground state of a quantum mechanical harmonic oscillator is a gaussian curve, as you see in Figure 4-1.

**Figure 4-1:**  
The ground  
state of a  
quantum  
mechanical  
harmonic  
oscillator.



### *Finding the wave function of the ground state*

As a gaussian curve, the ground state of a quantum oscillator is  $\psi_0(x) = A \exp(-x^2/2x_0^2)$ . How can you figure out A? Wave functions must be normalized, so the following has to be true:

$$1 = \int_{-\infty}^{\infty} |\psi_0(x)|^2 dx$$

Substituting for  $\psi_0(x)$  gives you this next equation:

$$1 = \int_{-\infty}^{\infty} \left| A \exp\left(-x^2/2x_0^2\right) \right|^2 dx$$

$$1 = A^2 \int_{-\infty}^{\infty} \left( \exp\left(-x^2/2x_0^2\right) \right)^2 dx$$

You can evaluate this integral to be

$$1 = A^2 \int_{-\infty}^{\infty} \left( \exp\left(-x^2/2x_0^2\right) \right)^2 dx = A^2 \int_{-\infty}^{\infty} \exp\left(-x^2/x_0^2\right) dx = A^2 \pi^{1/2} x_0$$

Therefore,

$$1 = A^2 \pi^{1/2} x_0$$

$$A = \frac{1}{\pi^{1/4} x_0^{1/2}}$$



This means that the wave function for the ground state of a quantum mechanical harmonic oscillator is

$$\psi_0(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left(-x^2 / 2x_0^2\right)$$

Cool. Now you've got an exact wave function.

### ***A little excitement: Finding the first excited state***

Okay, the preceding section shows you what  $\psi_0(x)$  looks like. What about the first excited state,  $\psi_1(x)$ ? Well, as you know,  $\psi_1(x) = \langle x | 1 \rangle$  and  $|1\rangle = a^\dagger |0\rangle$ , so

$$\psi_1(x) = \langle x | a^\dagger | 0 \rangle$$

And you know that  $a^\dagger$  is the following:

$$a^\dagger = \frac{1}{x_0 \sqrt{2}} \left( X - x_0^2 \frac{d}{dx} \right)$$

Therefore,  $\psi_1(x) = \langle x | a^\dagger | 0 \rangle$  becomes

$$\begin{aligned} \langle x | a^\dagger | 0 \rangle &= \frac{1}{x_0 \sqrt{2}} \langle x | \left( X - x_0^2 \frac{d}{dx} \right) | 0 \rangle \\ &= \frac{1}{x_0 \sqrt{2}} \left( X - x_0^2 \frac{d}{dx} \right) \langle x | 0 \rangle \end{aligned}$$

And because  $\psi_0(x) = \langle x | 0 \rangle$ , you get the following equation:

$$\begin{aligned} \psi_1(x) &= \frac{1}{x_0 \sqrt{2}} X - x_0^2 \frac{d}{dx} \psi_0(x) \\ &= \frac{1}{x_0 \sqrt{2}} \left( x - x_0^2 \frac{(-x)}{x_0^2} \right) \psi_0(x) \\ &= \frac{\sqrt{2}}{x_0} x \psi_0(x) \end{aligned}$$

You also know the following:

$$\psi_0(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left(-x^2 / 2x_0^2\right)$$

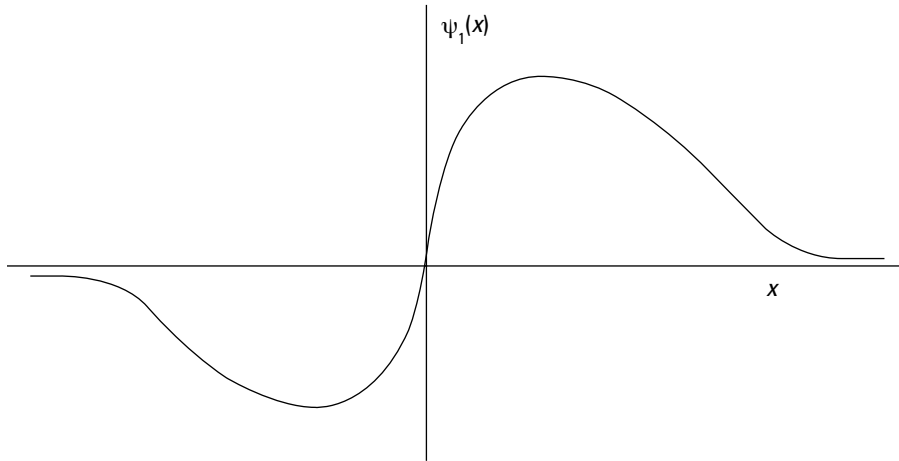
Therefore,  $\psi_1(x) = \frac{\sqrt{2}}{x_0} x \psi_0(x)$  becomes

$$\psi_1(x) = \frac{\sqrt{2}}{\pi^{1/4} x_0^{3/2}} x \exp\left(-x^2 / 2x_0^2\right)$$

