# Quantum Mechanics

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**In this chapter, we introduce quantum mechanics, an extremely successful theory** for explaining the behavior of

microscopic particles. This theory, devel-

**An opened flash drive of the type used as an external data storage device for a computer. Flash drives are employed extensively in computers, digital cameras, cell phones, and other devices. Writing data to and erasing data from flash drives incorporate the phenomenon of quantum tunneling, which we explore in this chapter.** *(Image copyright Vasilius, 2009. Used under license from Shutterstock.com)*

oped in the 1920s by Erwin Schrödinger, Werner Heisenberg, and others, enables us to understand a host of phenomena involving atoms, molecules, nuclei, and solids. The discussion in this chapter follows from the quantum particle model that was developed in Chapter 40 and incorporates some of the features of the waves under boundary conditions model that was explored in Chapter 18. We also discuss practical applications of quantum mechanics, including the scanning tunneling microscope and nanoscale devices that may be used in future quantum computers. Finally, we shall return to the simple harmonic oscillator that was introduced in Chapter 15 and examine it from a quantum mechanical point of view.





### 41.1 The Wave Function

In Chapter 40, we introduced some new and strange ideas. In particular, we concluded on the basis of experimental evidence that both matter and electromagnetic radiation are sometimes best modeled as particles and sometimes as waves, depending on the phenomenon being observed. We can improve our understanding of quantum physics by making another connection between particles and waves using the notion of probability, a concept that was introduced in Chapter 40.

 We begin by discussing electromagnetic radiation using the particle model. The probability per unit volume of finding a photon in a given region of space at an instant of time is proportional to the number of photons per unit volume at that time:

$$
\frac{\text{Probability}}{V} \propto \frac{N}{V}
$$

The number of photons per unit volume is proportional to the intensity of the radiation:

$$
\frac{N}{V} \propto I
$$

Now, let's form a connection between the particle model and the wave model by recalling that the intensity of electromagnetic radiation is proportional to the square of the electric field amplitude *E* for the electromagnetic wave (Eq. 34.24):

 $I \propto E^2$ 

Equating the beginning and the end of this series of proportionalities gives

Probability 
$$
\propto E^2
$$
 (41.1)

Therefore, for electromagnetic radiation, the probability per unit volume of finding a particle associated with this radiation (the photon) is proportional to the square of the amplitude of the associated electromagnetic wave.

 Recognizing the wave–particle duality of both electromagnetic radiation and matter, we should suspect a parallel proportionality for a material particle: the probability per unit volume of finding the particle is proportional to the square of the amplitude of a wave representing the particle. In Chapter 40, we learned that there is a de Broglie wave associated with every particle. The amplitude of the de Broglie wave associated with a particle is not a measurable quantity because the wave function representing a particle is generally a complex function as we discuss below. In contrast, the electric field for an electromagnetic wave is a real function. The matter analog to Equation 41.1 relates the square of the amplitude of the wave to the probability per unit volume of finding the particle. Hence, the amplitude of the wave associated with the particle is called the **probability amplitude,** or the **wave function,** and it has the symbol  $\Psi$ .

In general, the complete wave function  $\Psi$  for a system depends on the positions of all the particles in the system and on time; therefore, it can be written  $\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_j, \ldots, t)$ , where  $\vec{r}_j$  is the position vector of the *j*th particle in the system. For many systems of interest, including all those we study in this text, the wave function  $\Psi$  is mathematically separable in space and time and can be written as a product of a space function  $\psi$  for one particle of the system and a complex time function:<sup>1</sup>

 $\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_j, \ldots, t) = \psi(\vec{r}_j) e^{-i\omega t}$  (41.2)

where  $\omega$  (=  $2\pi f$ ) is the angular frequency of the wave function and  $i = \sqrt{-1}$ .

<sup>1</sup>The standard form of a complex number is  $a + ib$ . The notation  $e^{i\theta}$  is equivalent to the standard form as follows:  $e^{i\theta} = \cos \theta + i \sin \theta$ 

Therefore, the notation  $e^{-i\omega t}$  in Equation 41.2 is equivalent to cos  $(-\omega t) + i\sin(-\omega t) = \cos \omega t - i\sin \omega t$ .

