

# Quantum Mechanics II

# 6

## CHAPTER

*I think it is safe to say that no one understands quantum mechanics. Do not keep saying to yourself, if you can possibly avoid it, "But how can it be like that?" because you will get "down the drain" into a blind alley from which nobody has yet escaped. Nobody knows how it can be like that.*

**Richard Feynman**

*Those who are not shocked when they first come across quantum mechanics cannot possibly have understood it.*

**Niels Bohr**

As we discussed in Chapter 5, tremendous progress was made during the 1920s to correct the deficiencies of Bohr's atomic model. The origination of the quantum theory, also called **quantum mechanics**, is generally credited to Werner Heisenberg and Erwin Schrödinger, whose answers were clothed in very different mathematical formulations. Heisenberg (along with Max Born and Pascual Jordan) presented the *matrix formulation* of quantum mechanics in 1925 and 1926. The mathematical tools necessary to introduce matrix mechanics are not intrinsically difficult, but they would require too lengthy an exposition for us to study them here. The other solution, proposed in 1926 by Schrödinger, is called *wave mechanics*; its mathematical framework is similar to the classical wave descriptions we have already studied in elementary physics. Paul Dirac and Schrödinger himself (among others) later showed that the matrix and wave mechanics formulations give identical results and differ only in their mathematical form. We shall study only the wave theory of Schrödinger here.

In Chapter 5 we discussed the Copenhagen interpretation of quantum theory and the lack of universal agreement among physicists. Quantum theory is indeed a complex subject, and its probabilistic nature is contrary to the direct cause and effect seen in classical physics. We will do what thousands before us have done: "Shut up and calculate!"\* In this chapter we determine wave functions for some

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\*Many people credit this to Richard Feynman, but David Mermin (*Physics Today*, May 2004) says that this quote should not be attributed to Feynman. Certainly many students studying quantum physics have heard similar phrases uttered by their professors.



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**Erwin Schrödinger** (1887–1961) was an Austrian who worked at several European universities before fleeing Nazism in 1938 and accepting a position at the University of Dublin, where he remained until his retirement in 1956. His primary work on the wave equation was performed during the period he was in Zurich from 1920 to 1927. Schrödinger worked in many fields including philosophy, biology, history, literature, and language.

simple potentials and use these wave functions to predict the values of physical observables such as position and energy. We will see that particles are able to tunnel through potential barriers to exist in places that are not allowed by classical physics. Nuclear alpha decay and electronic tunnel diodes are examples of tunneling we will discuss.

## 6.1 The Schrödinger Wave Equation

The Austrian physicist Erwin Schrödinger (Nobel Prize, 1933) was presenting a seminar at the University of Zurich in November 1925 on de Broglie's wave theory for particles when Peter Debye suggested that there should be a wave equation. Within a few weeks Schrödinger had found a suitable wave equation based on what he knew about geometrical and wave optics.

In our previous study of elementary physics, we learned that Newton's laws, especially the second law of motion, govern the motion of particles. We need a similar set of equations to describe the wave motion of particles; that is, we need a **wave equation** that is dependent on the potential field (for example, the Coulomb or strong force field) that the particle experiences. We can then find the wave function  $\Psi$  (discussed in Chapter 5) that will allow us to calculate the probable values of the particle's position, energy, momentum, and so on.

We point out that although our procedure is similar to that followed in classical physics, we will no longer be able to calculate and specify the *exact* position, energy, and momentum simultaneously. Our calculations now must be consistent with the uncertainty principle and the notion of probability. It will take time and experience to get used to these new ideas (see the Feynman and Bohr quotes at the beginning of this chapter), and we will strive to give you that experience in this chapter.

There are several possible paths through which we could plausibly obtain the **Schrödinger wave equation**. Because none of the methods is actually a derivation, we prefer to present the equation and indicate its usefulness. Its ultimate correctness rests on its ability to explain and describe experimental results. The Schrödinger wave equation in its **time-dependent** form for a particle moving in a potential  $V$  in one dimension is

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V\Psi(x, t) \quad (6.1)$$

where  $i = \sqrt{-1}$  is an imaginary number and we have used partial derivatives. Both the potential  $V$  and wave function  $\Psi$  may be functions of space and time,  $V(x, t)$  and  $\Psi(x, t)$ .

The extension of Equation (6.1) into three dimensions is fairly straightforward.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V\Psi(x, y, z, t) \quad (6.2)$$

We will restrict ourselves to the one-dimensional form until Section 6.5.

Let's compare Equation (6.1) with the classical wave equation given by

$$\frac{\partial^2 \Psi(x, t)}{\partial x^2} - \frac{1}{v^2} \frac{\partial^2 \Psi(x, t)}{\partial t^2} \quad (6.3)$$

### Time-dependent Schrödinger wave equation

In Equation (6.3) the wave function may be as varied as the amplitude of a water wave, a guitar-string vibration, or even the electric field  $\vec{E}$  or magnetic field  $\vec{B}$ . Notice that the classical wave equation contains a second-order time derivative, whereas the Schrödinger wave equation contains only a first-order time derivative. This already gives us some idea that we are dealing with a somewhat different phenomenon.

Because the time-dependent Schrödinger Equation (6.1) is such a departure from our known physical laws, there is no derivation for it. We need *new* physical principles. Despite the fact that the Schrödinger wave equation has not been derived, it is still a useful tool because it describes experimental results. In science, and especially in physics, the test of a theoretical calculation is that it agrees with what we observe. In most of the remainder of this chapter, we apply the Schrödinger wave equation to several simple situations to illustrate its usefulness.



### EXAMPLE 6.1

The wave equation must be linear so that we can use the superposition principle to form wave packets using two or more waves. Prove that the wave function in Equation (6.1) is linear by showing that it is satisfied for the wave function

$$\Psi(x, t) = a\Psi_1(x, t) + b\Psi_2(x, t)$$

where  $a$  and  $b$  are constants, and  $\Psi_1$  and  $\Psi_2$  describe two waves each satisfying Equation (6.1).

**Strategy** We take the derivatives needed for Equation (6.1) and insert them in a straightforward manner. If Equation (6.1) is satisfied, then the wave equation is linear.

**Solution** We take each of the derivatives needed for Equation (6.1).

$$\begin{aligned}\frac{\partial \Psi}{\partial t} &= a \frac{\partial \Psi_1}{\partial t} + b \frac{\partial \Psi_2}{\partial t} \\ \frac{\partial \Psi}{\partial x} &= a \frac{\partial \Psi_1}{\partial x} + b \frac{\partial \Psi_2}{\partial x}\end{aligned}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = a \frac{\partial^2 \Psi_1}{\partial x^2} + b \frac{\partial^2 \Psi_2}{\partial x^2}$$

We insert these derivatives into Equation (6.1) to yield

$$\begin{aligned}i\hbar \left( a \frac{\partial \Psi_1}{\partial t} + b \frac{\partial \Psi_2}{\partial t} \right) &= -\frac{\hbar^2}{2m} \left( a \frac{\partial^2 \Psi_1}{\partial x^2} + b \frac{\partial^2 \Psi_2}{\partial x^2} \right) \\ &\quad + V(a\Psi_1 + b\Psi_2)\end{aligned}$$

Rearrangement of this equation gives

$$\begin{aligned}a \left( i\hbar \frac{\partial \Psi_1}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi_1}{\partial x^2} - V\Psi_1 \right) \\ + b \left( i\hbar \frac{\partial \Psi_2}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi_2}{\partial x^2} - V\Psi_2 \right) = 0\end{aligned}$$

Because  $\Psi_1$  and  $\Psi_2$  each satisfy Equation (6.1), the quantities in parentheses are identically zero, and therefore  $\Psi$  is also a solution.

In Section 5.4 we discussed wave motion and the formation of wave packets from waves. For a wave of wave number  $k$  and angular frequency  $\omega$  moving in the  $+x$  direction, the wave function is

$$\Psi(x, t) = A \sin(kx - \omega t + \phi) \quad (5.18)$$

Equation (5.18) is not the most general form of a wave function, which may include both sines and cosines. Our wave function is also not restricted to being real. Only the physically measurable quantities must be real, and Equation (6.1) already has an imaginary number. A more general form of wave function is

$$\Psi(x, t) = Ae^{i(kx - \omega t)} = A[\cos(kx - \omega t) + i \sin(kx - \omega t)] \quad (6.4)$$

which also describes a wave moving in the  $+x$  direction. In general the amplitude  $A$  may also be complex.



### EXAMPLE 6.2

Show that  $Ae^{i(kx-\omega t)}$  satisfies the time-dependent Schrödinger wave equation.

**Strategy** We take appropriate derivatives needed for Equation (6.1) and insert them into Equation (6.1) to see whether it is satisfied.

**Solution**

$$\frac{\partial \Psi}{\partial t} = -i\omega Ae^{i(kx-\omega t)} = -i\omega \Psi$$

$$\frac{\partial \Psi}{\partial x} = ik\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = i^2 k^2 \Psi = -k^2 \Psi$$

We insert these results into Equation (6.1) to yield

$$i\hbar \left( -i\omega \right) \Psi - \frac{\hbar^2}{2m} \left( -k^2 \right) \Psi + V\Psi = 0$$

$$\left( \hbar\omega - \frac{\hbar^2 k^2}{2m} - V \right) \Psi = 0$$

If we use  $E = \hbar\omega$  and  $p = \hbar k$ , we obtain

$$\left( E - \frac{p^2}{2m} - V \right) \Psi = 0$$

which is zero in our nonrelativistic formulation, because  $E = K + V = p^2/2m + V$ . Thus  $e^{i(kx-\omega t)}$  appears to be an acceptable solution at this point.

We showed in Example 6.2 that  $e^{i(kx-\omega t)}$  represents an acceptable solution to the Schrödinger wave equation. It is not true that all functions of  $\sin(kx - \omega t)$  and  $\cos(kx - \omega t)$  are solutions. We show this in the following example.



### EXAMPLE 6.3

Determine whether  $\Psi(x, t) = A \sin(kx - \omega t)$  is an acceptable solution to the time-dependent Schrödinger wave equation.

**Strategy** We again take the derivatives needed for Equation (6.1) and insert them into the equation to see whether it is satisfied.

**Solution**

$$\frac{\partial \Psi}{\partial t} = -\omega A \cos(kx - \omega t)$$

$$\frac{\partial \Psi}{\partial x} = kA \cos(kx - \omega t)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A \sin(kx - \omega t) = -k^2 \Psi$$

After we insert these relations into Equation (6.1), we have

$$-i\hbar\omega \cos(kx - \omega t) = \left( \frac{\hbar^2 k^2}{2m} + V \right) \Psi$$

$$= \left( \frac{\hbar^2 k^2}{2m} + V \right) A \sin(kx - \omega t) \quad (6.5)$$

(not true)

This equation is generally *not* satisfied for all  $x$  and  $t$ , and  $A \sin(kx - \omega t)$  is, therefore, not an acceptable wave function. This function is, however, a solution to the classical wave equation [Equation (6.3)].

## Normalization and Probability

We begin by reviewing the probability interpretation of the wave function that we discussed in Section 5.7. The probability  $P(x) dx$  of a particle being between  $x$  and  $x + dx$  was given in Equation (5.48).

$$P(x) dx = \Psi^*(x, t) \Psi(x, t) dx \quad (6.6)$$

The probability of the particle being between  $x_1$  and  $x_2$  is given by

$$P = \int_{x_1}^{x_2} \Psi^* \Psi dx \quad (6.7) \quad \text{Probability}$$

The wave function must also be normalized so that the probability of the particle being somewhere on the  $x$  axis is 1.

$$\int_{-\infty}^{\infty} \Psi^*(x, t) \Psi(x, t) dx = 1 \quad (6.8) \quad \text{Normalization}$$



### EXAMPLE 6.4

Consider a wave packet formed by using the wave function  $Ae^{-\alpha|x|}$ , where  $A$  is a constant to be determined by normalization. Normalize this wave function and find the probabilities of the particle being between 0 and  $1/\alpha$ , and between  $1/\alpha$  and  $2/\alpha$ .

**Strategy** This wave function is sketched in Figure 6.1. We will use Equation (6.8) to normalize  $\Psi$ . Then we will find the probability by using the limits in the integration of Equation (6.7).

**Solution** If we insert the wave function into Equation (6.8), we have

$$\int_{-\infty}^{\infty} A^2 e^{-2\alpha|x|} dx = 1$$

Because the wave function is symmetric about  $x = 0$ , we can integrate from 0 to  $\infty$ , multiply by 2, and drop the absolute value signs on  $|x|$ .

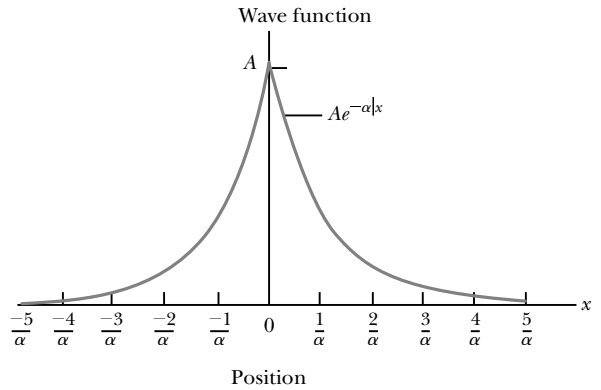
$$\begin{aligned} 2 \int_0^{\infty} A^2 e^{-2\alpha x} dx &= 1 = \frac{2A^2}{-2\alpha} e^{-2\alpha x} \Big|_0^{\infty} \\ 1 &= \frac{-A^2}{\alpha} (0 - 1) = \frac{A^2}{\alpha} \end{aligned}$$

The coefficient  $A = \sqrt{\alpha}$ , and the normalized wave function  $\Psi$  is

$$\Psi = \sqrt{\alpha} e^{-\alpha|x|}$$

We use Equation (6.7) to find the probability of the particle being between 0 and  $1/\alpha$ , where we again drop the absolute signs on  $|x|$  because  $x$  is positive.

$$P = \int_0^{1/\alpha} \alpha e^{-2\alpha x} dx$$



**Figure 6.1** The wave function  $Ae^{-\alpha|x|}$  is plotted as a function of  $x$ . Note that the wave function is symmetric about  $x = 0$ .

The integration is similar to the previous one.

$$P = \frac{\alpha}{-2\alpha} e^{-2\alpha x} \Big|_0^{1/\alpha} = -\frac{1}{2} (e^{-2} - 1) \approx 0.432$$

The probability of the particle being between  $1/\alpha$  and  $2/\alpha$  is

$$\begin{aligned} P &= \int_{1/\alpha}^{2/\alpha} \alpha e^{-2\alpha x} dx \\ P &= \frac{\alpha}{-2\alpha} e^{-2\alpha x} \Big|_{1/\alpha}^{2/\alpha} = -\frac{1}{2} (e^{-4} - e^{-2}) \approx 0.059 \end{aligned}$$

We conclude that the particle is much more likely to be between 0 and  $1/\alpha$  than between  $1/\alpha$  and  $2/\alpha$ . This is to be expected, given the shape of the wave function shown in Figure 6.1.

The wave function  $e^{i(kx-\omega t)}$  represents a particle under zero net force (constant  $V$ ) moving along the  $x$  axis. There is a problem with this wave function, because if we try to normalize it, we obtain an infinite result for the integral. This occurs because there is a finite probability for the particle to be anywhere along the  $x$  axis. Over the entire  $x$  axis, these finite probabilities add up, when integrated, to infinity. The only other possibility is a zero probability, but that is not an interesting physical result. Because this wave function has precise  $k$  and  $\omega$  values, it represents a particle having a definite energy and momentum. According to the uncertainty principle, because  $\Delta E = 0$  and  $\Delta p = 0$ , we must have  $\Delta t = \infty$  and  $\Delta x = \infty$ . We cannot know where the particle is at any time. We can still use such wave functions if we restrict the particle to certain positions in space, such as in a box or in an atom. We can also form wave packets from such functions in order to localize the particle.

### Properties of Valid Wave Functions

Besides the Schrödinger wave equation, there are certain properties (often called **boundary conditions**) that an acceptable wave function  $\Psi$  must also satisfy:

#### Boundary conditions

1. In order to avoid infinite probabilities,  $\Psi$  must be finite everywhere.
2. In order to avoid multiple values of the probability,  $\Psi$  must be single valued.
3. For finite potentials,  $\Psi$  and  $\partial\Psi/\partial x$  must be continuous. This is required because the second-order derivative term in the wave equation must be single valued. (There are exceptions to this rule when  $V$  is infinite.)
4. In order to normalize the wave functions,  $\Psi$  must approach zero as  $x$  approaches  $\pm\infty$ .

Solutions for  $\Psi$  that do not satisfy these properties do not generally correspond to physically realizable circumstances.

### Time-Independent Schrödinger Wave Equation

In many cases (and in most of the cases discussed here), the potential will not depend explicitly on time. The dependence on time and position can then be separated in the Schrödinger wave equation. Let

$$\Psi(x, t) = \psi(x)f(t) \quad (6.9)$$

We insert this  $\Psi(x, t)$  into Equation (6.1) and obtain

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

We divide by  $\psi(x)f(t)$  to yield

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} - \frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + V(x) \quad (6.10)$$

The left side of Equation (6.10) depends only on time, and the right side depends only on spatial coordinates. We have changed the partial derivatives to ordinary derivatives, because each side depends on only one variable. It follows that each side must be equal to a constant (which we label  $B$ ), because one variable may change independently of the other. We integrate the left side of Equation (6.10) in an effort to determine the value of  $B$ .

$$i\hbar \frac{1}{f} \frac{df}{dt} = B$$

$$i\hbar \int \frac{df}{f} = \int B dt$$

We integrate both sides and find

$$i\hbar \ln f = Bt + C$$

where  $C$  is an integration constant that we may choose to be 0. Therefore

$$\ln f = \frac{Bt}{i\hbar}$$

From this equation we determine  $f$  to be

$$f(t) = e^{Bt/i\hbar} = e^{-iEt/\hbar} \quad (6.11)$$

If we compare this function for  $f(t)$  to the free-particle wave function that has the time dependence  $e^{-i\omega t}$ , we see that  $B = \hbar\omega = E$ . This is a general result.