What's  $\psi_1(x)$  look like? You can see a graph of  $\psi_1(x)$  in Figure 4-2, where it has one *node* (transition through the  $x$  axis).

**Figure 4-2:**

The first excited state of a quantum mechanical harmonic oscillator.



### ***Finding the second excited state***

All right, how about finding  $\psi_2(x)$  and so on? You can find  $\psi_2(x)$  from this equation:

$$\psi_2(x) = \frac{1}{\sqrt{2!}} \langle x | (a^\dagger)^2 | 0 \rangle$$

Substituting for  $a^\dagger$ , the equation becomes

$$\psi_2(x) = \frac{1}{\sqrt{2!}} \frac{1}{2x_0^2} \left( x - x_0^2 \frac{d}{dx} \right) \psi_0(x)$$

### Using hermite polynomials to find any excited state

You can generalize the differential equation for  $\psi_n(x)$  like this:

$$\psi_n(x) = \frac{1}{\pi^{1/4} (2^n n!)^{1/2}} \frac{1}{x_0^{n+1/2}} \left( x - x_0^2 \frac{d}{dx} \right)^n \exp\left(-x^2 / 2x_0^2\right)$$

To solve this general differential equation, you make use of the fact that

$$\left( x - x_0^2 \frac{d}{dx} \right)^n \exp\left(-x^2 / 2x_0^2\right) = \exp\left(-x^2 / 2x_0^2\right) H_n\left(x / x_0\right)$$

$H_n(x)$  is the  $n$ th *hermite polynomial*, which is defined this way:

$$H_n(x) = (-1)^n \exp(x^2) \frac{d^n}{dx^n} \exp(-x^2)$$

Holy mackerel! What do the hermite polynomials look like? Here's  $H_0(x)$ ,  $H_1(x)$ , and so on:

$$\checkmark H_0(x) = 1$$

$$\checkmark H_1(x) = 2x$$

$$\checkmark H_2(x) = 4x^2 - 2$$

$$\checkmark H_3(x) = 8x^3 - 12x$$

$$\checkmark H_4(x) = 16x^4 - 48x^2 + 12$$

$$\checkmark H_5(x) = 32x^5 - 160x^3 + 120x$$

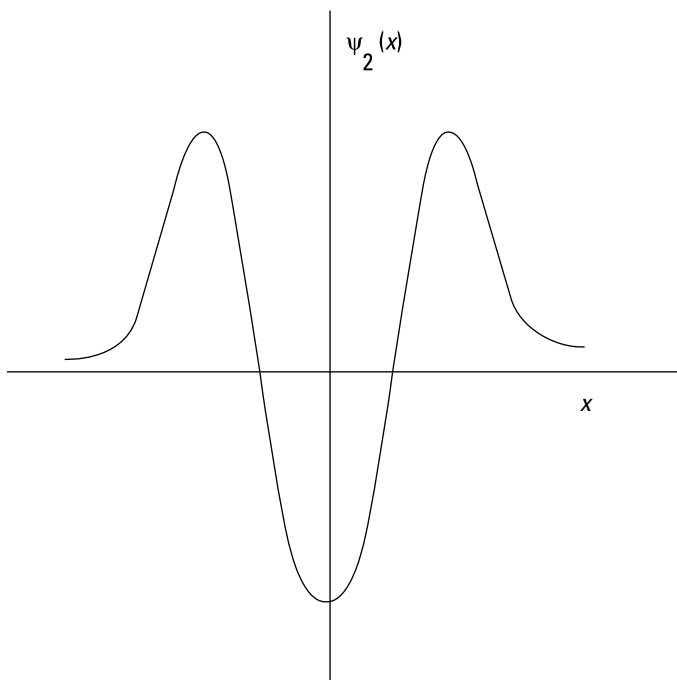
What does this buy you? You can express the wave functions for quantum mechanical harmonic oscillators like this, using the hermite polynomials  $H_n(x)$ :

$$\psi_n(x) = \frac{1}{\pi^{1/4} (2^n n! x_0)^{1/2}} H_n\left(x / x_0\right) \exp\left(-x^2 / 2x_0^2\right)$$

where  $x_0 = \left( \hbar / (m\omega) \right)^{1/2}$ .