Space- and time-dependent  $\blacktriangleright$ **wave function**  $\Psi$ 

 For any system in which the potential energy is time-independent and depends only on the positions of particles within the system, the important information about the system is contained within the space part of the wave function. The time part is simply the factor  $e^{-i\omega t}$ . Therefore, an understanding of  $\psi$  is the critical aspect of a given problem.

The wave function  $\psi$  is often complex-valued. The absolute square  $|\psi|^2 = \psi^* \psi$ , where  $\psi^*$  is the complex conjugate<sup>2</sup> of  $\psi$ , is always real and positive and is proportional to the probability per unit volume of finding a particle at a given point at some instant. The wave function contains within it all the information that can be known about the particle.

Although  $\psi$  cannot be measured, we can measure the real quantity  $|\psi|^2$ , which can be interpreted as follows. If  $\psi$  represents a single particle, then  $|\psi|^2$ —called the **probability density**—is the relative probability per unit volume that the particle will be found at any given point in the volume. This interpretation can also be stated in the following manner. If *dV* is a small volume element surrounding some point, the probability of finding the particle in that volume element is

$$
P(x, y, z) dV = |\psi|^2 dV \tag{41.3}
$$

 This probabilistic interpretation of the wave function was first suggested by Max Born (1882–1970) in 1928. In 1926, Erwin Schrödinger proposed a wave equation that describes the manner in which the wave function changes in space and time. The *Schrödinger wave equation,* which we shall examine in Section 41.3, represents a key element in the theory of quantum mechanics.

 The concepts of quantum mechanics, strange as they sometimes may seem, developed from classical ideas. In fact, when the techniques of quantum mechanics are applied to macroscopic systems, the results are essentially identical to those of classical physics. This blending of the two approaches occurs when the de Broglie wavelength is small compared with the dimensions of the system. The situation is similar to the agreement between relativistic mechanics and classical mechanics when  $v \ll c$ .

 In Section 40.5, we found that the de Broglie equation relates the momentum of a particle to its wavelength through the relation  $p = h/\lambda$ . If an ideal free particle has a precisely known momentum  $p_r$ , its wave function is an infinitely long sinusoidal wave of wavelength  $\lambda = h/p_x$  and the particle has equal probability of being at any point along the *x* axis (Fig. 40.18a). The wave function  $\psi$  for such a free particle moving along the *x* axis can be written as

$$
\psi(x) = Ae^{ikx} \tag{41.4}
$$

where *A* is a constant amplitude and  $k = 2\pi/\lambda$  is the angular wave number (Eq. 16.8) of the wave representing the particle.3

#### **One-Dimensional Wave Functions and Expectation Values**

This section discusses only one-dimensional systems, where the particle must be located along the *x* axis, so the probability  $|\psi|^2 dV$  in Equation 41.3 is modified to become  $|\psi|^2 dx$ . The probability that the particle will be found in the infinitesimal interval *dx* around the point *x* is

$$
P(x) \, dx = |\psi|^2 \, dx \tag{41.5}
$$

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

The real part of this wave function has the same form as the waves we added together to form wave packets in Section 40.6.

#### **4** Probability density  $|\psi|^2$

#### **Pitfall Prevention 41.1**

#### **The Wave Function Belongs to a System**

The common language in quantum mechanics is to associate a wave function with a particle. The wave function, however, is determined by the particle *and* its interaction with its environment, so it more rightfully belongs to a system. In many cases, the particle is the only part of the system that experiences a change, which is why the common language has developed. You will see examples in the future in which it is more proper to think of the system wave function rather than the particle wave function.

W **Wave function for a free particle**

<sup>&</sup>lt;sup>2</sup>For a complex number  $z = a + ib$ , the complex conjugate is found by changing  $i$  to  $-iz * = a - ib$ . The product of a complex number and its complex conjugate is always real and positive. That is,  $z^*z = (a - ib)(a + ib) = a^2 - (ib)^2 =$  $a^2 - (i)^2 b^2 = a^2 + b^2$ .