We now have, from the left and right sides of Equation (6.10),

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = E \quad (6.12)$$

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

**Time-independent  
Schrödinger wave equation**

Equation (6.13) is known as the **time-independent Schrödinger wave equation**, and it is a fundamental equation in quantum mechanics.

Equation (6.11) can be rewritten as

$$f(t) = e^{-i\omega t} \quad (6.14)$$

and the wave function  $\Psi(x, t)$  becomes

$$\Psi(x, t) = \psi(x)e^{-i\omega t} \quad (6.15)$$

We will restrict our attention for the present to time-independent potentials in one space dimension. Many important and useful results can be obtained from this nonrelativistic and one-dimensional form of quantum mechanics, because usually only the spatial part of the wave function  $\psi(x)$  is needed. Therefore, we need only use Equation (6.13), the time-independent form of the Schrödinger wave equation.

Let's examine the probability density  $\Psi^*\Psi$  discussed in Section 5.7. For the case of Equation (6.15), where the potential does not depend on time, we have

$$\Psi^*\Psi = \psi^2(x)(e^{i\omega t}e^{-i\omega t})$$

$$\Psi^*\Psi = \psi^2(x) \quad (6.16)$$

The probability distributions are constant in time. We have seen in introductory physics the phenomenon of *standing waves* (for example, oscillations of strings fixed at both ends). Such standing waves can be formed from traveling waves moving in opposite directions. In quantum mechanics, we say the system is in a **stationary state**.

**EXAMPLE 6.5**

Consider a metal in which there are free electrons, and the potential is zero. What mathematical form does the wave function  $\psi(x)$  take?

**Strategy** This is our first attempt to solve Equation (6.13), the time-independent Schrödinger wave equation. We let  $V(x) = 0$  in Equation (6.13) and try to solve the differential equation for  $\psi(x)$ .

**Solution** If we let  $V(x) = 0$  in Equation (6.13), we have

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

We drop the  $x$  dependence notation on  $\psi(x)$  and rewrite this equation as

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

We have seen the differential equation  $d^2\psi/dx^2 = -k^2\psi$  several times in calculus and in introductory physics. It occurs in small angle oscillations for pendula and in simple harmonic motion. If the energy  $E$  is positive, then  $k^2$  is real, and the wave function solution is sinusoidal [ $\psi(x) = A \sin kx + B \cos kx$ ]. However, for negative energy  $E$ , then  $k^2$  is negative, and  $k$  is imaginary. An exponential wave function [ $\psi(x) = Ce^{ikx}$ ] is appropriate.

**Comparison of Classical and Quantum Mechanics** We can gain insight by looking briefly at the similarities and differences between classical and quantum mechanics. Newton's second law ( $\vec{F} = d\vec{p}/dt$ ) and Schrödinger's wave equation are both differential equations. They are both postulated to explain certain observed behavior, and experiments show that they are successful. Newton's second law can be derived from the Schrödinger wave equation, so the latter is the more fundamental. Newton's laws may seem more fundamental—because they describe the precise values of the system's parameters, whereas the wave equation only produces wave functions that give probabilities—but by now we know from the uncertainty principle that it is not possible to know simultaneously precise values of both position and momentum and of both energy and time. Classical mechanics only appears to be more precise because it deals with macroscopic phenomena. The underlying uncertainties in macroscopic measurements are just too small to be significant.

An interesting parallel between classical mechanics and wave mechanics can be made by considering ray optics and wave optics. Throughout the 1700s, scientists argued about which of the optics formulations was the more fundamental; Newton favored ray optics. Finally, it was shown early in the 1800s that wave optics was needed to explain the observed phenomena of diffraction and interference. Ray optics is a good approximation as long as the wavelength of the radiation is much smaller than the dimensions of the apertures and obstacles it passes. Rays of light are characteristic of particle-like behavior. However, in order to describe interference phenomena, wave optics is required. Similarly for macroscopic objects, the de Broglie wavelength is so small that wave behavior is not apparent. However, advances in instrumentation and experimentation made it possible to observe behavior at the atomic level, and eventually the wave descriptions and quantum mechanics were required to understand all the data. Classical mechanics is a good macroscopic approximation and is accurate enough in the limit of large quantum numbers, but as far as we know now, there is only one correct theory, and that is quantum mechanics.



## 6.2 Expectation Values

In order to be useful, the wave equation formalism must be able to determine values of measurable quantities, including position, momentum, and energy. In this section we will discuss how the wave function is able to provide this information. We will do this here in only one dimension, but the discussion can be extended to three dimensions. We will also evaluate the values of the physical quantities for a given time  $t$ , because in general the whole system, including the values of the physical quantities, evolves with time.

Consider a measurement of the position  $x$  of a particular system (for example, the position of a particle in a box—see Section 5.8). If we make three measurements of the position, we are likely to obtain three different results. Nevertheless, if our method of measurement is inherently accurate, then there is some physical significance to the average of our measured values of  $x$ . Moreover, the precision of our result improves as more measurements are made. In quantum mechanics we use wave functions to calculate the expected result of the average of many measurements of a given quantity. We call this result the **expectation value**; the expectation value of  $x$  is denoted by  $\langle x \rangle$ . Any measurable quantity for which we can calculate the expectation value is called a **physical observable**. The expectation values of physical observables (for example, position, linear momentum, angular momentum, and energy) must be real, because the experimental results of measurements are real.

Expectation value

Physical observables

Let's first review the method of determining average values. Consider a particle that is constrained to move along the  $x$  axis. If we make many measurements of the particle, we may find the particle  $N_1$  times at  $x_1$ ,  $N_2$  times at  $x_2$ ,  $N_i$  times at  $x_i$ , and so forth. The average value of  $x$ , denoted by  $\bar{x}$  [or  $(x)_{av}$ ], is then

$$\bar{x} = \frac{N_1 x_1 + N_2 x_2 + N_3 x_3 + N_4 x_4 + \cdots}{N_1 + N_2 + N_3 + N_4 + \cdots} = \frac{\sum_i N_i x_i}{\sum_i N_i}$$

We can change from discrete to continuous variables by using the probability  $P(x, t)$  of observing the particle at a particular  $x$ . The previous equation then becomes

$$\bar{x} = \frac{\int_{-\infty}^{\infty} x P(x) dx}{\int_{-\infty}^{\infty} P(x) dx} \quad (6.17)$$

In quantum mechanics we must use the probability distribution given in Equation (6.6),  $P(x) dx = \Psi^*(x, t) \Psi(x, t) dx$ , to determine the average or expectation value. The procedure for finding the expectation value  $\langle x \rangle$  is similar to that followed in Equation (6.17):

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x \Psi^*(x, t) \Psi(x, t) dx}{\int_{-\infty}^{\infty} \Psi^*(x, t) \Psi(x, t) dx} \quad (6.18)$$

The denominator of Equation (6.18) is the normalization equation, previously shown as Equation (6.8). If the wave function is normalized, the denominator becomes 1. The expectation value is then given by

$$\langle x \rangle = \int_{-\infty}^{\infty} x \Psi^*(x, t) \Psi(x, t) dx \quad (6.19)$$

If the wave function has not been normalized, then Equation (6.18) should be used.

The same general procedure can be used to find the expectation value of any function  $g(x)$  for a normalized wave function  $\Psi(x, t)$ .

$$\langle g(x) \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) g(x) \Psi(x, t) dx \quad (6.20)$$

We emphasize again that the wave function can provide only the expectation value of a given function  $g(x)$  that can be written as a function of  $x$ . It cannot give us the value of each individual measurement. When we say the wave function provides a complete description of the system, we mean that the expectation values of the physical observables can be determined.

Any knowledge we might have of the simultaneous values of the position  $x$  and momentum  $p$  must be consistent with the uncertainty principle. To find the expectation value of  $p$ , we first need to represent  $p$  in terms of  $x$  and  $t$ . As an example, let's consider once more the wave function of the free particle,  $\Psi(x, t) = e^{i(kx - \omega t)}$ . If we take the derivative of  $\Psi(x, t)$  with respect to  $x$ , we have

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x} [e^{i(kx - \omega t)}] = i k e^{i(kx - \omega t)} = i k \Psi$$

But because  $k = p/\hbar$ , this becomes

$$\frac{\partial \Psi}{\partial x} = i \frac{p}{\hbar} \Psi$$

After rearrangement, this yields

$$p[\Psi(x, t)] = -i\hbar \frac{\partial \Psi(x, t)}{\partial x}$$

**Operators** An **operator** is a mathematical operation that transforms one function into another. For example, an operator, denoted by  $\hat{Q}$ , transforms the function  $f(x)$  by  $\hat{Q}f(x) = g(x)$ . In the previous wave function equation, the quantity  $-i\hbar(\partial/\partial x)$  is operating on the function  $\Psi(x, t)$  and is called the *momentum operator*  $\hat{p}$ , where the  $\hat{\phantom{p}}$  sign over the letter  $p$  indicates an operator.

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \quad (6.21)$$

The existence of the momentum operator is not unique. Each of the physical observables has an associated operator that is used to find that observable's expectation value. In order to compute the expectation value of some physical observable  $Q$ , the operator  $\hat{Q}$  must be placed between  $\Psi^*$  and  $\Psi$  so that it *operates* on  $\Psi(x, t)$  in the order shown:

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{Q} \Psi(x, t) dx \quad (6.22)$$

Thus, the expectation value of the momentum becomes

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial x} dx \quad (6.23)$$

The position  $x$  is its own operator. Operators for observables that are functions of both  $x$  and  $p$  can be constructed from  $x$  and  $\hat{p}$ .

Now let's take the time derivative of the free-particle wave function.

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t} [e^{i(kx - \omega t)}] = -i\omega e^{i(kx - \omega t)} = -i\omega \Psi$$

We substitute  $\omega = E/\hbar$ , and then rearrange to find

$$E[\Psi(x, t)] = i\hbar \frac{\partial \Psi(x, t)}{\partial t} \quad (6.24)$$

We call the quantity operating on  $\Psi(x, t)$  the *energy operator*.

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \quad (6.25)$$

It is used to find the expectation value  $\langle E \rangle$  of the energy.

$$\langle E \rangle = i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial t} dx \quad (6.26)$$

Although we have found the momentum and energy operators for only the free-particle wave functions, they are general results. We shall have occasion later to use these operators to determine the physical observables (position, momentum, and energy, for example) and compare with experimental results.



## EXAMPLE 6.6

Use the momentum and energy operators with the conservation of energy to produce the Schrödinger wave equation.

**Strategy** We first find the energy  $E$  as the sum of the kinetic and potential energies. Our treatment is entirely non-relativistic. We want to use the operator functions, so we write the kinetic energy in terms of momentum.

**Solution** The energy is

$$E = K + V = \frac{p^2}{2m} + V \quad (6.27)$$

We allow the operators of both sides of this equation to act on the wave function. The left side gives

$$\hat{E}\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (6.28)$$

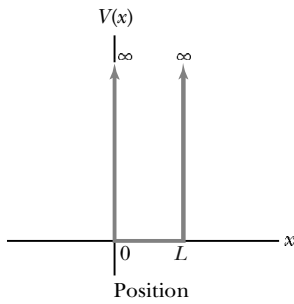
The application of the operators on the right side of Equation (6.27) on  $\Psi$  gives

$$\begin{aligned} \left[ \frac{1}{2m} (\hat{p})^2 + V \right] \Psi &= \frac{1}{2m} \left( -i\hbar \frac{\partial}{\partial x} \right)^2 \Psi + V\Psi \\ &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \end{aligned}$$

Notice that the operator  $(\hat{p})^2$  implies two successive applications of the  $\hat{p}$  operator, not the algebraic square of one  $\hat{p}$  operator. Now we set the previous equation equal to Equation (6.28) and obtain

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad (6.29)$$

which is the time-dependent Schrödinger wave equation, Equation (6.1). It should be noted that this example is not a determination of the Schrödinger wave equation, but rather a verification of the consistency of the definitions.



**Figure 6.2** Infinite square-well potential. The potential is  $V = \infty$  everywhere except the region  $0 < x < L$ , where  $V = 0$ .

## 6.3 Infinite Square-Well Potential

We have thus far established the time-independent Schrödinger wave equation and have discussed how the wave functions can be used to determine the physical observables. Now we would like to find the wave function for several possible potentials and see what we can learn about the behavior of a system having those potentials. In the process of doing this we will find that some observables, including energy, have quantized values. We begin by exploring the simplest such system—that of a particle trapped in a box with infinitely hard walls that the particle cannot penetrate. This is the same physical system as the particle in a box we presented in Section 5.8, but now we present the full quantum-mechanical solution.

The potential, called an *infinite square well*, is shown in Figure 6.2 and is given by

$$V(x) = \begin{cases} \infty & x < 0, x > L \\ 0 & 0 < x < L \end{cases} \quad (6.30)$$

The particle is constrained to move only between  $x = 0$  and  $x = L$ , where the particle experiences no forces. Although the infinite square-well potential is simple, we will see that it is useful because many physical situations can be approximated by it. We will also see that requiring the wave function to satisfy certain boundary conditions leads to energy quantization. We will use this fact to explore energy levels of simple atomic and nuclear systems.

As we stated previously, most of the situations we encounter allow us to use the time-independent Schrödinger wave equation. Such is the case here. If we insert  $V = \infty$  in Equation (6.13), we see that the only possible solution for the wave function is  $\psi(x) = 0$ . Therefore, there is zero probability for the particle to be located at  $x < 0$  or  $x > L$ . Because the kinetic energy of the particle must be finite, the particle can never penetrate into the region of infinite potential. However, when  $V = 0$ , Equation (6.13) becomes, after rearranging,

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

where we have used Equation (6.13) with  $V = 0$  and let the wave number  $k = \sqrt{2mE/\hbar^2}$ . A suitable solution to this equation that satisfies the properties given in Section 6.1 is

$$\psi(x) = A \sin kx + B \cos kx \quad (6.31)$$

where  $A$  and  $B$  are constants used to normalize the wave function. The wave function must be continuous, which means that  $\psi(x) = 0$  at both  $x = 0$  and  $x = L$  as already discussed. The proposed solution in Equation (6.31) therefore must have  $B = 0$  in order to have  $\psi(x = 0) = 0$ . If  $\psi(x = L) = 0$ , then  $A \sin(kL) = 0$ , and because  $A = 0$  leads to a trivial solution, we must have

$$kL = n\pi \quad (6.32)$$

where  $n$  is a positive integer. The value  $n = 0$  leads to  $\psi = 0$ , a physically uninteresting solution, and negative values of  $n$  do not give different physical solutions than the positive values. The wave function is now

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right) \quad (n = 1, 2, 3, \dots) \quad (6.33)$$

The property that  $d\psi/dx$  must be continuous is not satisfied in this case, because of the infinite step value of the potential at  $x = 0$  and  $x = L$ , but we were warned of this particular situation in Section 6.1, and it creates no problem. We normalize our wave function over the total distance  $-\infty < x < \infty$ .

$$\int_{-\infty}^{\infty} \psi_n^*(x) \psi_n(x) dx = 1$$

Substitution of the wave function yields

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

This is a straightforward integral (with the help of integral tables, see Appendix 3) and gives  $L/2$ , so that  $A^2(L/2) = 1$  and  $A = \sqrt{2/L}$ .

The normalized wave function becomes

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (n = 1, 2, 3, \dots) \quad (6.34)$$

These wave functions are identical to the ones obtained for a vibrating string with its ends fixed that are studied in elementary physics. The application of the boundary conditions here corresponds to fitting standing waves into the box. It is not a surprise to obtain standing waves in this case, because we are considering time-independent solutions. Because  $k_n = n\pi/L$  from Equation (6.32), we have

$$k_n = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}}$$

Notice the subscript  $n$  on  $k_n$  and  $E_n$  denoting that they depend on the integer  $n$  and have multiple values. This equation is solved for  $E_n$  to yield

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \quad (n = 1, 2, 3, \dots) \quad (6.35) \quad \text{Quantized energy levels}$$

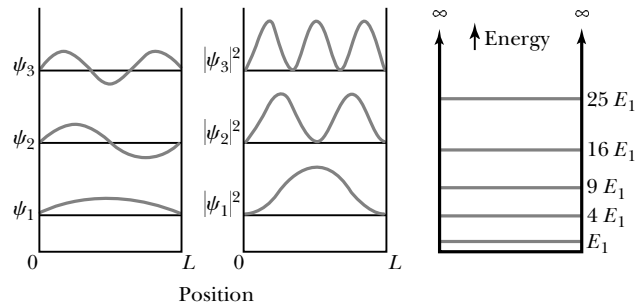
The possible energies  $E_n$  of the particle are quantized, and the integer  $n$  is a quantum number. Notice that the results for the quantized energy levels in Equation (6.35) are identical to those obtained in Equation (5.51) of Section 5.8, when we treated a particle in a one-dimensional box as a wave. The quantization of the energy occurs in a natural way from the application of the boundary conditions (standing waves) to possible solutions of the wave equation. Each wave function  $\psi_n(x)$  has associated with it a unique energy  $E_n$ . In Figure 6.3 (page 214) we show the wave function  $\psi_n$ , probability density  $|\psi_n|^2$ , and energy  $E_n$  for the lowest three values of  $n$  (1, 2, 3).