And that's what the wave function looks like for a quantum mechanical harmonic oscillator. Who knew it would've involved hermite polynomials?

You can see what  $\psi_2(x)$  looks like in Figure 4-3; note that there are two nodes here — in general,  $\psi_n(x)$  for the harmonic oscillator will have  $n$  nodes.

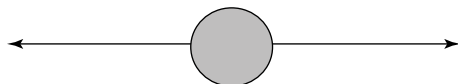


**Figure 4-3:**  
The second  
excited  
state of a  
quantum  
mechanical  
harmonic  
oscillator.

## Putting in some numbers

The preceding section gives you  $\psi_n(x)$ , and you've already solved for  $E_n$ , so you're on top of harmonic oscillators. Take a look at an example.

Say that you have a proton undergoing harmonic oscillation with  $\omega = 4.58 \times 10^{21} \text{ sec}^{-1}$ , as shown in Figure 4-4.



**Figure 4-4:**  
A proton  
undergoing  
harmonic  
oscillation.

What are the energies of the various energy levels of the proton? You know that in general,

$$E_n = \left( n + \frac{1}{2} \right) \hbar \omega \quad n = 0, 1, 2, \dots$$

So here are the energies of the proton, in megaelectron volts (MeV):

$$\checkmark E_0 = \frac{\hbar \omega}{2} = 1.51 \text{ MeV}$$

$$\checkmark E_1 = \frac{3\hbar \omega}{2} = 4.52 \text{ MeV}$$

$$\checkmark E_2 = \frac{5\hbar \omega}{2} = 7.54 \text{ MeV}$$

$$\checkmark E_3 = \frac{7\hbar \omega}{2} = 10.6 \text{ MeV}$$

And so on.

Now what about the wave functions? The general form of  $\psi_n(x)$  is

$$\psi_n(x) = \frac{1}{\pi^{1/4} (2^n n! x_0)^{1/2}} H_n \left( \frac{x}{x_0} \right) \exp \left( -\frac{x^2}{2x_0^2} \right)$$

where  $x_0 = \left( \frac{\hbar}{m\omega} \right)^{1/2}$ . So  $x_0 = 3.71 \times 10^{-15} \text{ m}$ .

Convert all length measurements into femtometers ( $1 \text{ fm} = 1 \times 10^{-15} \text{ m}$ ), giving you  $x_0 = 3.71 \text{ fm}$ . Here's  $\psi_0(x)$ , where  $x$  is measured in femtometers:

$$\psi_0(x) = \frac{1}{1.92\pi^{1/4}} \exp \left( -\frac{x^2}{27.5} \right)$$

Here are a couple more wave functions:

$$\checkmark \psi_1(x) = \frac{1}{2.72\pi^{1/4}} 2 \left( \frac{x}{3.71} \right) \exp \left( -\frac{x^2}{27.5} \right)$$

$$\checkmark \psi_2(x) = \frac{1}{5.45\pi^{1/4}} \left[ 4 \left( \frac{x}{3.71} \right)^2 - 2 \right] \exp \left( -\frac{x^2}{27.5} \right)$$

## *Looking at Harmonic Oscillator Operators as Matrices*

Because the harmonic oscillator has regularly spaced energy levels, people often view it in terms of matrices, which can make things simpler. For example, the following may be the ground state eigenvector (note that it's an infinite vector):

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

And this may be the first excited state:

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

And so on. The  $N$  operator, which just returns the energy level, would then look like this:

$$N = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 2 & 0 & \dots \\ 0 & 0 & 0 & 3 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

So  $N|2\rangle$  gives you

$$N|2\rangle = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 2 & 0 & \dots \\ 0 & 0 & 0 & 3 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

This is equal to

$$N|2\rangle = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 2 & 0 & \dots \\ 0 & 0 & 0 & 3 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} = 2 \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

In other words,  $N|2\rangle = 2|2\rangle$ .