 ${}^{3}$ For the free particle, the full wave function, based on Equation 41.2, is



**Figure 41.1** An arbitrary probability density curve for a particle.

#### **Normalization condition on**  $\psi$

**Expectation value > for position** *x*

**Expectation value for**  $\blacktriangleright$ **a function** *f***(***x***)**

 Although it is not possible to specify the position of a particle with complete certainty, it is possible through  $|\psi|^2$  to specify the probability of observing it in a region surrounding a given point *x.* The probability of finding the particle in the arbitrary interval  $a \leq x \leq b$  is

$$
P_{ab} = \int_{a}^{b} |\psi|^2 dx \tag{41.6}
$$

The probability  $P_{ab}$  is the area under the curve of  $|\psi|^2$  versus *x* between the points  $x = a$  and  $x = b$  as in Figure 41.1.

 Experimentally, there is a finite probability of finding a particle in an interval near some point at some instant. The value of that probability must lie between the limits 0 and 1. For example, if the probability is 0.30, there is a 30% chance of finding the particle in the interval.

 Because the particle must be somewhere along the *x* axis, the sum of the probabilities over all values of *x* must be 1:

$$
\int_{-\infty}^{\infty} |\psi|^2 \ dx = 1
$$
 (41.7)

Any wave function satisfying Equation 41.7 is said to be **normalized.** Normalization is simply a statement that the particle exists at some point in space.

 Once the wave function for a particle is known, it is possible to calculate the average position at which you would expect to find the particle after many measurements. This average position is called the **expectation value** of *x* and is defined by the equation

$$
\langle x \rangle \equiv \int_{-\infty}^{\infty} \psi^* x \psi \ dx
$$
 (41.8)

(Brackets,  $\langle \ldots \rangle$ , are used to denote expectation values.) Furthermore, one can find the expectation value of any function  $f(x)$  associated with the particle by using the following equation:4

$$
\langle f(x) \rangle \equiv \int_{-\infty}^{\infty} \psi^* f(x) \psi \ dx
$$
 (41.9)

*Quick Quiz* **41.1** Consider the wave function for the free particle, Equation 41.4. At what value of *x* is the particle most likely to be found at a given time? **(a)** at  $x = 0$  **(b)** at small nonzero values of  $x$  **(c)** at large values of  $x$  **(d)** anywhere along the *x* axis

#### *Example* **41.1 A Wave Function for a Particle**

Consider a particle whose wave function is graphed in Figure 41.2 and is given by

 $\psi(x) = Ae^{-ax^2}$ 

**(A)** What is the value of *A* if this wave function is normalized?

<sup>4</sup>Expectation values are analogous to "weighted averages," in which each possible value of a function is multiplied by the probability of the occurrence of that value before summing over all possible values. We write the expectation value as  $\int_{-\infty}^{\infty} \psi^* f(x) \psi \ dx$  rather than  $\int_{-\infty}^{\infty} f(x) \psi^2 \ dx$  because  $f(x)$  may be represented by an operator (such as a derivative) rather than a simple multiplicative function in more advanced treatments of quantum mechanics. In these situations, the operator is applied only to  $\psi$  and not to  $\psi^*$ .

### **41.1** *cont.*

### SOLUTION

**Conceptualize** The particle is not a free particle because the wave function is not a sinusoidal function. Figure 41.2 indicates that the particle is constrained to remain close to  $x = 0$  at all times. Think of a physical system in which the particle always stays close to a given point. Examples of such systems are a block on a spring, a marble at the bottom of a bowl, and the bob of a simple pendulum.

**Categorize** Because the statement of the problem describes the wave nature of a particle, this example requires a quantum approach rather than a classical approach.

 $\infty$ 

 $|\psi|^2 dx =$ 



**Figure 41.2** (Example 41.1) A symmetric wave function for a particle, given by  $\psi(x) = Ae^{-ax^2}$ .

 $e^{-2ax^2} dx = 1$ 

**Analyze** Apply the normalization condition, Equation  $\left\{\frac{41.7}{5}\right\}$ 

Express the integral as the sum of two integrals:

Change the integration variable from  $x$  to  $-x$  in the second integral:

Reverse the order of the limits, which introduces a negative sign:

Substitute this expression for the second integral in Equation (1):

Evaluate the integral with the help of Table B.6 in Appendix B:

Substitute this result into Equation (2) and solve for *A*:

**(B)** What is the expectation value of *x* for this particle?

#### **SOLUTION**

Evaluate the expectation value using Equation 41.8:

(1) 
$$
A^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = A^2 \left( \int_{0}^{\infty} e^{-2ax^2} dx + \int_{-\infty}^{0} e^{-2ax^2} dx \right) = 1
$$
  