The lowest energy level given by  $n = 1$  is called the *ground state*, and its energy is given by

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

Note that the lowest energy cannot be zero because we have ruled out the possibility of  $n = 0$  ( $\psi_0 = 0$ ). Classically, the particle can have zero or any positive energy. If we calculate  $E_n$  for a macroscopic object in a box (for example, a tennis ball in a tennis court), we will obtain a very small number for  $E_1$ . Adjacent

**Figure 6.3** Wave functions  $\psi_n$ , probability densities  $|\psi_n|^2$ , and energy levels  $E_n$  for the lowest quantum numbers for the infinite square-well potential.



energy levels would be so close together that we could not measure their differences. Macroscopic objects must have very large values of  $n$ .

Classically, the particle has equal probability of being anywhere inside the box. The classical probability density (see Section 6.2) is  $P(x) = 1/L$  (for  $0 < x < L$ , zero elsewhere) for the probability to be 1 for the particle to be in the box. According to Bohr's correspondence principle (see Section 4.4), we should obtain the same probability in the region where the classical and quantum results should agree, that is, for large  $n$ . The quantum probability density is  $(2/L)\sin^2(k_n x)$ . For large values of  $n$ , there will be many oscillations within the box. The average value of  $\sin^2 \theta$  over one complete cycle is  $1/2$ . The average value of  $\sin^2 \theta$  over many oscillations is also  $1/2$ . Therefore, the quantum probability approaches  $1/L$  in this limit, in agreement with the classical result.

### EXAMPLE 6.7

Show that the wave function  $\Psi_n(x, t)$  for a particle in an infinite square well corresponds to a standing wave in the box.

**Strategy** We have just found the wave function  $\psi_n(x)$  in Equation (6.34). According to Equation (6.14), we can obtain  $\Psi_n(x, t)$  by multiplying the wave function  $\psi_n(x)$  by  $e^{-i\omega_n t}$ .

**Solution** The product of  $\psi_n(x)$  from Equation (6.34) and  $f(t) = e^{-i\omega_n t}$  gives

$$\Psi_n(x, t) = \sqrt{\frac{2}{L}} \sin(k_n x) e^{-i\omega_n t}$$

We can write  $\sin(k_n x)$  as

$$\sin(k_n x) = \frac{e^{ik_n x} - e^{-ik_n x}}{2i}$$

so that the wave function\* becomes

$$\Psi_n(x, t) = \sqrt{\frac{2}{L}} \frac{e^{i(k_n x - \omega_n t)} - e^{-i(k_n x + \omega_n t)}}{2i}$$

This is the equation of a standing wave for a vibrating string, for example. It is the superposition of a wave traveling to the right with a wave traveling to the left. They interfere to produce a standing wave of angular frequency  $\omega_n$ .

\*The imaginary number  $i$  should be of no concern, because the probability values are determined by a product of  $\psi^* \psi$ , which gives a real number.



### EXAMPLE 6.8

Determine the expectation values for  $x$ ,  $x^2$ ,  $p$ , and  $p^2$  of a particle in an infinite square well for the first excited state.

**Strategy** The first excited state corresponds to  $n = 2$ , because  $n = 1$  corresponds to the lowest energy state or the ground state. Equation (6.34) gives us the wave function that we need to find the expectation values given in Section 6.2.

**Solution** The wave function for this case, according to Equation (6.34), is

$$\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

The expectation value  $\langle x \rangle_{n=2}$  is

$$\langle x \rangle_{n=2} = \frac{2}{L} \int_0^L x \sin^2\left(\frac{2\pi x}{L}\right) dx = \frac{L}{2}$$

We evaluate all these integrations by looking up the integral in Appendix 3. As we expect, the average position of the particle is in the middle of the box ( $x = L/2$ ), even though the actual probability of the particle being there is zero (see  $|\psi|^2$  in Figure 6.3).

The expectation value  $\langle x^2 \rangle_{n=2}$  of the square of the position is given by

$$\langle x^2 \rangle_{n=2} = \frac{2}{L} \int_0^L x^2 \sin^2\left(\frac{2\pi x}{L}\right) dx = 0.32L^2$$

The value of  $\sqrt{\langle x^2 \rangle_{n=2}}$  is  $0.57L$ , larger than  $\langle x \rangle_{n=2} = 0.5L$ . Does this seem reasonable? (*Hint:* look again at the shape of the wave function in Figure 6.3.)

The expectation value  $\langle p \rangle_{n=2}$  is determined by using Equation (6.23).

$$\langle p \rangle_{n=2} = (-i\hbar) \frac{2}{L} \int_0^L \sin\left(\frac{2\pi x}{L}\right) \left[ \frac{d}{dx} \sin\left(\frac{2\pi x}{L}\right) \right] dx$$

which reduces to

$$\langle p \rangle_{n=2} = -\frac{4i\hbar}{L^2} \int_0^L \sin\left(\frac{2\pi x}{L}\right) \cos\left(\frac{2\pi x}{L}\right) dx = 0$$

Because the particle is moving left as often as right in the box, the average momentum is zero.

The expectation value  $\langle p^2 \rangle_{n=2}$  is given by

$$\begin{aligned} \langle p^2 \rangle_{n=2} &= \frac{2}{L} \int_0^L \sin\left(\frac{2\pi x}{L}\right) \left( -i\hbar \frac{d}{dx} \right) \left( -i\hbar \frac{d}{dx} \right) \sin\left(\frac{2\pi x}{L}\right) dx \\ &= (-i\hbar)^2 \frac{2}{L} \int_0^L \sin\left(\frac{2\pi x}{L}\right) \left( \frac{2\pi}{L} \frac{d}{dx} \right) \cos\left(\frac{2\pi x}{L}\right) dx \\ &= -(\hbar^2) \frac{8\pi^2}{L^3} \int_0^L \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi x}{L}\right) dx \\ &= \frac{4\pi^2 \hbar^2}{L^2} \end{aligned}$$

This value can be compared with  $E_2$  [Equation (6.35)]:

$$E_2 = \frac{4\pi^2 \hbar^2}{2mL^2} = \frac{\langle p^2 \rangle_{n=2}}{2m}$$

which is correct, because nonrelativistically we have  $E = p^2/2m + V$  and  $V = 0$ .



### EXAMPLE 6.9

A typical diameter of a nucleus is about  $10^{-14}$  m. Use the infinite square-well potential to calculate the transition energy from the first excited state to the ground state for a proton confined to the nucleus. Of course, this is only a rough calculation for a proton in a nucleus.

**Strategy** To find the transition energy between the ground and first excited energy states, we use Equation (6.35) to find  $E_1$  and  $E_2$ .

**Solution** The energy of the ground state, from Equation (6.35), is

$$\begin{aligned} E_1 &= \frac{\pi^2 \hbar^2 c^2}{2mc^2 L^2} = \frac{1}{mc^2} \frac{\pi^2 (197.3 \text{ eV} \cdot \text{nm})^2}{2(10^{-5} \text{ nm})^2} \\ &= \frac{1}{mc^2} (1.92 \times 10^{15} \text{ eV}^2) \end{aligned}$$

The mass of the proton is  $938.3 \text{ MeV}/c^2$ , which gives

$$E_1 = \frac{1.92 \times 10^{15} \text{ eV}^2}{938.3 \times 10^6 \text{ eV}} = 2.0 \text{ MeV}$$

The first excited state energy is found [again from Equation (6.35)] to be  $E_2 = 4E_1 = 8 \text{ MeV}$ , and the transition energy is  $\Delta E = E_2 - E_1 = 6 \text{ MeV}$ . This is a reasonable value for protons in the nucleus.

If we had done a calculation, similar to that in the previous example, for an electron in the nucleus, we would find energies on the order of  $10^4$  MeV, much larger than the rest energy of the electron. A correct relativistic treatment is necessary, and it would give electron energies significantly less than  $10^4$  MeV but still much larger than those of electrons actually observed being emitted from the nucleus in  $\beta$  decay. Such reasoning indicates that electrons do not exist inside the nucleus.

## 6.4 Finite Square-Well Potential

We gained some experience in the last section in dealing with the time-independent Schrödinger wave equation. Now we want to look at a more realistic potential—one that is not infinite. The finite square-well potential is similar to the infinite one, but we let the potential be  $V_0$  rather than infinite in the region  $x < 0$  and  $x > L$ .

$$V(x) = \begin{cases} V_0 & x \leq 0 & \text{region I} \\ 0 & 0 < x < L & \text{region II} \\ V_0 & x \geq L & \text{region III} \end{cases} \quad (6.36)$$

The three regions of the potential are shown in Figure 6.4. We will consider a particle of energy  $E < V_0$  that classically is bound inside the well. We will find that quantum mechanics *allows the particle to be outside the well*. We set the potential  $V = V_0$  in the time-independent Schrödinger Equation (6.13) for regions I and III outside the square well. This gives

$$-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2\psi}{dx^2} = E - V_0 \quad \text{regions I, III} \quad (6.37)$$

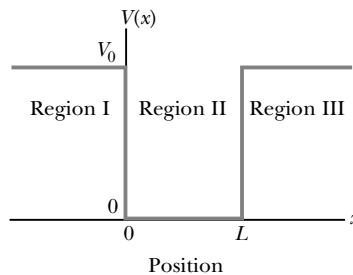
We rewrite this using  $\alpha^2 = 2m(V_0 - E)/\hbar^2$ , a positive constant.

$$\frac{d^2\psi}{dx^2} = \alpha^2\psi$$

The solution to this differential equation has exponentials of the form  $e^{\alpha x}$  and  $e^{-\alpha x}$ . In the region  $x > L$ , we can reject the positive exponential term, because it would become infinite as  $x \rightarrow \infty$ . Similarly, the negative exponential can be rejected for  $x < 0$ . The wave functions become

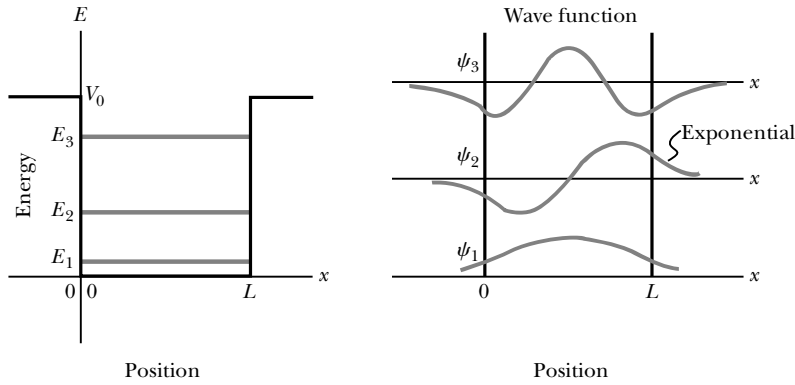
$$\psi_I(x) = Ae^{\alpha x} \quad \text{region I, } x < 0 \quad (6.38)$$

$$\psi_{III}(x) = Be^{-\alpha x} \quad \text{region III, } x > L \quad (6.39)$$



**Figure 6.4** A finite square-well potential has the value  $V_0$  everywhere except  $0 < x < L$ , where  $V = 0$ . The three regions I, II, and III are indicated.





**Figure 6.5** The energy levels  $E_n$  and wave functions  $\psi_n$  for the lowest quantum numbers for the finite square-well potential. Notice that  $\psi$  extends past  $x < 0$  and  $x > L$ , where classically the particle is forbidden. *From Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles, 2nd ed., by Robert Eisberg and Robert Resnick. Copyright 1985 by John Wiley & Sons, Inc. Reproduced with permission of John Wiley & Sons, Inc.*

Inside the square well, where the potential  $V$  is zero, the wave equation becomes

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

where  $k = \sqrt{(2mE)/\hbar^2}$ . Instead of a sinusoidal solution, we can write it as

$$\psi_{II} = Ce^{ikx} + De^{-ikx} \quad \text{region II, } 0 < x < L \quad (6.40)$$

We now want to satisfy the boundary-value properties listed in Section 6.1. We have already made sure that all but properties 2 and 3 have been satisfied. The wave functions are finite everywhere, both inside and outside the well. In order for the wave functions to be single valued, we must have  $\psi_I = \psi_{II}$  at  $x = 0$  and  $\psi_{II} = \psi_{III}$  at  $x = L$ . Both  $\psi$  and  $\partial\psi/\partial x$  must be continuous at  $x = 0$  and  $x = L$ . We will not perform these tedious procedures here, but the results for the wave functions are presented graphically in Figure 6.5.

The application of the boundary conditions leads to quantized energy values  $E_n$  and to particular wave functions  $\psi_n(x)$ . One remarkable result is that the particle has a finite probability of being outside the square well, as indicated by Figure 6.5. Notice that the wave functions join smoothly at the edges of the well and approach zero exponentially outside the well.

What other differences can we easily discern between the infinite and finite square well? For example, by examination of Figures 6.5 and 6.3, we can see that the de Broglie wavelength is larger for the finite square well because the waves extend past the square well. This in turn leads to a smaller momentum and lower energy levels. The number of energy levels will, of course, be limited because of the potential height  $V_0$  (see Figure 6.5). When  $E > V_0$  the particle is unbound, a situation that will be discussed in Section 6.7.

The occurrence of the particle outside the square well is clearly prohibited classically, but it occurs naturally in quantum mechanics. Note that because of the exponential decrease of the wave functions  $\psi_I$  and  $\psi_{III}$ , the probability of the particle penetrating a distance greater than  $\delta x \approx 1/\alpha$  begins to decrease markedly.

$$\delta x \approx \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}} \quad (6.41)$$

We call  $\delta x$  the *penetration depth*. However, later we will find values of  $\delta x$  as large as  $10/\alpha$  and  $20/\alpha$  for electrons tunneling through semiconductors (Example 6.14)

and for nuclear alpha decay (Example 6.17), respectively. The fraction of particles that successfully tunnel through in these cases is exceedingly small, but the results have important applications, especially in electronics.

It should not be surprising to find that the penetration distance that violates classical physics is proportional to Planck's constant  $\hbar$ . This result is also consistent with the uncertainty principle because in order for the particle to be in the barrier region, the uncertainty  $\Delta E$  of the energy must be very large. According to the uncertainty principle ( $\Delta E \Delta t > \hbar/2$ ), this can occur for only a very short period of time  $\Delta t$ .

## 6.5 Three-Dimensional Infinite-Potential Well

In order to use quantum theory to solve the atomic physics problems that we shall face in Chapters 7 and 8, it is necessary to extend the Schrödinger equation to three dimensions. This is easily accomplished with the operator notation already developed in Section 6.2. After obtaining the three-dimensional equation, we shall use it to study the problem of a three-dimensional infinite-potential well.

We anticipate that there will be time-independent solutions, so we shall start with the time-independent Schrödinger wave equation. The wave function  $\psi$  must be a function of all three spatial coordinates, that is,  $\psi = \psi(x, y, z)$ . We could just directly modify Equation (6.13) to three dimensions, but there is a simple method to arrive at the Schrödinger equation. We begin with the conservation of energy:

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

We multiply this equation times the wave function  $\psi$ , which gives

$$\frac{p^2}{2m}\psi + V\psi = E\psi \quad (6.42)$$

We now use Equation (6.21) to express  $p^2$  as an operator to act on  $\psi$ . But because  $p^2 = p_x^2 + p_y^2 + p_z^2$ , we must apply the momentum operator in all three dimensions.

$$\hat{p}_x\psi = -i\hbar \frac{\partial\psi}{\partial x}$$

$$\hat{p}_y\psi = -i\hbar \frac{\partial\psi}{\partial y}$$

$$\hat{p}_z\psi = -i\hbar \frac{\partial\psi}{\partial z}$$

The application of  $\hat{p}^2$  in Equation (6.42) gives

**Time-independent  
Schrödinger wave equation  
in three dimensions**

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} \right) + V\psi = E\psi \quad (6.43)$$

This is the time-independent Schrödinger wave equation in three dimensions.

You may recognize the expression in parentheses as the Laplacian operator in mathematics. It is usually written with the shorthand notation

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (6.44)$$

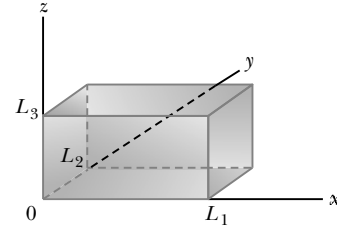
With this notation, we can write

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \quad (6.45)$$



### EXAMPLE 6.10

Consider a free particle inside a box with lengths  $L_1$ ,  $L_2$ , and  $L_3$  along the  $x$ ,  $y$ , and  $z$  axes, respectively, as shown in Figure 6.6. The particle is constrained to be inside the box. Find the wave functions and energies. Then find the ground-state energy and wave function and the energy of the first excited state for a cube of sides  $L$ .



**Figure 6.6** A three-dimensional box that contains a free particle. The potential is infinite outside the box, so the particle is constrained to be inside the box.

**Strategy** We employ some of the same strategies to solve this problem as we used for the one-dimensional case. First, because we are considering the walls of the box to be absolutely closed, they are infinite potential barriers, and the wave function  $\psi$  must be zero at the walls and beyond. We expect to see standing waves similar to Equation (6.31).