How about the  $a$  (lowering) operator? That looks like this:

$$a = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$



In this representation, what is  $a|1\rangle$ ? In general,  $a|n\rangle = n^{1/2}|n-1\rangle$ , so  $a|1\rangle$  should equal  $|0\rangle$ . Take a look:

$$a|1\rangle = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

This matrix multiplication equals the following:

$$a|1\rangle = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

In other words,  $a|1\rangle = |0\rangle$ , just as expected.

So how about the  $a^\dagger$  (raising) operator? Here's how it works in general:  $a^\dagger|n\rangle = (n+1)^{1/2}|n+1\rangle$ . In matrix terms,  $a^\dagger$  looks like this:

$$a^\dagger = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{4} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

For example, you expect that  $a^\dagger|1\rangle = \sqrt{2}|2\rangle$ . Does it? The matrix multiplication is

$$a^\dagger|1\rangle = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{4} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

This equals the following:

$$a^\dagger |1\rangle = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{4} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \sqrt{2} \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

So  $a^\dagger |1\rangle = \sqrt{2} |2\rangle$ , as it should.

How about taking a look at the Hamiltonian, which returns the energy of an eigenstate,  $H|n\rangle = E_n|n\rangle$ ? In matrix form, the Hamiltonian looks like this:

$$H = \frac{\hbar\omega}{2} \begin{bmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 3 & 0 & 0 & \dots \\ 0 & 0 & 5 & 0 & \dots \\ 0 & 0 & 0 & 7 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

So if you prefer the matrix way of looking at things, that's how it works for the harmonic oscillator.

## A Jolt of Java: Using Code to Solve the Schrödinger Equation Numerically

Here's the one-dimensional Schrödinger equation:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

And for harmonic oscillators, you can write the equation like this, where

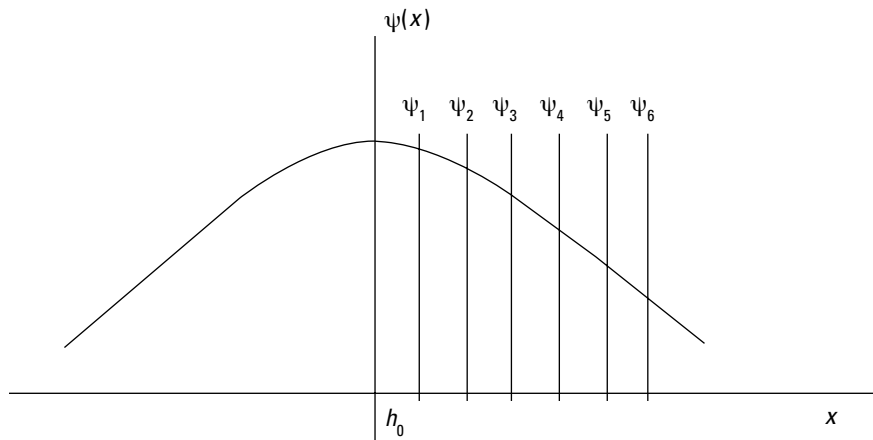
$$k^2(x) = 2m \left( \frac{E - V(x)}{\hbar^2} \right);$$

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

In general, as the potential  $V(x)$  gets more and more complex, using a computer to solve the Schrödinger equation begins to look more and more attractive. In this section, I show you how to do just that for the harmonic oscillator Schrödinger equation.

### Making your approximations

In computer terms, you can approximate  $\psi(x)$  as a collection of points,  $\psi_1, \psi_2, \psi_3, \psi_4, \psi_5$ , and so on, as you see in Figure 4-5.



**Figure 4-5:**  
Dividing  
 $\psi(x)$  along  
the  $x$  axis.

Each point along  $\psi(x)$  —  $\psi_1, \psi_2, \psi_3, \psi_4, \psi_5$ , and so on — is separated from its neighbor by a distance,  $h_0$ , along the  $x$  axis. And because  $d\psi/dx$  is the slope of  $\psi(x)$ , you can make the approximation that

$$\frac{d\psi}{dx} \approx \frac{\psi_{n+1} - \psi_n}{h_0}$$

In other words, the slope,  $d\psi/dx$ , is approximately equal to  $\Delta y/\Delta x$ , which is equal to  $\psi_{n+1} - \psi_n (= \Delta y)$  divided by  $h_0 (= \Delta x)$ .