\n $\int_{-\infty}^{0} e^{-2ax^2} dx = \int_{\infty}^{0} e^{-2a(-x)^2} (-dx) = -\int_{\infty}^{0} e^{-2ax^2} dx$   
\n $- \int_{\infty}^{0} e^{-2ax^2} dx = \int_{0}^{\infty} e^{-2ax^2} dx$   
\n $A^2 \left( \int_{0}^{\infty} e^{-2ax^2} dx + \int_{0}^{\infty} e^{-2ax^2} dx \right) = 1$   
\n(2)  $2A^2 \int_{0}^{\infty} e^{-2ax^2} dx = 1$   
\n $\int_{0}^{\infty} e^{-2ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{2a}}$   
\n $2A^2 \left( \frac{1}{2} \sqrt{\frac{\pi}{2a}} \right) = 1 \longrightarrow A = \left( \frac{2a}{\pi} \right)^{1/4}$ 

 $(Ae^{-ax^2})^2 dx = A^2$ 

$$
\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx = \int_{-\infty}^{\infty} (A e^{-ax^2}) x (A e^{-ax^2}) \, dx
$$

$$
= A^2 \int_{-\infty}^{\infty} x e^{-2ax^2} dx
$$

$$
(3) \quad \langle x \rangle = A^2 \Big( \int_{0}^{\infty} x e^{-2ax^2} dx + \int_{-\infty}^{0} x e^{-2ax^2} dx \Big)
$$

As in part (A), express the integral as a sum of two integrals:

*continued*

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**41.1** *cont.*

Change the integration variable from  $x$  to  $-x$  in the second integral:

Reverse the order of the limits, which introduces a negative sign:

Substitute this expression for the second integral in Equation (3):

$$
\int_{-\infty}^{0} xe^{-2ax^{2}} dx = \int_{\infty}^{0} -xe^{-2a(-x)^{2}} (-dx) = \int_{\infty}^{0} xe^{-2ax^{2}} dx
$$

$$
\int_{\infty}^{0} xe^{-2ax^2} dx = -\int_{0}^{\infty} xe^{-2ax^2} dx
$$

$$
\langle x \rangle = A^2 \bigg( \int_0^\infty x e^{-2ax^2} dx - \int_0^\infty x e^{-2ax^2} dx \bigg) = 0
$$

**Finalize** Given the symmetry of the wave function around  $x = 0$  in Figure 41.2, it is not surprising that the average position of the particle is at  $x = 0$ . In Section 41.7, we show that the wave function studied in this example represents the lowest-energy state of the quantum harmonic oscillator.

This figure is a *pictorial representation* showing a particle of mass *m* and speed *u* bouncing between two impenetrable walls separated by a distance *L*.



 $\frac{1}{2}$  x *L* b **Figure 41.3** (a) The particle in a

box. (b) The potential energy function for the system.

### 41.2 Analysis Model: Quantum Particle Under Boundary Conditions

The free particle discussed in Section 41.1 has no boundary conditions; it can be anywhere in space. The particle in Example 41.1 is not a free particle. Figure 41.2 shows that the particle is always restricted to positions near  $x = 0$ . In this section, we shall investigate the effects of restrictions on the motion of a quantum particle.

#### **A Particle in a Box**

We begin by applying some of the ideas we have developed to a simple physical problem, a particle confined to a one-dimensional region of space, called the *particle-in-a-box* problem (even though the "box" is one-dimensional!). From a classical viewpoint, if a particle is bouncing elastically back and forth along the *x* axis between two impenetrable walls separated by a distance *L* as in Figure 41.3a, it can be modeled as a particle under constant speed. If the speed of the particle is *u,* the magnitude of its momentum *mu* remains constant as does its kinetic energy. (Recall that in Chapter 39 we used *u* for particle speed to distinguish it from *v,* the speed of a reference frame.) Classical physics places no restrictions on the values of a particle's momentum and energy. The quantum-mechanical approach to this problem is quite different and requires that we find the appropriate wave function consistent with the conditions of the situation.