But how should we write the wave function so as to properly include the  $x$ ,  $y$ , and  $z$  dependence of the wave function? In this case the mathematics will follow from the physics. The particle is free within the box. Therefore, the  $x$ -,  $y$ -, and  $z$ -dependent parts of the wave function must be independent of each other. Inside the box  $V = 0$ , so the wave equation we must solve is

$$\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \quad (6.46)$$

It is therefore reasonable to try a wave function of the form

$$\psi(x, y, z) = A \sin(k_1 x) \sin(k_2 y) \sin(k_3 z) \quad (6.47)$$

where  $A$  is a normalization constant. The quantities  $k_i$  ( $i = 1, 2, 3$ ) are determined by applying the appropriate boundary conditions. To find the energies, we substitute the wave function into the Schrödinger equation and solve for  $E$ .

**Solution** The condition that  $\psi = 0$  at  $x = L_1$  requires that  $k_1 L_1 = n_1 \pi$  or  $k_1 = n_1 \pi / L_1$ . The values for the  $k_i$  are

$$k_1 = \frac{n_1 \pi}{L_1} \quad k_2 = \frac{n_2 \pi}{L_2} \quad k_3 = \frac{n_3 \pi}{L_3} \quad (6.48)$$

where  $n_1$ ,  $n_2$ , and  $n_3$  are integers. Not surprisingly, we have found that in three dimensions, it is necessary to use *three* quantum numbers to describe the physical state.

In order to find the energies using Equation (6.43), we first need to take the appropriate derivatives of the wave function. We do this first for the variable  $x$ .

$$\begin{aligned} \frac{\partial \psi}{\partial x} &= \frac{\partial}{\partial x} [A \sin(k_1 x) \sin(k_2 y) \sin(k_3 z)] \\ &= k_1 A \cos(k_1 x) \sin(k_2 y) \sin(k_3 z) \\ \frac{\partial^2 \psi}{\partial x^2} &= \frac{\partial}{\partial x} [k_1 A \cos(k_1 x) \sin(k_2 y) \sin(k_3 z)] \\ &= -(k_1)^2 A \sin(k_1 x) \sin(k_2 y) \sin(k_3 z) \\ &= -k_1^2 \psi \end{aligned}$$

The derivatives for  $y$  and  $z$  are similar, and Equation (6.43) becomes

$$\frac{\hbar^2}{2m}(k_1^2 + k_2^2 + k_3^2)\psi = E\psi$$

This gives

$$E = \frac{\hbar^2}{2m}(k_1^2 + k_2^2 + k_3^2)$$

We substitute the values of  $k_i$  from Equation (6.48) in this equation to obtain

$$E = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right) \quad (6.49)$$

The allowed energy values depend on the values of the three quantum numbers  $n_1$ ,  $n_2$ , and  $n_3$ .

For the *cubical* box, with  $L_1 = L_2 = L_3 = L$ . The energy values of Equation (6.49) can be expressed as

$$E = \frac{\pi^2 \hbar^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) \quad (6.50)$$

For the ground state we have  $n_1 = n_2 = n_3 = 1$ , so the ground state energy is

$$E_{\text{gs}} = \frac{3\pi^2 \hbar^2}{2mL^2} \quad (6.51)$$

and the ground state wave function is

$$\psi_{\text{gs}} = A \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right) \quad (6.52)$$

What is the energy of the first excited state? Higher values of the quantum numbers  $n_i$  correspond to higher energies; therefore, it is logical to try something like  $n_1 = 2$ ,  $n_2 = 1$ , and  $n_3 = 1$ . But we could just as well assign quantum numbers  $n_1 = 1$ ,  $n_2 = 2$ ,  $n_3 = 1$  to the first excited state, or  $n_1 = 1$ ,  $n_2 = 1$ ,  $n_3 = 2$ . In each of these cases the total energy is

$$E_{\text{1st}} = \frac{\pi^2 \hbar^2}{2mL^2} (2^2 + 1^2 + 1^2) = \frac{3\pi^2 \hbar^2}{mL^2}$$

### Degenerate state

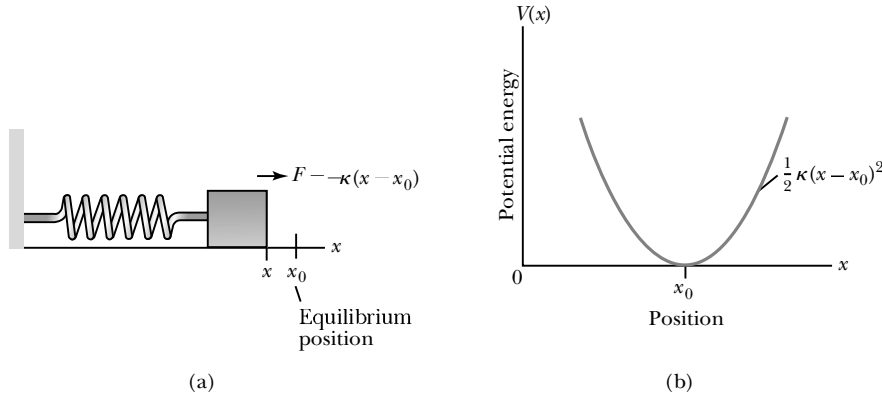
In physics we say that a given state is **degenerate** when there is more than one wave function for a given energy. We have this situation in Example 6.10, where all three possible wave functions for the first excited state have the same energy. The degeneracy in this case is a result of the symmetry of the cube. If the box had sides of three different lengths, we say the *degeneracy is removed*, because the three quantum numbers in different orders (211, 121, 112) would result in three different energies. Degeneracy is not a new phenomenon. It also occurs in classical physics, for example, in planetary motion, where orbits with different eccentricities may have the same energy. Degeneracy results from particular properties of the potential energy function that describes the system. A *perturbation* of the potential energy can remove the degeneracy. Energy levels can be split (and the degeneracy removed) by applying external magnetic fields (Zeeman effect, Section 7.4) and external electric fields (Stark effect, discussed in the Chapter 8 Special Topic, “Rydberg Atoms”).

## 6.6 Simple Harmonic Oscillator

Because of their common occurrence in nature, we now want to examine simple harmonic oscillators. In introductory physics you studied the case of a mass oscillating in one dimension on the end of a spring. Consider a spring having spring constant\*  $\kappa$  that is in equilibrium at  $x = x_0$ . The restoring force (see Figure 6.7a) along the  $x$  direction is  $F = -\kappa(x - x_0)$ , and the potential energy stored in the spring is  $V = \kappa(x - x_0)^2/2$  (see Figure 6.7b). The resulting motion is called *simple harmonic motion* (SHM), and the equations describing it are well known.

Besides springs and pendula (small oscillations), many phenomena in nature can be approximated by SHM, for example, diatomic molecules and atoms in a solid lattice of atoms. Systems can also be approximated by SHM in a general way. As an example, consider a lattice in which the force on the atoms depends on the distance  $x$  from some equilibrium position  $x_0$ . If we expand the potential in a Taylor series in terms of the distance  $(x - x_0)$  from equilibrium, we obtain

\*We let the lowercase Greek letter *kappa* ( $\kappa$ ) be the spring constant in this section rather than the normal  $k$  to avoid confusion with the wave number. It is important to note the context in which variables such as  $k$  and  $\kappa$  are used, because either might be used as wave number or spring constant.



**Figure 6.7** (a) The restoring force for a spring having a spring constant  $\kappa$  is  $F = -\kappa(x - x_0)$ . (b) The potential energy has the form  $\kappa(x - x_0)^2/2$ .

$$V(x) = V_0 + V_1(x - x_0) + \frac{1}{2}V_2(x - x_0)^2 + \cdots \quad (6.53)$$

where  $V_0$ ,  $V_1$ , and  $V_2$  are constants, and we have kept only the three lowest terms of the series, because  $(x - x_0) \approx 0$  for small excursions from the equilibrium position  $x_0$ . At  $x = x_0$  we have a minimum of the potential, so  $dV/dx = 0$  at  $x = x_0$ . This requires that  $V_1 = 0$ , and if we redefine the zero of potential energy to require  $V_0 = 0$ , then the lowest term of the potential  $V(x)$  is

$$V(x) = \frac{1}{2}V_2(x - x_0)^2$$

This is the origin of the  $V = \kappa x^2/2$  potential energy term that occurs so often. Near the equilibrium position a parabolic form as displayed in Figure 6.8 may approximate many potentials.

We want to study the quantum description of simple harmonic motion by inserting a potential  $V = \kappa x^2/2$  (we let  $x_0 = 0$ , see Figure 6.9a, page 222) into Equation (6.13), the time-independent Schrödinger wave equation.

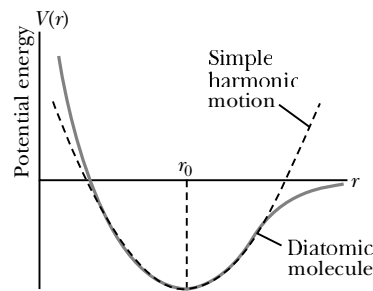
$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left(E - \frac{\kappa x^2}{2}\right)\psi = \left(-\frac{2mE}{\hbar^2} + \frac{m\kappa x^2}{\hbar^2}\right)\psi \quad (6.54)$$

If we let

$$\alpha^2 = \frac{m\kappa}{\hbar^2} \quad (6.55a)$$

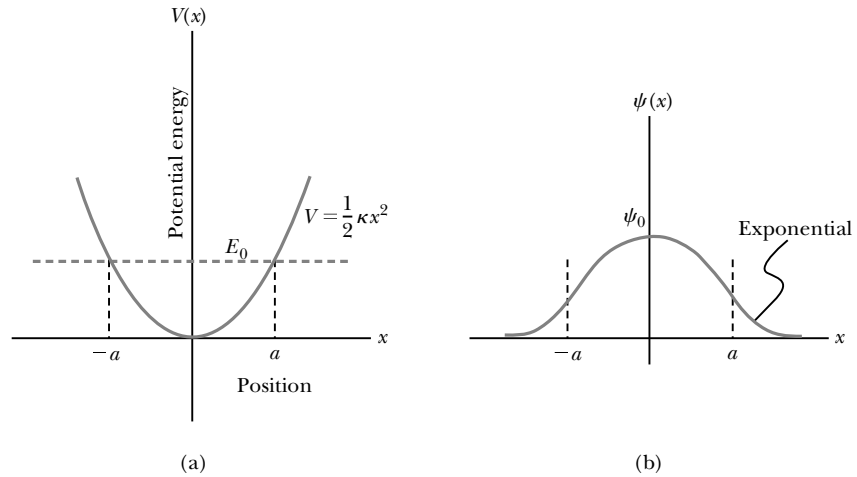
and

$$\beta = \frac{2mE}{\hbar^2} \quad (6.55b)$$



**Figure 6.8** Many potentials in nature can be approximated near their equilibrium position by the simple harmonic potential (black dashed curve). Such is the case here for the potential energy  $V(r)$  of a diatomic molecule near its equilibrium position  $r_0$  (blue curve).

**Figure 6.9** (a) The potential  $V = \kappa x^2/2$  for a simple harmonic oscillator. The classical turning points  $\pm a$  are determined for the ground state when the lowest energy  $E_0$  is equal to the potential energy. (b) Notice that the wave function  $\psi_0(x)$  for the ground state is symmetric and decays exponentially outside  $\pm a$  where  $V > E_0$ .



then

$$\frac{d^2\psi}{dx^2} = (\alpha^2 x^2 - \beta)\psi \quad (6.56)$$

Before discussing the solution of Equation (6.56), let us first examine what we can learn about the problem qualitatively. Because the particle is confined to the potential well, centered at  $x = 0$ , it has zero probability of being at  $x = \pm\infty$ . Therefore,  $\psi(x) \rightarrow 0$  as  $x \rightarrow \pm\infty$ .

What is the lowest energy level possible for the harmonic oscillator? Is  $E = 0$  possible? If  $E = 0$ , then  $x = 0$  and  $V = 0$  to allow  $E \geq V$ . But if  $E$  and  $V$  are zero, then the kinetic energy  $K = 0$ , and the momentum  $p = 0$ . Simultaneously having both  $x = 0$  and  $p = 0$  (that is, both  $x$  and  $p$  are known exactly) violates the uncertainty principle. Therefore, the minimum energy  $E$  cannot be zero. In fact, the energy levels must all be positive, because  $E > V > 0$ . The state having the lowest energy, denoted here by  $E_0$ , as shown in Figure 6.9a, and the wave function  $\psi_0$  for that state will most likely be a simple wave fitting inside the region defined by the potential (see Figure 6.9b). Let  $E_0 = V_0 = \kappa a^2/2$ . The distances  $\pm a$  define the classical limits of the particle, but we know from the previous section that the particle has a small probability of being outside the potential well dimensions of  $\pm a$ . Therefore, the wave function will not be zero at  $x = \pm a$  but will have a finite value that decreases rapidly to zero on the other side of the barrier. Thus a plausible guess for the lowest-order wave function  $\psi_0$  is like that shown in Figure 6.9b. We shall find the minimum energy  $E_0$ , called the *zero-point energy*, in the following example.



### EXAMPLE 6.11

Estimate the minimum energy of the simple harmonic oscillator allowed by the uncertainty principle.

**Strategy** In introductory physics you learned that the average kinetic energy is equal to the average potential energy

for simple harmonic oscillators over the range of motion (from  $-x$  to  $+x$ ), and both the average potential and kinetic energies are equal to one half the total energy. By relating the mean square deviation values to the uncertainty values  $\Delta x$  and  $\Delta p$ , we will determine the minimum energy.

**Solution** The energies are related by

$$K_{\text{av}} = \frac{1}{2}E = \frac{1}{2}\kappa(x^2)_{\text{av}} = \frac{1}{2m}(p^2)_{\text{av}}$$

The mean value of  $x$  is zero, but the mean value of  $(x^2)_{\text{av}}$  is the mean square deviation  $(\Delta x)^2$ . Similarly,  $(p^2)_{\text{av}} = (\Delta p)^2$ . From the previous equation, we therefore have the energy  $E = \kappa(\Delta x)^2 = (\Delta p)^2/m$  and, as a result, we must have  $\Delta x = \Delta p/\sqrt{m\kappa}$ . From the uncertainty principle we have  $\Delta p\Delta x \geq \hbar/2$ , so the minimum value of  $\Delta x = \hbar/(2\Delta p)$ . Now we have for the lowest energy  $E_0$

$$E_0 = \kappa(x^2)_{\text{av}} = \kappa(\Delta x)^2 = \kappa\left(\frac{\Delta p}{\sqrt{m\kappa}}\right)\left(\frac{\hbar}{2\Delta p}\right)$$

$$E_0 = \frac{\hbar}{2}\sqrt{\frac{\kappa}{m}} = \frac{\hbar\omega}{2}$$

Our estimate for the zero-point energy of the harmonic oscillator is  $\hbar\omega/2$ . This agrees with the zero-point energy found by more rigorous means.

The zero-point energy is not just a curious oddity. For example, the zero-point energy for  $^4\text{He}$  is large enough to prevent liquid  $^4\text{He}$  from freezing at atmospheric pressure, no matter how cold the system, even near 0 K.

The wave function solutions  $\psi_n$  for Equation (6.56) are

$$\psi_n = H_n(x)e^{-\alpha x^2/2} \quad (6.57)$$

where  $H_n(x)$  are polynomials of order  $n$ , and  $n$  is an integer  $\geq 0$ . The functions  $H_n(x)$  are related by a constant to the *Hermite polynomial functions* tabulated in many quantum mechanics books. The first few values of  $\psi_n$  and  $|\psi_n|^2$  are shown in Figure 6.10. In contrast to the particle in a box, where the oscillatory wave function is a sinusoidal curve, in this case the oscillatory behavior is due to the polynomial, which dominates at small  $x$ . The exponential tail is provided by the Gaussian function, which dominates at large  $x$ .