You can rearrange the equation to this:

$$\psi_{n+1} \approx h_0 \frac{d\psi}{dx} + \psi_n$$

That's a crude approximation for  $\psi_{n+1}$ , given  $\psi_n$ . So, for example, if you know  $\psi_4$ , you can find the approximate value of  $\psi_5$ , if you know  $d\psi/dx$  in the region of  $\psi_4$ .

You can, of course, find better approximations for  $\psi_{n+1}$ . In particular, physicists often use the *Numerov algorithm* when solving the Schrödinger equation, and that algorithm gives you  $\psi_{n+1}$  in terms of  $\psi_n$  and  $\psi_{n-1}$ . Here's what the Numerov algorithm says:

$$\psi_{n+1} = \frac{2 \left( 1 - \left( \frac{5h_0^2 k_n^2(x)}{12} \right) \right) \psi_n - \left( 1 + \left( \frac{h_0^2 k_{n-1}^2(x)}{12} \right) \right) \psi_{n-1}}{1 + \frac{h_0^2 k_{n+1}^2(x)}{12}}$$

In this equation, for the harmonic oscillator,  $k_n^2(x) = \frac{2m}{\hbar^2} \left( E_n - \frac{m\omega^2 x^2}{2} \right)$

and the boundary conditions are  $\psi(-\infty) = \psi(\infty) = 0$ . Wow. Imagine having to calculate this by hand. Why not leave it up to the computer?

For a proton undergoing harmonic oscillation with  $\omega = 4.58 \times 10^{21} \text{ sec}^{-1}$ , the exact ground state energy is

$$E_0 = \frac{\hbar\omega}{2} = 1.51 \text{ MeV}$$

You solve this problem exactly earlier in this chapter. The following sections have you try to get this same result using the Numerov algorithm and a computer.

## Building the actual code

To calculate the ground state energy of the harmonic oscillator using the Numerov algorithm, this section uses the Java programming language, which you can get for free from `java.sun.com`.

Here's how you use the program: You choose a trial value of the energy for the ground state,  $E_0$ , and then calculate  $\psi(x)$  at  $\infty$ , which should be zero — and if it's not, you can adjust your guess for  $E_0$  and try again. You keep going until  $\psi(\infty) = 0$  (or if not actually 0, a very small number in computer terms) — and when it does, you know you've guessed the correct energy.

### Approximating $\psi(\infty)$

How do you calculate  $\psi(\infty)$ ? After all, infinity is a pretty big number, and the computer is going to have trouble with that. In practical terms, you have to use a number that approximates infinity. In this case, you can use the classical turning points of the proton — the points where all the proton's energy is potential energy and it has stopped moving in preparation for reversing its direction.

At the turning points,  $x_t$ ,  $E_0 = \frac{m\omega^2 x_t^2}{2}$  (that is, all the energy is in potential energy), so

$$x_t = \left( \frac{2E_0}{m\omega^2} \right)^{1/2}$$

And this is on the order of  $\pm 5$  femtometers (fm), so you assume that  $\psi(x)$  should surely be zero at, say,  $\pm 15$  fm. Here's the interval over which you calculate  $\psi(x)$ :

$$\checkmark x_{\min} = -15 \text{ fm}$$

$$\checkmark x_{\max} = 15 \text{ fm}$$

Divide this 30 fm interval into 200 segments, making the width of each segment,  $h_0$ , equal to  $(x_{\max} - x_{\min})/200 = h_0 = 0.15 \text{ fm}$ .

Okay, you're making progress. You'll start by assuming that  $\psi(x_{\min}) = 0$ , guess a value of  $E_0$ , and then calculate  $\psi(x_{\max}) = \psi_{200}$  (because there are 200 segments, at  $x = x_{\max}$ ,  $\psi_n = \psi_{200}$ ), which should equal zero when you get  $E_0$ .

Here's what the results tell you:

- ✓ **Correct:** If  $\text{abs}(\psi_{200})$  is zero, or in practical terms, less than, say, your maximum allowed value of  $\psi_{\text{max}} = 1 \times 10^{-8}$ , then you're done — the  $E_0$  you guessed was correct.
- ✓ **Too high:** If  $\text{abs}(\psi_{200})$  is larger than your maximum allowed  $\psi$ ,  $\psi_{\text{max}}$  ( $= 1 \times 10^{-8}$ ), and  $\psi_{200}$  is *positive*, the energy you chose for  $E_0$  was too high. You have to subtract a small amount of energy,  $\Delta E$  — say  $1 \times 10^{-7}$  MeV — from your guess for the energy; then calculate  $\text{abs}(\psi_{200})$  again and see whether it's still higher than your maximum allowed  $\psi$ ,  $\psi_{\text{max}}$ . If so, you have to repeat the process again.
- ✓ **Too low:** If  $\text{abs}(\psi_{200})$  is larger than your maximum allowed  $\psi$ ,  $\psi_{\text{max}}$  ( $= 1 \times 10^{-8}$ ), and  $\psi_{200}$  is *negative*, the energy you chose for  $E_0$  was too low. You have to add a small amount of energy,  $\Delta E$ , to your guess for the energy; then calculate  $\text{abs}(\psi_{200})$  again and see whether it's still higher than your maximum allowed  $\psi$ ,  $\psi_{\text{max}}$ . If so, you have to repeat the process.

So how do you calculate  $\psi_{200}$ ? Given two starting values,  $\psi_0$  and  $\psi_1$ , use the Numerov algorithm:

$$\psi_{n+1} = \frac{2 \left( 1 - \left( \frac{5h_0^2 k_n(x)^2}{12} \right) \right) \psi_n - \left( 1 + \left( \frac{h_0^2 k_{n-1}(x)^2}{12} \right) \right) \psi_{n-1}}{1 + \frac{h_0^2 k_{n+1}(x)^2}{12}}$$

Keep calculating successive points along  $\psi(x)$ :  $\psi_2$ ,  $\psi_3$ ,  $\psi_4$ , and so on. The last point is  $\psi_{200}$ .

Okay, you're on our way. You're going to start the code with the assumption that  $\psi_0 = 0$  and  $\psi_1$  is a very small number (you can choose any small number you like). Because you know that the exact ground level energy is actually 1.50 MeV, start the code with the guess that  $E_0 = 1.4900000$  MeV and let the computer calculate the actual value using increments of  $\Delta E = 1 \times 10^{-7}$  MeV.

Note also this equation depends on  $k_n(x)^2$ ,  $k_{n-1}(x)^2$ , and  $k_{n+1}(x)^2$ . Here's how you can find these values, where  $E_{\text{current}}$  is the current guess for the ground state energy (substitute  $n$ ,  $n-1$ , and  $n+1$  for  $j$ ):

$$k_j^2(x_j) = \frac{2m}{\hbar^2} \left( E_{\text{current}} - \frac{m\omega^2 x_j^2}{2} \right)$$

And you know that  $\omega = 4.58 \times 10^{21} \text{ sec}^{-1}$ , so

$$\checkmark \frac{m^2 \omega^2}{\hbar^2} = 5.63 \times 10^{-3} \text{ fm}^{-4}$$

$$\checkmark \frac{2m}{\hbar^2} = 0.05 \text{ MeV}^{-1} \text{ fm}^{-2}$$

Therefore,  $k_j^2(x_j) = 0.05E_{\text{current}} - 5.63 \times 10^{-3}x_j^2$ , where  $x_j$  for a particular segment  $j$  is  $x_j = jh_0 + x_{\text{min}}$ .

### Writing the code

Okay, now I'm going to put together all the info from the preceding section into some Java code. You start with a Java class, *se* (for Schrödinger Equation), in a file you name *se.java*:

```
public class se
{
    .
    .
    .
}
```

Then you set up the variables and constants you'll need, including an array for the values you calculate for  $\psi$  (because to find  $\psi_{n+1}$ , you'll have had to store the already-calculated values of  $\psi_n$  and  $\psi_{n-1}$ ):

```
public class se
{
    double psi[];
    double ECurrent;
    double Emin = 1.490;
    double xMin = -15.;
    double xMax = 15.;
    double hZero;
    double EDelta = 0.0000001;
    double maxPsi = 0.00000001;
    int numberDivisions = 200;
    .
    .
    .
}
```

The *se* class's constructor gets run first, so you initialize values there, including  $\psi_0$  ( $= \psi(x_{\text{min}}) = 0$ ) and  $\psi_1$  (any small number you want) to get the calculation going. In the main method, called *after the constructor*, you create an object of the *se* class and call it *calculate method* to get things started:



```

public class se
{
    double psi[];
    double ECurrent;
    double Emin = 1.490;
    double xMin = -15.;
    double xMax = 15.;
    double hZero;
    double EDelta = 0.00000001;
    double maxPsi = 0.00000001;
    int numberDivisions = 200;

    public se()
    {
        ECurrent = Emin;
        psi = new double[numberDivisions + 1];
        psi[0] = 0;
        psi[1] = -0.0000000001;
        psi[numberDivisions] = 1.0;
        hZero = (xMax - xMin) / numberDivisions;
    }

    public static void main(String [] argv)
    {
        se de = new se();
        de.calculate();
    }
    .
    .
    .
}