 Because the walls are impenetrable, there is zero probability of finding the particle outside the box, so the wave function  $\psi(x)$  must be zero for  $x < 0$  and  $x > L$ . To be a mathematically well-behaved function,  $\psi(x)$  must be continuous in space. There must be no discontinuous jumps in the value of the wave function at any point.<sup>5</sup> Therefore, if  $\psi$  is zero outside the walls, it must also be zero *at* the walls; that is,  $\psi(0) = 0$  and  $\psi(L) = 0$ . Only those wave functions that satisfy these boundary conditions are allowed.

 Figure 41.3b, a graphical representation of the particle-in-a-box problem, shows the potential energy of the particle–environment system as a function of the position of the particle. As long as the particle is inside the box, the potential energy

<sup>5</sup>If the wave function were not continuous at a point, the derivative of the wave function at that point would be infinite. This result leads to difficulties in the Schrödinger equation, for which the wave function is a solution as discussed in Section 41.3.



#### **ACTIVE FIGURE 41.4**

The first three allowed states for a particle confined to a onedimensional box. The states are shown superimposed on the potential energy function of Figure 41.3b. The wave functions and probability densities are plotted vertically from separate axes that are offset vertically for clarity. The positions of these axes on the potential energy function suggest the relative energies of the states.

of the system does not depend on the location of the particle and we can choose its constant value to be zero. Outside the box, we must ensure that the wave function is zero. We can do so by defining the system's potential energy as infinitely large if the particle were outside the box. Therefore, the only way a particle could be outside the box is if the system has an infinite amount of energy, which is impossible.

 The wave function for a particle in the box can be expressed as a real sinusoidal function:6

$$
\psi(x) = A \sin\left(\frac{2\pi x}{\lambda}\right)
$$
\n(41.10)

where  $\lambda$  is the de Broglie wavelength associated with the particle. This wave function must satisfy the boundary conditions at the walls. The boundary condition  $\psi(0) = 0$  is satisfied already because the sine function is zero when  $x = 0$ . The boundary condition  $\psi(L) = 0$  gives

$$
\psi(L) = 0 = A \sin\left(\frac{2\pi L}{\lambda}\right)
$$

which can only be true if

$$
\frac{2\pi L}{\lambda} = n\pi \quad \rightarrow \quad \lambda = \frac{2L}{n} \tag{41.11}
$$

where  $n = 1, 2, 3, \ldots$ . Therefore, only certain wavelengths for the particle are allowed! Each of the allowed wavelengths corresponds to a quantum state for the system, and *n* is the quantum number. Incorporating Equation 41.11 in Equation 41.10 gives

$$
\psi(x) = A \sin\left(\frac{2\pi x}{2L/n}\right) = A \sin\left(\frac{n\pi x}{L}\right)
$$
\n(41.12)

normalizing this wave function shows that  $A = \sqrt{2/L}$ . (See Problem 17.) Therefore, the normalized wave function for the particle in a box is

$$
\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)
$$
\n(41.13)

Active Figures 41.4a and b on page 1226 are graphical representations of  $\psi$  versus *x* and  $|\psi|^2$  versus *x* for *n* = 1, 2, and 3 for the particle in a box.<sup>7</sup> Although  $\psi$  can

W **Wave functions for a particle in a box**

#### W **Normalized wave function for a particle in a box**

<sup>6</sup>We shall show this result explicitly in Section 41.3.

#### **Pitfall Prevention 41.2**

#### **Reminder: Energy Belongs to a System**

We often refer to the energy of a particle in commonly used language. As in Pitfall Prevention 41.1, we are actually describing the energy of the *system* of the particle and whatever environment is establishing the impenetrable walls. For the particle in a box, the only type of energy is kinetic energy belonging to the particle, which is the origin of the common description.



#### **ACTIVE FIGURE 41.5**

Energy-level diagram for a particle confined to a one-dimensional box of length *L.*

be positive or negative,  $|\psi|^2$  is always positive. Because  $|\psi|^2$  represents a probability density, a negative value for  $|\psi|^2$  would be meaningless.

Further inspection of Active Figure 41.4b shows that  $|\psi|^2$  is zero at the boundaries, satisfying our boundary conditions. In addition,  $|\psi|^2$  is zero at other points, depending on the value of *n*. For  $n = 2$ ,  $|\psi|^2 = 0$  at  $x = L/2$ ; for  $n = 3$ ,  $|\psi|^2 = 0$  at  $x = L/3$  and at  $x = 2L/3$ . The number of zero points increases by one each time the quantum number increases by one.