The energy levels are given by

$$E_n = (n + \frac{1}{2})\hbar\sqrt{\kappa/m} = (n + \frac{1}{2})\hbar\omega \quad (6.58)$$

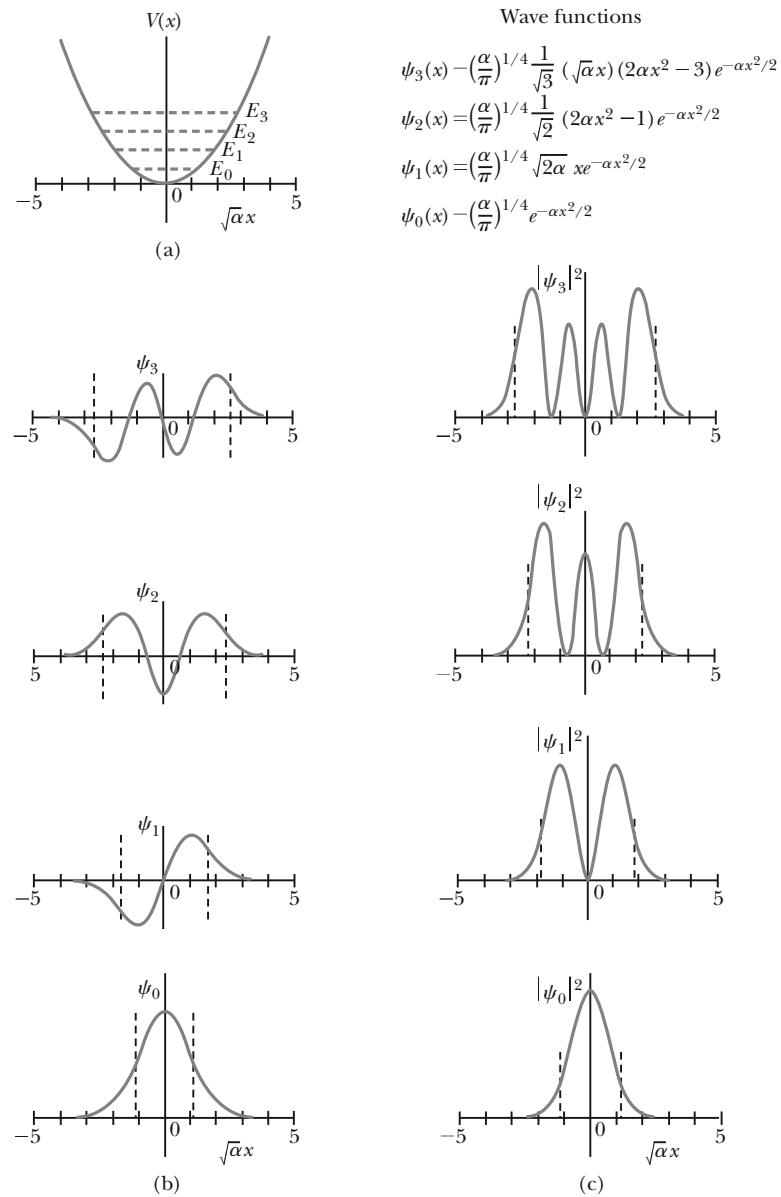
where  $\omega^2 = \kappa/m$ , and  $\omega$  is the classical angular frequency. From Equation (6.58) we see that the *zero-point energy*  $E_0$  is

$$E_0 = \frac{1}{2}\hbar\omega \quad (6.59)$$

Notice that this result for  $E_0$  is precisely the value found in Example 6.11 by using the uncertainty principle. The uncertainty principle is responsible for the minimum energy of the simple harmonic oscillator. In Section 5.6 we mentioned that the minimum value (that is, the equality sign) of the uncertainty principle is found for Gaussian wave packets. We note here that the wave functions for the simple harmonic oscillators are of just the Gaussian form (see Figure 6.10, page 224). The minimum energy  $E_0$  allowed by the uncertainty principle, sometimes called the *Heisenberg limit*, is found for the ground state of the simple harmonic oscillator.

Finally, let us compare the motion as described by classical and quantum theory. We recall the classical motion of the mass at the end of a spring. The speed is greatest as it passes through its equilibrium position. The speed is lowest (zero) at the two ends (compressed or extended positions of the spring), when the mass stops and reverses direction. Classically, the probability of finding the mass is greatest at the ends of motion and smallest at the center (that is, proportional to the amount of time the mass spends at each position). The classical probability is shown by the black dashed line in Figure 6.11 (page 224).

The quantum theory probability density for the lowest energy state ( $\psi_0^2$ , see Figure 6.10) is contrary to the classical one. The largest probability for this lowest energy state is for the particle to be at the center. We are not surprised to see such a marked difference between classical and quantum predictions (see Section 4.4).

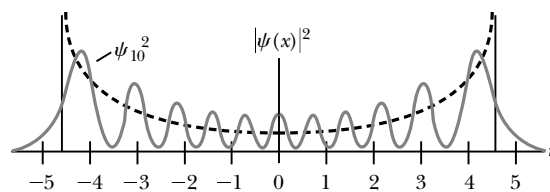


**Figure 6.10** Results for simple harmonic oscillator potential.

(a) The energy levels for the lowest four energy states are shown with the corresponding wave functions listed. (b) The wave functions for the four lowest energy states are displayed. Notice that even quantum numbers have symmetric  $\psi_n(x)$ , and the odd quantum numbers have antisymmetric  $\psi_n(x)$ . (c) The probability densities  $|\psi_n|^2$  for the lowest four energy states are displayed.

However, from the correspondence principle we would expect the classical and quantum probabilities to be similar as the quantum number  $n$  becomes very large. In Figure 6.11 we show  $\psi_{10}^2$  for the case of  $n = 10$ , and we see that the average probabilities become similar. As  $n$  continues to increase, the peaks and valleys of the quantum probabilities are hardly observable, and the average value approaches the classical result.

**Figure 6.11** The probability distribution  $|\psi_{10}|^2$  for the  $n = 10$  state is compared with the classical probability (dashed line). As  $n$  increases, the two probability distributions become more similar.







### EXAMPLE 6.12

Normalize the ground state wave function  $\psi_0$  for the simple harmonic oscillator and find the expectation values  $\langle x \rangle$  and  $\langle x^2 \rangle$ .

**Strategy** We can use Equation (5.49) for the normalization process. Let's assume that all we know about the wave function  $\psi_0$  is the form given in Equation (6.57).  $H_0(x)$  has no dependence on  $x$ , so we take it to be a constant  $A$ . We find the expectation values as discussed in Section 6.2.

**Solution** If we let  $H_0(x) = A$ , the ground state wave function becomes

$$\psi_0(x) = Ae^{-\alpha x^2/2}$$

The normalization determines  $A$ .

$$\begin{aligned}\int_{-\infty}^{\infty} \psi_0^*(x)\psi_0(x) dx &= 1 \\ A^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} dx &= 1 \\ 2A^2 \int_0^{\infty} e^{-\alpha x^2} dx &= 1\end{aligned}$$

We determine this integral with the help of integral tables (see Appendix 6), with the result

$$\begin{aligned}2A^2 \left( \frac{1}{2} \sqrt{\frac{\pi}{\alpha}} \right) &= 1 \\ A^2 &= \sqrt{\frac{\alpha}{\pi}} \\ A &= \left( \frac{\alpha}{\pi} \right)^{1/4}\end{aligned}$$

For the ground state wave function, this gives

$$\psi_0(x) = \left( \frac{\alpha}{\pi} \right)^{1/4} e^{-\alpha x^2/2} \quad (6.60)$$

This is precisely the wave function given in Figure 6.10 and is of the Gaussian form.

The expectation value of  $x$  is

$$\begin{aligned}\langle x \rangle &= \int_{-\infty}^{\infty} \psi_0^*(x)x\psi_0(x) dx \\ &= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} x e^{-\alpha x^2} dx\end{aligned}$$

The value of  $\langle x \rangle$  must be zero, because we are integrating an odd function of  $x$  over symmetric limits from  $-\infty$  to  $+\infty$  (see Appendix 6). Both classical and quantum mechanics predict the average value of  $x$  to be zero because of the symmetric nature of the potential,  $\kappa x^2/2$ .

The expectation value  $\langle x^2 \rangle$ , however, must be positive, because  $x^2$  is never negative.

$$\begin{aligned}\langle x^2 \rangle &= \int_{-\infty}^{\infty} \psi_0^*(x)x^2\psi_0(x) dx \\ &= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx \\ &= 2\sqrt{\frac{\alpha}{\pi}} \int_0^{\infty} x^2 e^{-\alpha x^2} dx\end{aligned}$$

This integral can be found in a table of integrals (see Appendix 6), and the result is

$$\langle x^2 \rangle = 2\sqrt{\frac{\alpha}{\pi}} \left( \frac{\sqrt{\pi}}{4\alpha^{3/2}} \right) = \frac{1}{2\alpha}$$

Inserting the value of the constant  $\alpha$  from Equation (6.55a) gives

$$\langle x^2 \rangle = \frac{\hbar}{2\sqrt{m\kappa}}$$

Because  $\omega = \sqrt{\kappa/m}$ , we have

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \quad (6.61)$$

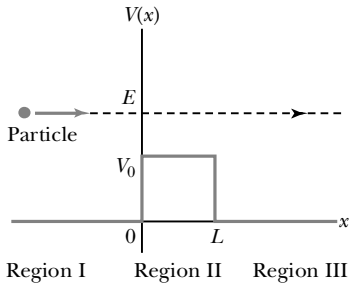
In Example 6.11 we argued that

$$(x^2)_{av} = (\Delta x)^2 = \frac{E_0}{\kappa}$$

and showed that  $E_0 = \hbar\omega/2$ , the minimum energy allowed by the uncertainty principle. We can now see that these results are consistent, because

$$\langle x^2 \rangle = (x^2)_{av} = \frac{E_0}{\kappa} = \frac{\hbar\omega}{2\kappa} = \frac{\hbar\omega}{2m\omega^2} = \frac{\hbar}{2m\omega}$$

as we determined in Equation (6.61).



**Figure 6.12** A particle having energy  $E$  approaches a potential barrier of width  $L$  and height  $V_0$  with  $E > V_0$ . The one-dimensional space is divided into three regions as shown.

## 6.7 Barriers and Tunneling

The methods we have already seen for studying particles in potential wells can be applied to the problem of a particle approaching a potential barrier. As you will see, potential barriers are real physical phenomena, and our results have immediate applications.

### Potential Barrier with $E > V_0$

Consider a particle of energy  $E$  approaching a potential barrier of height  $V_0$  for  $0 < x < L$ . The potential elsewhere is zero. First, let us consider the case where the particle's energy is  $E > V_0$  as shown in Figure 6.12. Classically we know the particle would pass the barrier, moving with reduced velocity in the region of  $V_0$  ( $K = mv^2/2 = E - V_0$ , rather than  $K = mv^2/2 = E$ ). On the other side of the barrier, where  $V = 0$ , the particle will have its original velocity again. According to quantum mechanics, the particle will behave differently because of its wavelike character. In regions I and III (where  $V = 0$ ) the wave numbers are

$$k_I = k_{III} = \frac{\sqrt{2mE}}{\hbar} \quad \text{where } V = 0 \quad (6.62a)$$

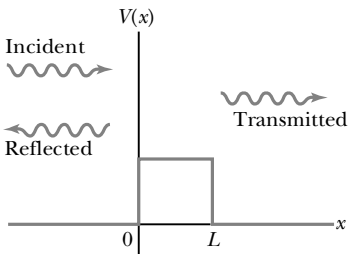
In the barrier region, however, we have

$$k_{II} = \frac{\sqrt{2m(E - V_0)}}{\hbar} \quad \text{where } V = V_0 \quad (6.62b)$$

We consider an analogy with optics. When light in air penetrates another medium (for example, glass), the wavelength changes because of the index of refraction. Some of the light will be reflected, and some will be transmitted into the medium. Because we must consider the wave behavior of particles interacting with potential barriers, we might expect similar behavior. The wave function will consist of an incident wave, a reflected wave, and a transmitted wave (see Figure 6.13). These wave functions can be determined by solving the Schrödinger wave equation, subject to appropriate boundary conditions. The difference from classical wave theories is that the wave function allows us to compute only probabilities.

Classical mechanics allows *no* reflection if  $E > V_0$  and *total* reflection for  $E < V_0$ . Quantum mechanics predicts almost total *transmission* for  $E \gg V_0$  and almost complete *reflection* for  $E \ll V_0$ . In the regime where  $E$  is comparable to  $V_0$ , unusual nonclassical phenomena may appear.

The potentials and the Schrödinger equation for the three regions are as follows:



**Figure 6.13** The incident particle in Figure 6.12 can be either transmitted or reflected.

$$\text{Region I } (x < 0) \quad V = 0 \quad \frac{d^2\psi_I}{dx^2} + \frac{2m}{\hbar^2}E\psi_I = 0$$

$$\text{Region II } (0 < x < L) \quad V = V_0 \quad \frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_{II} = 0$$

$$\text{Region III } (x > L) \quad V = 0 \quad \frac{d^2\psi_{III}}{dx^2} + \frac{2m}{\hbar^2}E\psi_{III} = 0$$

The wave functions obtained for these equations are

$$\text{Region I } (x < 0) \quad \psi_I = Ae^{ik_1x} + Be^{-ik_1x} \quad (6.63a)$$

$$\text{Region II } (0 < x < L) \quad \psi_{II} = Ce^{ik_1x} + De^{-ik_1x} \quad (6.63b)$$

$$\text{Region III } (x > L) \quad \psi_{III} = Fe^{ik_1x} + Ge^{-ik_1x} \quad (6.63c)$$

We assume that we have incident particles coming from the left moving along the  $+x$  direction. In this case the term  $Ae^{ik_1x}$  in region I represents the incident particles. The term  $Be^{-ik_1x}$  represents the reflected particles moving in the  $-x$  direction. In region III there are no particles initially moving along the  $-x$  direction, so the only particles present must be those transmitted through the barrier. Thus  $G = 0$ , and the only term in region III is  $Fe^{ik_1x}$ . We summarize these wave functions as follows:

$$\text{Incident wave} \quad \psi_I(\text{incident}) = Ae^{ik_1x} \quad (6.64a)$$

$$\text{Reflected wave} \quad \psi_I(\text{reflected}) = Be^{-ik_1x} \quad (6.64b)$$

$$\text{Transmitted wave} \quad \psi_{III}(\text{transmitted}) = Fe^{ik_1x} \quad (6.64c)$$

The probability of particles being reflected or transmitted is determined by the ratio of the appropriate  $\psi^*\psi$ . The probabilities are

$$R = \frac{|\psi_I(\text{reflected})|^2}{|\psi_I(\text{incident})|^2} = \frac{B^*B}{A^*A} \quad (6.65) \quad \text{Probability of reflection}$$

$$T = \frac{|\psi_{III}(\text{transmitted})|^2}{|\psi_I(\text{incident})|^2} = \frac{F^*F}{A^*A} \quad (6.66) \quad \text{Probability of transmission}$$

where  $R$  and  $T$  are reflection and transmission probabilities, respectively. Because the particles must be either reflected or transmitted, we must have  $R + T = 1$ , the probability of the wave being either reflected or transmitted has to be unity.

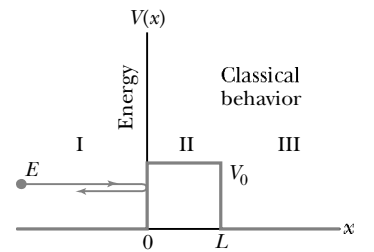
The values of  $R$  and  $T$  are found by applying the properties (boundary conditions) of Section 6.1 as  $x \rightarrow +\infty$ ,  $x = 0$ , and  $x = L$ . These conditions will result in relationships between the coefficients  $A$ ,  $B$ ,  $C$ ,  $D$ , and  $F$ . We will not go through the long algebra steps here, but the result for the transmission probability is

$$T = \left[ 1 + \frac{V_0^2 \sin^2(k_1 L)}{4E(E - V_0)} \right]^{-1} \quad (6.67)$$

Notice that there is a situation in which the transmission probability is 1. This occurs when  $k_1 L = n\pi$ , where  $n$  is an integer. It is possible for particles moving along the  $+x$  direction to be reflected both at  $x = 0$  and  $x = L$ . Their path difference back toward the  $-x$  direction is  $2L$ . When  $2L$  equals an integral number of the wavelengths inside the potential barrier, the incident and reflected wave functions are precisely out of phase and cancel completely.

### Potential Barrier with $E < V_0$

Now we consider the situation in which classically the particle does not have enough energy to surmount the potential barrier,  $E < V_0$ . We show the situation in Figure 6.14. In the classical situation, the particle cannot penetrate the barrier because its kinetic energy ( $K = E - V_0$ ) is negative. The particle is reflected at  $x = 0$  and returns. The quantum mechanical result, however, is one of the most



**Figure 6.14** A particle having energy  $E$  approaches a potential barrier of height  $V_0$  with  $E < V_0$ . Classically, the particle is always reflected.

remarkable features of modern physics, and there is ample experimental proof of its existence. There is a small, but finite, probability that the particle can penetrate the barrier and even emerge on the other side. Such a surprising result requires a careful inspection of the wave functions. Fortunately, there are only a few changes to the equations already presented, and they occur in region II. The wave function in region II becomes  $\psi_{II} = Ce^{\kappa x} + De^{-\kappa x}$  where

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \quad (6.68)$$

The parameter  $\kappa$  is a positive, real number, because  $V_0 > E$ . The application of the boundary conditions will again relate the coefficients of the wave functions.

The equations for the reflection and transmission probabilities of Equations (6.65) and (6.66) are unchanged, but the results will be modified by changing  $ik_{II} \rightarrow \kappa$ . Quantum mechanics allows the particle to actually be on the other side of the potential barrier despite the fact that all the incident particles came in from the left moving along the  $+x$  direction (Figure 6.15). This effect is called **tunneling**. The result for the transmission probability in this case is

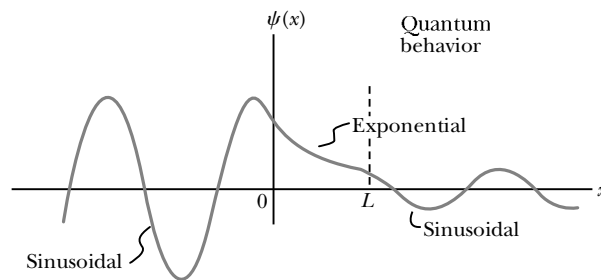
**Tunneling**

$$T = \left[ 1 + \frac{V_0^2 \sinh^2(\kappa L)}{4E(V_0 - E)} \right]^{-1} \quad (6.69)$$

Note that the sine function in Equation (6.67) has been replaced by the hyperbolic sine ( $\sinh$ ). When  $\kappa L \gg 1$ , the transmission probability equation (6.67) reduces to

$$T = 16 \frac{E}{V_0} \left( 1 - \frac{E}{V_0} \right) e^{-2\kappa L} \quad (6.70)$$

**Figure 6.15** According to quantum mechanics, the particle approaching the potential barrier of Figure 6.14 may actually pass into the barrier and has a small probability of tunneling through the barrier and emerging at  $x = L$ . The particle may also be reflected at each boundary.