```

The real work takes place in the *calculate method*, where you use the current guess for the energy and calculate  $\psi_{200}$ :

- ✓ If  $\text{abs}(\psi_{200})$  is less than your maximum allowed value of  $\psi$ ,  $\psi_{\text{max}}$ , you've found the answer — your current guess for the energy is right on.
- ✓ If  $\text{abs}(\psi_{200})$  is greater than  $\psi_{\text{max}}$  and  $\psi_{200}$  is positive, you have to subtract  $\Delta E$  from your current guess for the energy and try again.
- ✓ If  $\text{abs}(\psi_{200})$  is greater than  $\psi_{\text{max}}$  and  $\psi_{200}$  is negative, you have to add  $\Delta E$  to your current guess for the energy and then try again.

Here's what all this looks like in code:

```
public void calculate()
{
    while(Math.abs(psi[numberDivisions])> maxPsi){
        for (int i = 1; i <numberDivisions; i++){
            psi[i + 1] = calculateNextPsi(i);
        }
        if (psi[numberDivisions]> 0.0) {
            ECurrent = ECurrent - EDelta;
        }
        else {
            ECurrent = ECurrent + EDelta;
        }
        System.out.println("Psi200: " + psi[numberDivisions]
            + " E: " + round(ECurrent));
    }
    System.out.println("\nThe ground state energy is " +
        round(ECurrent) + " MeV.");
}
```

Note that the next value of  $\psi$  (that is,  $\psi_{n+1}$ ) is calculated with a method named *calculateNextPsi*. Here's where you use the Numerov algorithm — given  $\psi_n$ ,  $\psi_{n-1}$ , you can calculate  $\psi_{n+1}$ :

```
public double calculateNextPsi(int n)
{
    double KSqNMinusOne = calculateKSquared(n - 1);
    double KSqN = calculateKSquared(n);
    double KSqNPlusOne = calculateKSquared(n + 1);
    double nextPsi = 2.0 * (1.0 - (5.0 * hZero * hZero *
        KSqN / 12.0)) * psi[n];
    nextPsi = nextPsi - (1.0 + (hZero * hZero *
        KSqNMinusOne / 12.0)) * psi[n - 1];
    nextPsi = nextPsi / (1.0 + (hZero * hZero * KSqNPlusOne
        / 12.0));
    return nextPsi;
}
```

Finally, note that to calculate  $\psi_{n+1}$ , you need  $k_n$ ,  $k_{n-1}$ , and  $k_{n+1}$ , which you find with a method named *calculateKSquared*, which uses the numeric values you've already figured out for this problem:

```
public double calculateKSquared(int n)
{
    double x = (hZero * n) + xMin;
    return (((0.05) * ECurrent) - ((x * x) * 5.63e-3));
}
```

Whew. Here's the whole program, *se.java*:

[illegible]

```

    }

    public double calculateKSquared(int n)
    {
        double x = (hZero * n) + xMin;
        return (((0.05) * ECurrent) - ((x * x) * 5.63e-3));
    }

    public double calculateNextPsi(int n)
    {
        double KSqNMinusOne = calculateKSquared(n - 1);
        double KSqN = calculateKSquared(n);
        double KSqNPlusOne = calculateKSquared(n + 1);
        double nextPsi = 2.0 * (1.0 - (5.0 * hZero * hZero *
            KSqN / 12.0)) * psi[n];
        nextPsi = nextPsi - (1.0 + (hZero * hZero *
            KSqNMinusOne / 12.0)) * psi[n - 1];
        nextPsi = nextPsi / (1.0 + (hZero * hZero * KSqNPlusOne
            / 12.0));
        return nextPsi;
    }

    public double round(double val)
    {
        double divider = 100000;
        val = val * divider;
        double temp = Math.round(val);
        return (double)temp / divider;
    }
}

```

Okay, now you can compile the code with `javac`, the Java compiler (if `javac` isn't in your computer's path, be sure to add the correct path to your command-line command, such as `C:>C:\java\bin\javac se.java`).

```
C:>javac se.java
```