### CONCEPTUAL EXAMPLE 6.13

Which is more effective in preventing tunneling, the barrier potential height or the barrier width?

**Solution** The probability of penetration is dominated by the exponentially decreasing term. The exponential factor in Equation (6.70) depends linearly on the barrier width but

only on the square root of the potential barrier height ( $\kappa \sim \sqrt{V_0 - E}$ ). Thus, the width of the barrier is more effective than the potential height in preventing tunneling. It comes as no surprise that tunneling is observed only at the smallest distances on the atomic scale.



### EXAMPLE 6.14

In a particular semiconductor device, electrons that are accelerated through a potential of 5 V attempt to tunnel through a barrier of width 0.8 nm and height 10 V. What fraction of the electrons are able to tunnel through the barrier if the potential is zero outside the barrier?

**Strategy** We use either Equation (6.69) or (6.70) to calculate the tunneling probability, depending on the value of  $\kappa L$ . We need to know  $V_0$ ,  $\kappa$ ,  $L$ , and  $E$ . We are given  $L$  and the fact that the potential barrier has  $V_0 = 10$  eV and is zero outside the barrier. We determine from the accelerating voltage that the energy  $E$  of the electrons is  $K = 5$  eV. We find the value of  $\kappa$  from a variation of Equation (6.62b) where we let  $i\hbar_{II} \rightarrow \kappa$ .

**Solution** We determine  $\kappa$  by using the mass of the electron and the appropriate energies.

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$\begin{aligned} &= \frac{\sqrt{2(0.511 \times 10^6 \text{ eV}/c^2)(10 \text{ eV} - 5 \text{ eV})}}{6.58 \times 10^{-16} \text{ eV} \cdot \text{s}} \\ &= \frac{3.43 \times 10^{18} \text{ s}^{-1}}{c} = \frac{3.43 \times 10^{18} \text{ s}^{-1}}{3 \times 10^8 \text{ m/s}} = 1.15 \times 10^{10} \text{ m}^{-1} \end{aligned}$$

The value of  $\kappa L = (1.15 \times 10^{10} \text{ m}^{-1})(0.8 \times 10^{-9} \text{ m}) = 9.2$ , which might be considered to be much greater than 1, so we can try Equation (6.70). Let's calculate the transmission probability using both equations. The approximate Equation (6.70) gives

$$T = 16 \left( \frac{5 \text{ eV}}{10 \text{ eV}} \right) \left( 1 - \frac{5 \text{ eV}}{10 \text{ eV}} \right) e^{-18.4} = 4.1 \times 10^{-8}$$

The more accurate Equation (6.69) gives

$$T = \left[ \frac{1 + (10 \text{ eV})^2 \sinh^2(9.2)}{4(5 \text{ eV})(5 \text{ eV})} \right]^{-1} = 4.1 \times 10^{-8} \quad (6.71)$$

The approximate equation, valid when  $\kappa L \gg 1$ , works well in this case.



### EXAMPLE 6.15

Consider Equation (6.70) and let all the factors multiplying the exponential term be denoted by  $M$ :

$$T = 16 \frac{E}{V_0} \left( 1 - \frac{E}{V_0} \right) e^{-2\kappa L} = M e^{-2\kappa L} \quad (6.72)$$

Consider the value of  $M$  and assign an average value. Calculate the probability of the electron tunneling through the barrier of the previous example.

**Strategy** We first consider a range of values  $E/V_0$  and estimate an average value. Then we use Equation (6.72) to determine the tunneling probability and compare with the value found in Equation (6.71) of Example 6.14.

**Solution** The maximum value of

$$M = 16 \frac{E}{V_0} \left( 1 - \frac{E}{V_0} \right)$$

will be  $M = 4$  when  $E/V_0 = 0.5$ . The values of  $M$  are symmetric around  $E/V_0 = 0.5$ , and  $M = 1.4$  when  $E/V_0 = 0.1$ . A typical value of  $M$  might be 2, so Equation (6.72) becomes

$$T \approx 2e^{-2\kappa L} \quad (6.73)$$

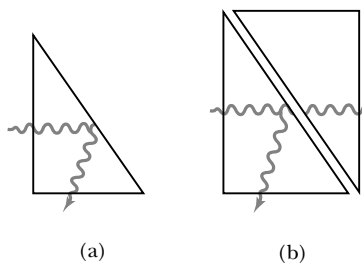
We emphasize that Equation (6.73) is only an estimate to give an order of magnitude value for the tunneling probability.

For the values in Example 6.14,  $\kappa L = 9.2$ , and we have

$$T \approx 2e^{-2(9.2)} = 2e^{-18.4} = 2 \times 10^{-8}$$

As we expected, Equation (6.73) gives a result that agrees in order of magnitude with Example 6.14.

A simple argument based on the uncertainty principle helps us understand tunneling. Inside the barrier region (where  $0 < x < L$ ), the wave function  $\psi_{II}$  is dominated by the  $e^{-\kappa x}$  term, and  $|\psi_{II}|^2 \approx e^{-2\kappa x}$ , so that over the interval  $\Delta x = \kappa^{-1}$ , the probability density of observing the particle has decreased markedly ( $e^{-2} = 0.14$ ). Because  $\Delta p \Delta x \geq \hbar$ , we have  $\Delta p \geq \hbar / \Delta x = \hbar \kappa$ . The minimum kinetic energy in this interval must be



**Figure 6.16** (a) A light wave will be totally reflected inside a prism if the reflection angle is greater than the critical angle. (b) If a second prism is brought close to the first, there is a small probability for the wave to pass through the air gap and emerge in the second prism.

$$K_{\min} = \frac{(\Delta p)^2}{2m} = \frac{\pi^2 \kappa^2}{2m} = V_0 - E$$

where we have substituted for  $\kappa$  in the last step. The violation allowed by the uncertainty principle ( $K_{\min}$ ) is equal to the *negative* kinetic energy required! The particle is allowed by quantum mechanics and the uncertainty principle to penetrate into a classically forbidden region.

Let us return briefly to our analogy with wave optics. If light passing through a glass prism reflects from an internal surface with an angle greater than the critical angle, total internal reflection occurs as seen in Figure 6.16a. However, the electromagnetic field is not exactly zero just outside the prism. If we bring another prism very close to the first one, experiment shows that the electromagnetic wave (light) appears in the second prism (see Figure 6.16b). The situation is analogous to the tunneling described here. This effect was observed by Newton and can be demonstrated with two prisms and a laser. The intensity of the second light beam decreases exponentially as the distance between the two prisms increases.\*

\*See D. D. Coon, *American Journal of Physics* **34**, 240 (1966).



### EXAMPLE 6.16

Consider a particle of kinetic energy  $K$  approaching the step function of Figure 6.17 from the left, where the potential barrier steps from 0 to  $V_0$  at  $x = 0$ . Find the penetration distance  $\Delta x$ , where the probability of the particle penetrating into the barrier drops to  $1/e$ . Calculate the penetration distance for a 5-eV electron approaching a step barrier of 10 eV.

**Strategy** We use the results of this section to find the wave functions in the two regions  $x < 0$  and  $x > 0$ .

$$\begin{aligned}\psi_I &= Ae^{ikx} + Be^{-ikx} & x < 0 \\ \psi_{II} &= Ce^{\kappa x} + De^{-\kappa x} & x > 0\end{aligned}$$

where

$$\begin{aligned}k &= \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2mK}}{\hbar} \\ \kappa &= \frac{\sqrt{2m(V_0 - E)}}{\hbar}\end{aligned}$$

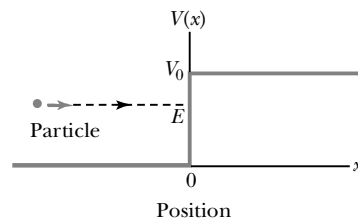
Because the wave function  $\psi_{II}$  must go to zero when  $x \rightarrow \infty$ , the coefficient  $C = 0$ , so we have

$$\psi_{II} = De^{-\kappa x} \quad x > 0$$

The probability distribution for  $x > 0$  is given by  $|\psi_{II}|^2$ . We need to find the value of  $x$  when the probability has dropped to  $e^{-1}$ . Let's call this distance  $\ell$ .

**Solution** For the penetration distance  $\ell$ , we have

$$e^{-1} = \frac{|\psi_{II}(x = \ell)|^2}{|\psi_{II}(x = 0)|^2} = e^{-2\kappa\ell}$$



**Figure 6.17** A particle of energy  $E$  approaches a potential barrier from the left. The step potential is  $V = 0$  for  $x < 0$  and  $V = V_0$  for  $x > 0$ .

From this equation we have  $1 = 2\kappa\ell$ , and the penetration distance becomes

$$\ell = \frac{1}{2\kappa} = \frac{\hbar}{2\sqrt{2m(V_0 - E)}}$$

This is the result we needed.

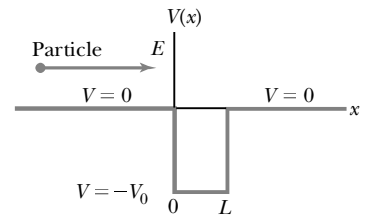
Now we find the penetration distance for the  $E = K = 5$ -eV electron.

$$\begin{aligned}\ell &= \frac{\hbar c}{2\sqrt{2mc^2(V_0 - E)}} \\ &= \frac{197.3 \text{ eV} \cdot \text{nm}}{2\sqrt{2(0.511 \times 10^6 \text{ eV})(10 \text{ eV} - 5 \text{ eV})}} = 0.044 \text{ nm}\end{aligned}$$

Electrons do not penetrate very far into the classically forbidden region.

## Potential Well

Consider a particle of energy  $E > 0$  passing through the potential well region (Figure 6.18), rather than into a potential barrier. Let  $V = -V_0$  in the region  $0 < x < L$  and zero elsewhere. Classically, the particle would accelerate passing the well region, because  $K = mv^2/2 = E + V_0$ . According to quantum mechanics, reflection and transmission may occur, but the wavelength inside the potential well is smaller than outside. When the width of the potential well is precisely equal to half-integral or integral units of the wavelength, the reflected waves may be out of phase or in phase with the original wave, and cancellations or resonances may occur. The reflection/cancellation effects can lead to almost pure transmission or pure reflection for certain wavelengths. For example, at the second boundary ( $x = L$ ) for a wave passing to the right, the wave may reflect and be out of phase with the incident wave. The effect would be a cancellation of the wave function inside the well.

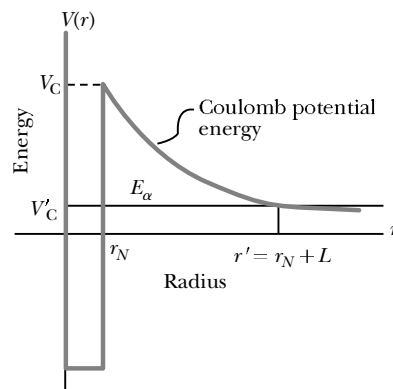


**Figure 6.18** A particle of energy  $E$  approaches a potential well from the left. The potential is  $V = 0$  everywhere except between  $0 < x < L$ , where  $V = -V_0$ .

## Alpha-Particle Decay

The phenomenon of tunneling explains the alpha-particle decay of radioactive nuclei. Many nuclei heavier than lead are natural emitters of alpha particles, but their emission rates vary over a factor of  $10^{13}$ , whereas their energies tend to range only from 4 to 8 MeV. Inside the nucleus, an alpha particle feels the strong, short-range attractive nuclear force as well as the repulsive Coulomb force. An approximate potential well is shown in Figure 6.19. The nuclear force dominates inside the nuclear radius  $r_N$ , and the potential can be approximated by a square well. However, outside the nucleus, the Coulomb force dominates. The so-called Coulomb potential energy barrier of Figure 6.19 can be several times the typical kinetic energy  $K$  ( $\sim 5$  MeV) of an alpha particle.

The alpha particle therefore is trapped inside the nucleus. Classically, it does not have enough energy to surmount the Coulomb potential barrier. According to quantum mechanics, however, the alpha particle can “tunnel” through the barrier. The widely varying rates of alpha emission from radioactive nuclei can be explained by small changes in the potential barrier (both height and width). A small change in the barrier can manifest itself greatly in the transmission probability (see Conceptual Example 6.13), because of the exponential behavior in  $e^{-2\kappa L}$ .



**Figure 6.19** An  $\alpha$  particle of energy  $E_\alpha$  is trapped inside a heavy nucleus by the large nuclear potential. Classically, it can never escape, but quantum mechanics allows it to tunnel through and escape.



# Special Topic

## Scanning Probe Microscopes

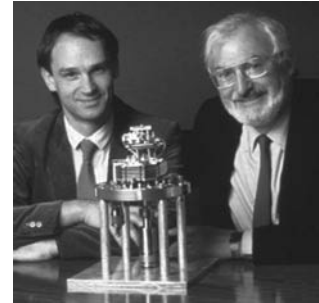
Scanning probe microscopes allow a computer-generated contour map of a surface, atom by atom (see Figure 1.7). They consist of two types, **scanning tunneling microscopes** (STM) and **atomic force microscopes** (AFM), which have revolutionized the imaging of atomic surfaces. Gerd Binnig and Heinrich Rohrer (Nobel Prize, 1986) invented the STM in the early 1980s at the IBM Research Laboratory in Zurich, Switzerland. Later while Binnig was on leave at Stanford University and IBM's Almaden Research Center, he thought up the concept of the AFM, which he developed in 1985 with Christoph Gerber of IBM and Calvin Quate of Stanford.

In the most common form of the STM a constant bias voltage of appropriate polarity is applied between the atoms of a tip and the sample to be examined (Figure A). As the tip runs over the surface of the sample just an atom's diameter away, electrons attracted to the needle tunnel across the gap, and the sensitivity of the tunneling current to the gap distance is the key to the STM capability. This tunneling current can be as small as a few pA ( $10^{-12}$  A), and a change in the tunneling gap of only 0.4 nm can cause a factor of  $10^4$  in the tunneling current. A highly sensitive feedback mechanism regulates the position of the tip to maintain a steady current of electrons. The resulting up and down movements of the tip effectively trace the contours of the sample atoms, producing something like a topographic map. The resulting image (path of the tip) is shown by the solid black line in Figure A.

The AFM depends on the interatomic forces between the tip and sample atoms as shown in Figure B. In some systems, the sample atoms are scanned horizontally while the sample is moved up and down to keep the force between the tip and sample atoms constant. The interatomic forces cause the very sensitive cantilever to bend. A laser is reflected off the end of the cantilever arm into an optical sensor, and the feedback signal from this sensor controls the sample height, giving the topography of the atomic surface. The tip is scanned over the surface for a constant cantilever deflection and a constant interatomic force between tip and atom.

The interaction between tip and sample is much like that of a record player stylus moving across the

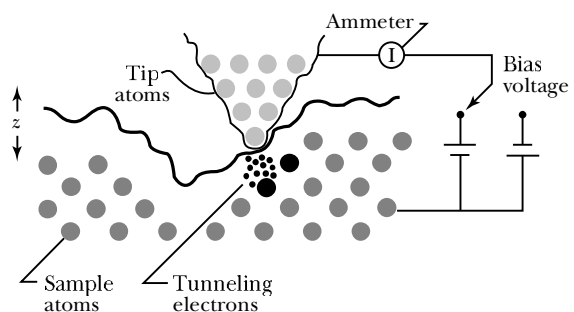
**Heinrich Rohrer** (right, 1933–) and **Gerd Binnig** (1947–) received the Nobel Prize for Physics in 1986 for their design of the scanning tunneling microscope. The Swiss Rohrer was educated at the Swiss Federal Institute of Technology in Zurich and joined the IBM Research Laboratory in Zurich in 1963. The German Binnig received his doctorate from the University of Frankfurt (Germany) in 1978 and then joined the same IBM Research Laboratory. He moved to the IBM Physics Group in Munich in 1984.



Courtesy of IBM Zurich Research Laboratory.

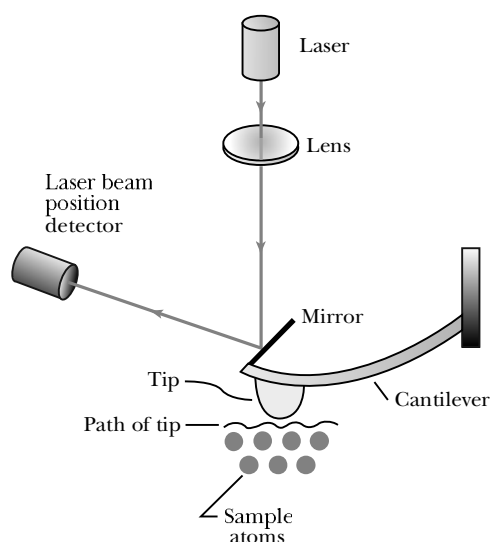
record but is about a million times more sensitive. The optical feedback system prevents the tip from actually damaging or distorting the sample atoms. Cantilevers having spring constants as small as 0.1 N/m have been microfabricated from silicon and silicon compounds. The cantilever lateral dimensions are on the order of 100  $\mu\text{m}$  with thicknesses of about 1  $\mu\text{m}$ . In comparison the spring constant of a piece of household aluminum foil 4 mm by 1 mm is about 1 N/m. The tapered tips may have an end dimension of only 50 nm. The tracking forces felt by the cantilever can be as small as  $10^{-9}$  N.

Advantages of the AFM compared with the STM are that a conducting surface is not required, and neither special sample preparation nor expensive



**Figure A** Highly schematic diagram of the scanning tunneling microscope process. Electrons, represented in the figure as small dots, tunnel across the gap between the atoms of the tip and sample. A feedback system that keeps the tunneling current constant causes the tip to move up and down, tracing the contours of the sample atoms.

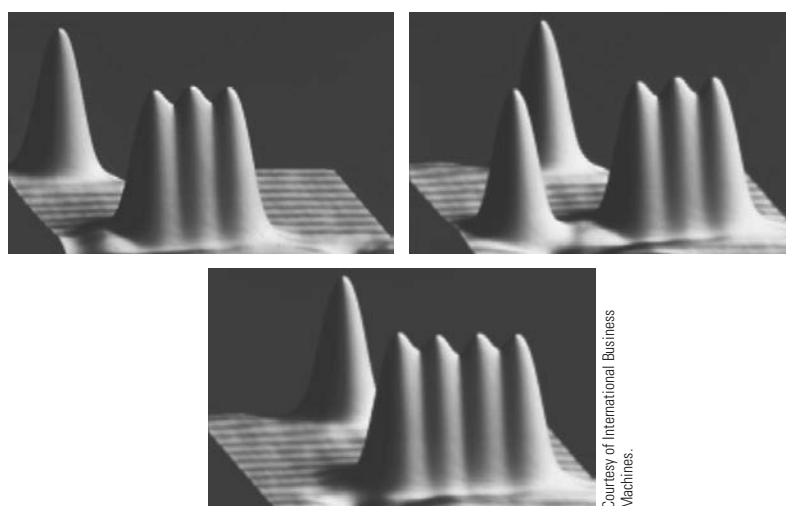




**Figure B** Highly schematic diagram of the atomic force microscope. A feedback signal from the detection of the laser beam reflecting off the mirror that is mounted on the cantilever provides a signal to move the sample atoms up or down to keep the cantilever force constant. The movement of the sample atoms traces the contours of the sample atoms.

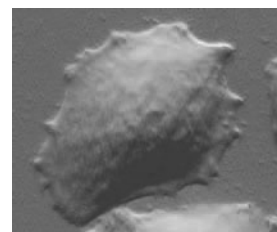
vacuum equipment is needed. Because the AFM works for both insulators and conductors, it can be used for ceramics, polymers, optical surfaces, and biological specimens. However, special vibrational insulation is needed for AFM to dampen air currents and even human voices. Figure 1.7 is a photo indicating individual atoms that was taken using an STM. Those atoms can be individually moved as shown in Figure C.

In addition to providing individual atomic images, the STM and AFM open tremendous possibilities for investigation of a variety of atomic surface features. The topographical images produced by these microscopes allow scientists to examine the gross features of a sample, such as the flatness of materials, grain structures, and the breakup of thin films. Industrial applications of this technology include the inspections of magnetic bit shapes, integrated circuit topography, lubricant thicknesses, optical disk stampers (Figure D), and measurement of line widths on integrated circuit masks. Biological applications of AFM include the imaging of amino acids, DNA, proteins, and even leaf sections from a plant. The AFM



**Figure C** These three photos, taken with an STM, show xenon atoms placed on a nickel surface. The xenon atoms are 0.16 nm high and adjacent xenon atoms are 0.5 nm apart (the vertical scale has been exaggerated). The small force between the STM tip and an atom is enough to drag one xenon atom at a time across the nickel. The nickel atoms are represented by the black-and-white stripes on the horizontal surface. See also Figure 1.7. The image is magnified about 5 million times.

**Figure D** An atomic force microscope scan of a live cancer cell, size  $50\text{ }\mu\text{m} \times 50\text{ }\mu\text{m}$ . This lung cancer cell was grown for four days.



has been used to observe the polymerization of fibrin, a blood-clotting protein. Real-time imaging of biological samples offers incredible possibilities, for example, the attachment of the AIDS virus onto cell membranes. Now that STM and AFM instruments are both available commercially, new applications for this revolutionary technology are being developed that include such diverse techniques as developing x-ray mirrors by moving atoms to increase reflectivity, “nanoengineering” electronics to improve performance, and repairing organic molecules on an atomic basis.



### EXAMPLE 6.17

Consider the  $\alpha$ -particle emission from a  $^{238}\text{U}$  nucleus, which emits a 4.2-MeV  $\alpha$  particle. We represent the potentials as shown in Figure 6.19. The  $\alpha$  particle is contained inside the nuclear radius of  $r_N \approx 7 \times 10^{-15}$  m. Find the barrier height and the distance the  $\alpha$  particle must tunnel and use a square-top potential to calculate the tunneling probability.

**Strategy** We shall calculate the barrier height [ $V_C(r = r_N)$  in Figure 6.19] by calculating the Coulomb potential between an  $\alpha$  particle and the remainder of the uranium nucleus for a separation of the nuclear radius,  $7 \times 10^{-15}$  m. We find the tunneling distance by setting the kinetic energy equal to the Coulomb potential and then use Equation (6.70) to determine the tunneling probability.

**Solution** The Coulomb potential is

$$\begin{aligned} V_C &= \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r_N} \\ &= \frac{2(92)(1.6 \times 10^{-19} \text{ C})^2 (9 \times 10^9 \text{ N} \cdot \text{m}^2 / \text{C}^2)}{7 \times 10^{-15} \text{ m}} \\ &\quad \times \frac{10^{-6} \text{ MeV}}{1.6 \times 10^{-19} \text{ J}} \\ &= 38 \text{ MeV} \end{aligned}$$

We determine the distance  $r'$  through which the  $\alpha$  particle must tunnel by setting  $K = V_C(r = r')$  at that distance (see Figure 6.19). Because  $K = 4.2$  MeV, we have

$$4.2 \text{ MeV} = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r'}$$

We solve this equation for  $r'$ :

$$r' = \frac{38 \text{ MeV}}{4.2 \text{ MeV}} r_N = 6.3 \times 10^{-14} \text{ m} = 63 \text{ fm}$$

where we have used the values above for  $V_C$  and  $r_N$ .

We make a simple, but rough, approximation of a square-top potential where  $V = 38$  MeV for  $7 \text{ fm} < r < 63 \text{ fm}$ . We then find

$$\begin{aligned} \kappa &= \frac{\sqrt{2m(V - E)}}{\hbar} \\ &= \frac{\sqrt{2(3727 \text{ MeV}/c^2)(38 \text{ MeV} - 4.2 \text{ MeV})}}{6.58 \times 10^{-22} \text{ MeV} \cdot \text{s}} \\ &= 2.5 \times 10^{15} \text{ m}^{-1} \end{aligned}$$

where the mass of the  $\alpha$  particle is  $3727 \text{ MeV}/c^2$ . The barrier width  $L$  is the difference between  $r'$  and  $r_N$ .

$$\begin{aligned} L &= r' - r_N \\ &= 63 \text{ fm} - 7 \text{ fm} = 56 \text{ fm} \end{aligned}$$

The value of  $\kappa L = (2.5 \times 10^{15} \text{ m}^{-1})(56 \times 10^{-15} \text{ m}) = 140$ . Because  $\kappa L \gg 1$ , we use Equation (6.70) to calculate the tunneling probability.

$$\begin{aligned} T &= 16 \left( \frac{4.2 \text{ MeV}}{38 \text{ MeV}} \right) \left( 1 - \frac{4.2 \text{ MeV}}{38 \text{ MeV}} \right) e^{-280} \\ &= 1.6e^{-280} = 4 \times 10^{-121} \end{aligned}$$

which is an extremely small number.

Our assumption of a square-top potential of the full height and full width is unrealistic. A closer approximation to the potential shown in Figure 6.19 would be a square-top potential of only half the maximum Coulomb potential (19 MeV rather than 38 MeV) and a barrier width of only half  $L$  (28 fm rather than 56 fm). If we use 19 MeV in the calculation of  $\kappa$  we obtain  $1.7 \times 10^{15} \text{ m}^{-1}$ . The tunneling probability now becomes

$$\begin{aligned} T &= 16 \frac{4.2 \text{ MeV}}{18 \text{ MeV}} \left( 1 - \frac{4.2 \text{ MeV}}{18 \text{ MeV}} \right) \\ &\quad \times \exp[-2(1.7 \times 10^{15} \text{ m}^{-1})(2.8 \times 10^{-14} \text{ m})] \\ &= 2.8 \exp(-95) = 1.5 \times 10^{-41} \end{aligned}$$

This still seems like a very low probability, but let us see if we can determine how much time it takes the  $\alpha$  particle to tunnel out. If the  $\alpha$  particle has a kinetic energy of 4.2 MeV, its speed is determined nonrelativistically by

$$\begin{aligned} K &= \frac{1}{2}mv^2 \\ v &= \sqrt{\frac{2K}{m}} = \sqrt{\frac{2(4.2 \text{ MeV})}{3727 \text{ MeV}/c^2}} = 0.047c = 1.4 \times 10^7 \text{ m/s} \end{aligned}$$

The diameter of the nucleus is about  $1.4 \times 10^{-14}$  m, so it takes the  $\alpha$  particle  $(1.4 \times 10^{-14} \text{ m})/(1.4 \times 10^7 \text{ m/s}) \approx 10^{-21}$  s to cross. The  $\alpha$  particle must make many traverses back and forth across the nucleus before it can escape. According to our probability calculation it must make about  $10^{41}$  attempts, so we estimate the  $\alpha$  particle may tunnel through in about  $10^{20}$  s. The half-life of a  $^{238}\text{U}$  nucleus is  $4.5 \times 10^9$  y or about  $10^{17}$  s. Our rough estimate does not seem all that bad.

**Tunnel Diode** An extremely useful application of tunneling is that of a tunnel diode, which is a special kind of semiconductor. The tunnel diode was discovered by a Japanese Ph.D. student, Leo Esaki, in 1957. He received the Nobel Prize in Physics in 1973 for his discovery. In a tunnel diode, electrons may pass from one region through a junction into another region. We can depict the behavior by considering a potential barrier over the region of the junction, which may be only 10 nm wide. Both positive and negative bias voltages may be applied to change the barrier height to allow the electrons to tunnel either way through the barrier. In a normal semiconductor junction, the electrons (and holes) diffuse through, a relatively slow process. In a tunnel diode, the electrons tunnel through quite rapidly when the tunneling probability is relatively high. Because the applied bias voltage can be changed rapidly, a tunnel diode is an extremely fast device. It has had important uses in switching circuits and high-frequency oscillators but is rarely used now except for space applications, in which its longevity and resistance to radiation make it particularly useful.

## Summary

Werner Heisenberg and Erwin Schrödinger developed modern quantum theory in the 1920s. The time-dependent Schrödinger wave equation for the wave function  $\Psi(x, t)$  is expressed as

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V\Psi(x, t) \quad (6.1)$$

The time-independent form for the spatial dependence (in one dimension) of  $\psi(x)$ , where  $\Psi(x, t) = \psi(x)e^{-iEt/\hbar}$ , is

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (6.13)$$

Certain properties of  $\Psi$  and  $\partial\Psi/\partial x$  lead to quantized behavior. The wave function  $\Psi(x, t)$  must be finite, single valued, and continuous;  $\partial\Psi/\partial x$  must be continuous. The wave function must be normalized for use in determining probabilities.

Average values of the physical observables are determined by calculating the expectation values using the wave functions. The expectation value of a function  $g(x)$  is found from

$$\langle g(x) \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t)g(x)\Psi(x, t) dx \quad (6.20)$$

To find the expectation values of the momentum and energy, we need to know the appropriate operators. In these two cases the operators are

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \quad (6.21)$$

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \quad (6.25)$$

and the expectation values  $\langle p \rangle$  and  $\langle E \rangle$  are

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial x} dx \quad (6.23)$$

$$\langle E \rangle = i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial t} dx \quad (6.26)$$

The infinite square-well potential is a particularly simple application of the Schrödinger wave equation, and it leads to quantized energy levels and quantum numbers. The three-dimensional infinite square-well potential leads to the concept of degenerate states, different physical states with the same energy.

The simple harmonic oscillator, where the potential is  $V(x) = \kappa x^2/2$ , is an important application of the Schrödinger wave equation because it approximates many complex systems in nature but is exactly soluble. The energy levels of the simple harmonic oscillator are  $E_n = (n + \frac{1}{2})\hbar\omega$ , where  $n = 0$  represents the ground state energy  $E_0 = \hbar\omega/2$ . The fact that the minimum energy is not zero—that the oscillator exhibits zero-point motion—is a consequence of the uncertainty principle.

Finite potentials lead to the possibility of a particle entering a region that is classically forbidden, where  $V_0 > E$  (negative kinetic energy). This quantum process is called tunneling and is studied by considering various potential barrier shapes. Important examples of quantum tunneling are alpha decay and tunnel diodes. Tunneling is consistent with the uncertainty principle and occurs only for short distances.

## Questions

1. Why can we use the nonrelativistic form of the kinetic energy in treating the structure of the hydrogen atom?
2. How do you reconcile the fact that the probability density for the ground state of the quantum harmonic oscillator (Figure 6.10c) has its peak at the center and its minima at its ends, whereas the classical harmonic oscillator's probability density (Figure 6.11) has a minimum at the center and peaks at each end? If you do this experiment with an actual mass and spring, what experimental result for its position distribution would you expect to obtain? Why?
3. Notice for the finite square-well potential that the wave function  $\Psi$  is not zero outside the well despite the fact that  $E < V_0$ . Is it possible classically for a particle to be in a region where  $E < V_0$ ? Explain this result.
4. In a given tunnel diode the  $pn$  junction (see Chapter 11) width is fixed. How can we change the time response of the tunnel diode most easily? Explain.
5. A particle in a box has a first excited state that is 3 eV above its ground state. What does this tell you about the box?
6. Does the wavelength of a particle change after it tunnels through a barrier as shown in Figure 6.15? Explain.
7. Can a particle be observed while it is tunneling through a barrier? What would its wavelength, momentum, and kinetic energy be while it tunnels through the barrier?
8. Is it easier for an electron or a proton of the same energy to tunnel through a given potential barrier? Explain.
9. Can a wave packet be formed from a superposition of wave functions of the type  $e^{i(kx - \omega t)}$ ? Can it be normalized?
10. Given a particular potential  $V$  and wave function  $\Psi$ , how could you prove that the given  $\Psi$  is correct? Could you determine an appropriate energy  $E$  if the potential is independent of time?
11. Compare the infinite square-well potential with the finite one. Where is the Schrödinger wave equation the same? Where is it different?
12. Tunneling can occur for an electron trying to pass through a very thin tunnel diode. Can a baseball tunnel through a very thin window? Explain.
13. For the three-dimensional cubical box, the ground state is given by  $n_1 = n_2 = n_3 = 1$ . Why is it not possible to have one  $n_i = 1$  and the other two equal to zero?

## Problems

Note: The more challenging problems have their problem numbers shaded by a blue box.

### 6.1 The Schrödinger Wave Equation

1. Try to normalize the wave function  $e^{i(kx - \omega t)}$ . Why can't it be done over all space? Explain why this is not possible.
2. (a) In what direction does a wave of the form  $A \sin(kx - \omega t)$  move? (b) What about  $B \sin(kx + \omega t)$ ? (c) Is  $e^{i(kx - \omega t)}$  a real number? Explain. (d) In what direction is the wave in (c) moving? Explain.
3. Show directly that the trial wave function  $\Psi(x, t) = e^{i(kx - \omega t)}$  satisfies Equation (6.1).
4. Normalize the wave function  $e^{i(kx - \omega t)}$  in the region  $x = 0$  to  $a$ .
5. Normalize the wave function  $Are^{-r/\alpha}$  from  $r = 0$  to  $\infty$  where  $\alpha$  and  $A$  are constants. See Appendix 3 for useful integrals.
6. Property 2 of the boundary conditions for wave functions specifies that  $\Psi$  must be continuous in order to avoid discontinuous probability values. Why can't we have discontinuous probabilities?

7. Consider the wave function  $Ae^{-\alpha|x|}$  that we used in Example 6.4. (a) Does this wave function satisfy the boundary conditions of Section 6.1? (b) What does your analysis in part (a) imply about this wave function? (c) If the wave function is unacceptable as is, how could it be fixed?

### 6.2 Expectation Values

8. A set of measurements has given the following result for the measurement of  $x$  (in some units of length): 3.4, 3.9, 5.2, 4.7, 4.1, 3.8, 3.9, 4.7, 4.1, 4.5, 3.8, 4.5, 4.8, 3.9, and 4.4. Find the average value of  $x$ , called  $\bar{x}$  or  $\langle x \rangle$ , and average value of  $x^2$ , represented by  $\langle x^2 \rangle$ . Show that the standard deviation of  $x$ , given by

$$\sigma = \sqrt{\frac{\sum (x_i - \bar{x})^2}{N}}$$

where  $x_i$  is the individual measurement and  $N$  is the number of measurements, is also given by  $\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ . Find the value of  $\sigma$  for the set of data given here.

9. If the potential  $V(x)$  for a one-dimensional system is independent of time, show that the expectation value for  $x$  is independent of time.
10. A wave function  $\Psi$  is  $A(e^{ix} + e^{-ix})$  in the region  $-\pi < x < \pi$  and zero elsewhere. Normalize the wave function and find the probability of the particle being (a) between  $x = 0$  and  $x = \pi/8$ , and (b) between  $x = 0$  and  $x = \pi/4$ .
11. A wave function has the value  $A \sin x$  between  $x = 0$  and  $\pi$  but zero elsewhere. Normalize the wave function and find the probability that the particle is (a) between  $x = 0$  and  $x = \pi/4$  and (b) between  $x = 0$  and  $\pi/2$ .