This creates `se.class` from `se.java`, and you can run `se.class` with Java itself (adding the correct path if needed):

```
C:>java se
```

## *Running the code*

When you run the java code for the harmonic oscillator Schrödinger equation, it displays the successive values of  $\psi_{200}$  as it adjusts the current guess for the energy as it narrows in on the right answer — which it displays at the end of the run. Here's what you see:

```
C:>java se
PSI200: -1.0503644097337778E-4 E: 1.49
PSI200: -1.050354423295303E-4 E: 1.49
PSI200: -1.0503444368533108E-4 E: 1.49
PSI200: -1.0503344504260495E-4 E: 1.49
.
.
.
PSI200: -6.12820872814324E-8 E: 1.50066
PSI200: -6.031127521356655E-8 E: 1.50066
PSI200: -5.934046348307554E-8 E: 1.50066
PSI200: -5.836965180600015E-8 E: 1.50066
PSI200: -5.739883979461778E-8 E: 1.50066
PSI200: -5.6428029151212084E-8 E: 1.50066
PSI200: -5.5457218252899224E-8 E: 1.50066
PSI200: -5.4486408066519986E-8 E: 1.50066
PSI200: -5.351559702201636E-8 E: 1.50066
PSI200: -5.254478723976338E-8 E: 1.50066
PSI200: -5.157397714326237E-8 E: 1.50066
PSI200: -5.060316801012202E-8 E: 1.50066
PSI200: -4.963235841725704E-8 E: 1.50066
PSI200: -4.866154915227413E-8 E: 1.50066
PSI200: -4.7690740419271214E-8 E: 1.50066
PSI200: -4.6719932089691944E-8 E: 1.50066
PSI200: -4.574912368974434E-8 E: 1.50066
PSI200: -4.4778315322587505E-8 E: 1.50066
PSI200: -4.380750790476514E-8 E: 1.50066
PSI200: -4.28367005783992E-8 E: 1.50066
PSI200: -4.186589345217578E-8 E: 1.50066
PSI200: -4.0895085873184064E-8 E: 1.50066
PSI200: -3.992427935226201E-8 E: 1.50066
PSI200: -3.8953472673066213E-8 E: 1.50066
PSI200: -3.79826665057731E-8 E: 1.50066
PSI200: -3.701186038502826E-8 E: 1.50066
PSI200: -3.604105453620266E-8 E: 1.50066
PSI200: -3.507024949509914E-8 E: 1.50066
PSI200: -3.4099444217875174E-8 E: 1.50066
PSI200: -3.312863911389194E-8 E: 1.50066
PSI200: -3.2157834719961815E-8 E: 1.50066
PSI200: -3.1187030089902856E-8 E: 1.50066
PSI200: -3.021622619594536E-8 E: 1.50066
```

```
PSI200: -2.9245421985136167E-8 E: 1.50066
PSI200: -2.8274618172375295E-8 E: 1.50066
PSI200: -2.7303815344369703E-8 E: 1.50066
PSI200: -2.633301196069577E-8 E: 1.50066
PSI200: -2.5362208888510866E-8 E: 1.50066
PSI200: -2.439140632085814E-8 E: 1.50066
PSI200: -2.342060424823075E-8 E: 1.50066
PSI200: -2.244980221960756E-8 E: 1.50066
PSI200: -2.147900005347249E-8 E: 1.50067
PSI200: -2.0508198285622532E-8 E: 1.50067
PSI200: -1.9537397616823192E-8 E: 1.50067
PSI200: -1.8566596602866105E-8 E: 1.50067
PSI200: -1.7595795286272332E-8 E: 1.50067
PSI200: -1.6624994703779555E-8 E: 1.50067
PSI200: -1.565419461892862E-8 E: 1.50067
PSI200: -1.4683394780836424E-8 E: 1.50067
PSI200: -1.3712594592034165E-8 E: 1.50067
PSI200: -1.2741795159638587E-8 E: 1.50067
PSI200: -1.177099622966848E-8 E: 1.50067
PSI200: -1.0800197142733883E-8 E: 1.50067
PSI200: -9.82939798529632E-9 E: 1.50067
```

The ground state energy is 1.50067 MeV.

And there you have it — the program approximates the ground state energy as 1.50067 MeV, pretty darn close to the value you calculated theoretically in the earlier section “Making your approximations”: 1.50 MeV.

Very cool.