### 6.3 Infinite Square-Well Potential

12. Find an equation for the difference between adjacent energy levels ( $\Delta E_n = E_{n+1} - E_n$ ) for the infinite square-well potential. Calculate  $\Delta E_1$ ,  $\Delta E_8$ , and  $\Delta E_{800}$ .
13. Determine the average value of  $\psi_n^2(x)$  inside the well for the infinite square-well potential for  $n = 1, 5, 10$ , and 100. Compare these averages with the classical probability of detecting the particle inside the box.
14. A particle in an infinite square-well potential has ground-state energy 4.3 eV. (a) Calculate and sketch the energies of the next three levels, and (b) sketch the wave functions on top of the energy levels.
15. We can approximate an electron moving in a nanowire (a small, thin wire) as a one-dimensional infinite square-well potential. Let the wire be  $2.0 \mu\text{m}$  long. The nanowire is cooled to a temperature of 13 K, and we assume the electron's average kinetic energy is that of gas molecules at this temperature ( $= 3kT/2$ ). (a) What are the three lowest possible energy levels of the electrons? (b) What is the approximate quantum number of electrons moving in the wire?
16. An electron moves with a speed  $v = 1.25 \times 10^{-4}c$  inside a one-dimensional box ( $V = 0$ ) of length 48.5 nm. The potential is infinite elsewhere. The particle may not escape the box. What approximate quantum number does the electron have?
17. For the infinite square-well potential, find the probability that a particle in its ground state is in each third of the one-dimensional box:  $0 \leq x \leq L/3$ ,  $L/3 \leq x \leq 2L/3$ ,  $2L/3 \leq x \leq L$ . Check to see that the sum of the probabilities is one.
18. Repeat the previous problem using the first excited state.
19. Repeat Example 6.9 for an electron inside the nucleus. Assume nonrelativistic equations and find the transition energy for an electron. (See Example 6.9 for an interpretation of the result.)
20. What is the minimum energy of (a) a proton and (b) an  $\alpha$  particle trapped in a one-dimensional region the size of a uranium nucleus (radius  $= 7.4 \times 10^{-15} \text{ m}$ )?
21. An electron is trapped in an infinite square-well potential of width 0.70 nm. If the electron is initially in the  $n = 4$  state, what are the various photon energies that can be emitted as the electron jumps to the ground state?

### 6.4 Finite Square-Well Potential

22. Consider a finite square-well potential well of width  $3.00 \times 10^{-15} \text{ m}$  that contains a particle of mass  $1.88 \text{ GeV}/c^2$ . How deep does this potential well need to be to contain three energy levels? (This situation approximates a deuteron inside a nucleus.)
23. Compare the results of the infinite and finite square-well potentials. (a) Are the wavelengths longer or shorter for the finite square well compared with the infinite well? (b) Use physical arguments to decide whether the energies (for a given quantum number  $n$ ) are (i) larger or (ii) smaller for the finite square well than for the infinite square well? (c) Why will there be a finite number of bound energy states for the finite potential?
24. Apply the boundary conditions to the finite square-well potential at  $x = 0$  to find the relationships between the coefficients  $A$ ,  $C$ , and  $D$  and the ratio  $C/D$ .
25. Apply the boundary conditions to the finite square-well potential at  $x = L$  to find the relationship between the coefficients  $B$ ,  $C$ , and  $D$  and the ratio  $C/D$ .

### 6.5 Three-Dimensional Infinite-Potential Well

26. Find the energies of the second, third, fourth, and fifth levels for the three-dimensional cubical box. Which energy levels are degenerate?
27. Write the possible (unnormalized) wave functions for each of the first four excited energy levels for the cubical box.
28. Find the normalization constant  $A$  for the ground state wave function for the cubical box in Equation (6.52).
29. Complete the derivation of Equation (6.49) by substituting the wave function given in Equation (6.47) into Equation (6.46). What is the origin of the three quantum numbers?
30. Find the normalization constant  $A$  [in Equation (6.47)] for the first excited state of a particle trapped in a cubical potential well with sides  $L$ . Does it matter which of the three degenerate excited states you consider?
31. A particle is trapped in a rectangular box having sides  $L$ ,  $2L$ , and  $4L$ . Find the energy of the ground state and first three excited states. Are any of these states degenerate?

### 6.6 Simple Harmonic Oscillator

32. In Figure 6.9 we showed a plausible guess for the wave function  $\psi_0$  for the lowest energy level  $E_0$  of the simple harmonic oscillator. Explain the shape of the wave function and explain why it is a maximum at  $x = 0$  and not zero when  $E = V_0$ .

33. What is the energy level difference between adjacent levels  $\Delta E_n = E_{n+1} - E_n$  for the simple harmonic oscillator? What are  $\Delta E_0$ ,  $\Delta E_2$ , and  $\Delta E_{20}$ ? How many possible energy levels are there?
34. The wave function for the first excited state  $\psi_1$  for the simple harmonic oscillator is  $\psi_1 = A x e^{-\alpha x^2/2}$ . Normalize the wave function to find the value of the constant  $A$ . Determine  $\langle x \rangle$ ,  $\langle x^2 \rangle$  and  $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ .
35. A nitrogen atom of mass  $2.32 \times 10^{-26}$  kg oscillates in one dimension at a frequency of  $10^{13}$  Hz. What are its effective force constant and quantized energy levels?
36. One possible solution for the wave function  $\psi_n$  for the simple harmonic oscillator is

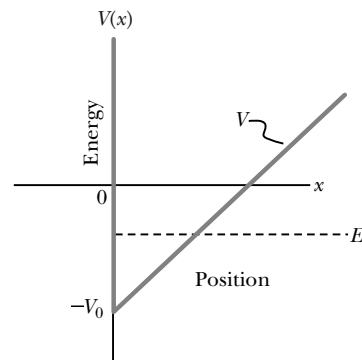
$$\psi_n = A(2\alpha x^2 - 1)e^{-\alpha x^2/2}$$

where  $A$  is a constant. What is the value of the energy level  $E_n$ ?

37. What would you expect for  $\langle p \rangle$  and  $\langle p^2 \rangle$  for the ground state of the simple harmonic oscillator? (*Hint*: Use symmetry and energy arguments.)
38. Show that the energy of a simple harmonic oscillator in the  $n = 1$  state is  $3\hbar\omega/2$  by substituting the wave function  $\psi_1 = A x e^{-\alpha x^2/2}$  directly into the Schrödinger equation.
39. An  $\text{H}_2$  molecule can be approximated by a simple harmonic oscillator with a force constant  $k = 1.1 \times 10^3$  N/m. Find (a) the energy levels and (b) the possible wavelengths of photons emitted when the  $\text{H}_2$  molecule decays from the third excited state eventually to the ground state.

### 6.7 Barriers and Tunneling

40. The creation of elements in the early universe and in stars involves protons tunneling through nuclei. Find the probability of the proton tunneling through  $^{12}\text{C}$  when the temperature of the star containing the proton and carbon is 12,000 K.
41. Compare the wavelength of a particle when it passes a barrier of height (a)  $+V_0$  (see Figure 6.12) and (b)  $-V_0$  where  $E > |V_0|$  (see Figure 6.18). Calculate the momentum and kinetic energy for both cases.
42. (a) Calculate the transmission probability of an  $\alpha$  particle of energy  $E = 5.0$  MeV through a Coulomb barrier of a heavy nucleus that is approximated by a square barrier with  $V_0 = 15$  MeV and barrier width  $L = 1.3 \times 10^{-14}$  m. Also, calculate the probability (b) by doubling the potential barrier height and (c) by using the original barrier height but doubling the barrier width. Compare all three probabilities.
43. Consider a particle of energy  $E$  trapped inside the potential well shown in the accompanying figure. Make an approximate sketch of possible wave functions inside and outside the potential well. Explain your sketch.



**Problem 43** A potential well is infinite for  $x \leq 0$  but increases linearly from  $V = -V_0$  at  $x = 0$ .

44. When a particle of energy  $E$  approaches a potential barrier of height  $V_0$ , where  $E \gg V_0$ , show that the reflection coefficient is about  $\{[V_0 \sin(kL)]/2E\}^2$ .
45. Let 12.0-eV electrons approach a potential barrier of height 4.2 eV. (a) For what barrier thickness is there no reflection? (b) For what barrier thickness is the reflection a maximum?
46. A 1.0-eV electron has a  $2.0 \times 10^{-4}$  probability of tunneling through a 2.5-eV potential barrier. What is the probability of a 1.0-eV proton tunneling through the same barrier?
47. An electron is attempting to tunnel through a square barrier potential. (a) Draw a potential function with zero potential on either side of a square-top potential similar to Figure 6.12. Draw the wave function before, after, and inside the barrier. (b) Let the barrier be twice as wide and repeat part (a). (c) Let the barrier be about twice as tall as in (a) and repeat (a). Do not perform calculations; make estimates only.
48. Use the approximate Equation (6.73) to estimate the probability of (a) a 1.4-eV electron tunneling through a 6.4-eV-high barrier of width 2.8 nm, and (b) a 4.4-MeV  $\alpha$  particle tunneling through a uranium nucleus where the potential barrier is 19.2 MeV and 7.4 fm wide. (c) Discuss whether the approximation was valid for these two cases. Explain.

### General Problems

49. Check to see whether the simple linear combination of sine and cosine functions

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

satisfies the time-independent Schrödinger equation for a free particle ( $V = 0$ ).

50. (a) Check to see whether the simple linear combination of sine and cosine functions

$$\Psi(x, t) = A \sin(kx - \omega t) + B \cos(kx - \omega t)$$

where  $A$  and  $B$  are real numbers, satisfies the time-dependent Schrödinger equation for a free particle ( $V = 0$ ). (b) Repeat for the modified version

$$\Psi(x, t) = A \cos(kx - \omega t) - i A \sin(kx - \omega t)$$

51. A particle of mass  $m$  is trapped in a three-dimensional rectangular potential well with sides of length  $L$ ,  $L/\sqrt{2}$ , and  $2L$ . Inside the box  $V = 0$ , outside  $V = \infty$ . Assume that

$$\psi = A \sin(k_1 x) \sin(k_2 y) \sin(k_3 z)$$

inside the well. Substitute this wave function into the Schrödinger equation and apply appropriate boundary conditions to find the allowed energy levels. Find the energy of the ground state and first four excited levels. Which of these levels are degenerate?

52. For a region where the potential  $V = 0$ , the wave function is given by  $\sqrt{2/\alpha} \sin(3\pi x/\alpha)$ . Calculate the energy of this system.
53. Consider the semi-infinite-well potential in which  $V = \infty$  for  $x \leq 0$ ,  $V = 0$  for  $0 < x < L$ , and  $V = V_0$  for  $x \geq L$ . (a) Show that possible wave functions are  $A \sin kx$  inside the well and  $B e^{-\kappa x}$  for  $x > L$ , where  $k = \sqrt{2mE}/\hbar$  and  $\kappa = \sqrt{2m(V_0 - E)}/\hbar$ . (b) Show that the application of the boundary conditions gives  $\kappa \tan(kL) = -k$ .
54. Assume that  $V_0 = \hbar^2/2mL^2$  and show that the ground state energy of a particle in the semi-infinite well of the previous problem is given by  $0.04\hbar^2/2mL^2$ .
55. Prove that there are a limited number of bound solutions for the semi-infinite well.
56. Use the semi-infinite-well potential to model a deuteron, a nucleus consisting of a neutron and a proton. Let the well width be  $3.5 \times 10^{-15}$  m and  $V_0 - E = 2.2$  MeV. Determine the energy  $E$ . How many excited states are there, and what are their energies?
57. Consider as a model of a hydrogen atom a particle trapped in a one-dimensional, infinite potential well of width  $2a_0$  (the ground-state hydrogen atom's diameter). Find the electron's ground-state energy and comment on the result.
58. (a) Repeat the preceding problem using a cubical infinite potential well, with each side of the cube equal to  $2a_0$ .
59. In the lab you make a simple harmonic oscillator with a 0.15-kg mass attached to a 12-N/m spring. (a) If the oscillation amplitude is 0.10 m, what is the corresponding quantum number  $n$  for the quantum harmonic oscillator? (b) What would be the amplitude of the quantum ground state for this oscillator? (c) What is the energy of a photon emitted when this oscillator makes a transition between adjacent energy levels? Comment on each of your results.
60. In gravity-free space, a 2.0-mg dust grain is confined to move back and forth between rigid walls 1.0 mm apart. (a) What is the speed of the dust grain if it is in the quantum ground state? (b) If it is actually moving at a speed of 0.25 mm/s, what is the quantum number associated with its quantum state?

61. The wave function for the  $n = 2$  state of a simple harmonic oscillator is  $A(1 - 2\alpha x^2)e^{-\alpha x^2/2}$ . (a) Show that its energy level is  $5\hbar\omega/2$  by substituting the wave function into the Schrödinger equation. (b) Find  $\langle x \rangle$  and  $\langle x^2 \rangle$ .
62. A particle is trapped inside an infinite square-well potential between  $x = 0$  and  $x = L$ . Its wave function is a superposition of the ground state and first excited state. The wave function is given by

$$\psi(x) = \frac{1}{2}\psi_1(x) + \frac{\sqrt{3}}{2}\psi_2(x)$$

Show that the wave function is normalized.

63. The *Morse potential* is a good approximation for a real potential to describe diatomic molecules. It is given by  $V(r) = D(1 - e^{-\alpha(r-r_e)})^2$  where  $D$  is the molecular dissociation energy, and  $r_e$  is the equilibrium distance between the atoms. For small vibrations,  $r - r_e$  is small, and  $V(r)$  can be expanded in a Taylor series to reduce to a simple harmonic potential. Find the lowest term of  $V(r)$  in this expansion and show that it is quadratic in  $(r - r_e)$ .

64. Show that the vibrational energy levels  $E_v$  for the Morse potential of the previous problem are given by

$$E_v = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\hbar^2\omega^2}{4D}\left(n + \frac{1}{2}\right)^2$$

where

$$\omega = a\sqrt{\frac{2D}{m_r}}$$

and  $n$  is the vibrational quantum number,  $m_r$  is the reduced mass, and  $E_v \ll D$ . Find the three lowest energy levels for KCl where  $D = 4.42$  eV, and  $a = 7.8$  nm<sup>-1</sup>.

65. Consider a particle of mass  $m$  trapped inside a two-dimensional square box of sides  $L$  aligned along the  $x$  and  $y$  axes. Show that the wave function and energy levels are given by

$$\psi(x, y) = \frac{2}{L} \sin \frac{n_x \pi x}{L} \sin \frac{n_y \pi y}{L}$$

$$E = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2)$$

Plot the first six energy levels and give their quantum numbers.

66. Make a sketch for each of the following situations for both the infinite square-well and finite square-well potentials in one dimension: (a) the four lowest energy levels and (b) the probability densities for the four lowest states. (c) Discuss the differences between the two potentials and why they occur.
67. Two nanowires are separated by 1.3 nm as measured by STM. Inside the wires the potential energy is zero, but between the wires the potential energy is greater than the electron's energy by only 0.9 eV. Estimate the probability that the electron passes from one wire to the other.

- 68.** The WKB approximation is useful to obtain solutions to the one-dimensional time-independent Schrödinger equation in cases where  $E > V(x)$  and the potential  $V(x)$  changes slowly and gradually with  $x$ . In this case the wavelength  $\lambda(x)$  varies with  $x$  because of the  $V(x)$  dependence on  $x$ . (a) Argue that we can write the wavelength as

$$\lambda(x) = \frac{h}{\sqrt{2m[E - V(x)]}}$$

for a particle of mass  $m$  in a potential  $V(x)$ . (b) By considering the number of oscillations that can be fit into a distance  $dx$ , show that the following equation is valid, where  $n$  is an integer and represents the number of standing waves that fit inside the potential well.

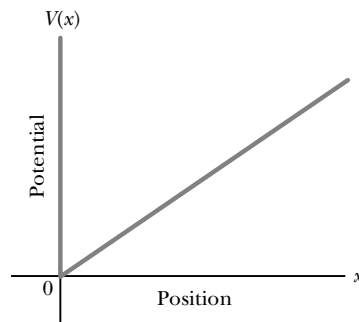
$$2 \int \sqrt{2m[E - V(x)]} dx = n\hbar \quad \text{where } n \text{ is an integer} \quad (6.74)$$

This is the WKB approximation. (*Hint:* the equation

$$\int \frac{dx}{\lambda(x)} = \frac{n}{2}$$

might be helpful.)

- 69.** Use the WKB approximation of Equation (6.74) in the previous problem with the potential shown in the accompanying figure.  $V(x) = \infty$  for  $x \leq 0$ , and  $V(x) = Ax$  for  $x > 0$ . (a) Find the quantized energy values, and (b) sketch the wave functions on top of the  $V(x)$  function for the three lowest states.



**Problem 69** The potential  $V(x) = \infty$  for  $x \leq 0$  and  $V(x) = Ax$  for  $x > 0$ .

- 70.** In the special topic box in Section 6.7, the extreme sensitivity of scanning tunneling microscopes (STM) was described. It was reported that a change in the tunneling gap of only 0.4 nm between STM sample and probe can change the tunneling current by a factor of  $10^4$ . Check the plausibility of this statement by using the “wide-barrier” approximation in Equation (6.70) to find the difference between the electron energy and barrier height that would produce such a situation. Report your answer in eV and comment in the result.





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