Because the wavelengths of the particle are restricted by the condition  $\lambda = 2L/n$ , the magnitude of the momentum of the particle is also restricted to specific values, which can be found from the expression for the de Broglie wavelength, Equation 40.15:

$$
p = \frac{h}{\lambda} = \frac{h}{2L/n} = \frac{nh}{2L}
$$

We have chosen the potential energy of the system to be zero when the particle is inside the box. Therefore, the energy of the system is simply the kinetic energy of the particle and the allowed values are given by

$$
E_n = \frac{1}{2}mu^2 = \frac{p^2}{2m} = \frac{(nh/2L)^2}{2m}
$$

$$
E_n = \left(\frac{h^2}{8mL^2}\right)n^2 \quad n = 1, 2, 3, ... \tag{41.14}
$$

This expression shows that the energy of the particle is quantized. The lowest allowed energy corresponds to the **ground state,** which is the lowest energy state for any system. For the particle in a box, the ground state corresponds to  $n = 1$ , for which  $E_1 = h^2/8mL^2$ . Because  $E_n = n^2E_1$ , the **excited states** corresponding to  $n = 2, 3, 4, \ldots$  have energies given by  $4E_1, 9E_1, 16E_1, \ldots$ 

 Active Figure 41.5 is an energy-level diagram describing the energy values of the allowed states. Because the lowest energy of the particle in a box is not zero, then, according to quantum mechanics, the particle can never be at rest! The smallest energy it can have, corresponding to  $n = 1$ , is called the **ground-state energy.** This result contradicts the classical viewpoint, in which  $E = 0$  is an acceptable state, as are *all* positive values of *E.*

*Quick Quiz* **41.2** Consider an electron, a proton, and an alpha particle (a helium nucleus), each trapped separately in identical boxes. **(i)** Which particle corresponds to the highest ground-state energy? (a) the electron (b) the proton (c) the alpha particle (d) The ground-state energy is the same in all three cases. **(ii)** Which particle has the longest wavelength when the system is in the ground state? (a) the electron (b) the proton (c) the alpha particle (d) All three particles have the same wavelength.

*Quick Quiz* **41.3** A particle is in a box of length *L.* Suddenly, the length of the box is increased to 2*L.* What happens to the energy levels shown in Active Figure 41.5? **(a)** nothing; they are unaffected. **(b)** They move farther apart. **(c)** They move closer together.

<sup>&</sup>lt;sup>7</sup>Note that  $n = 0$  is not allowed because, according to Equation 41.12, the wave function would be  $\psi = 0$ , which is not a physically reasonable wave function. For example, it cannot be normalized because  $\int_{-\infty}^{\infty} |\psi|^2 dx = \int_{-\infty}^{\infty} (0) dx = 0$ , but Equation 41.7 tells us that this integral must equal 1.

*Example* **41.2 Microscopic and Macroscopic Particles in Boxes**

**(A)** An electron is confined between two impenetrable walls 0.200 nm apart. Determine the energy levels for the states  $n = 1, 2,$  and 3.

#### **SOLUTION**

**Conceptualize** In Figure 41.3a, imagine that the particle is an electron and the walls are very close together.

**Categorize** We evaluate the energy levels using an equation developed in this section, so we categorize this example as a substitution problem.

Use Equation 41.14 for the  $n = 1$  state:

Using  $E_n = n^2 E_1$ , find the energies of the  $n = 2$  and  $n = 3$  states:

**(B)** Find the speed of the electron in the  $n = 1$  state.

#### **SOLUTION**

Solve the classical expression for kinetic energy for the particle speed:

Recognize that the kinetic energy of the particle is equal to the system energy and substitute  $E_n$  for  $K$ :

Substitute numerical values from part (A):

Simply placing the electron in the box results in a *minimum* speed of the electron equal to 
$$
0.6\%
$$
 of the speed of light!

**(C)** A 0.500-kg baseball is confined between two rigid walls of a stadium that can be modeled as a box of length 100 m. Calculate the minimum speed of the baseball.

#### SOLUTION

**Conceptualize** In Figure 41.3a, imagine that the particle is a baseball and the walls are those of the stadium.

**Categorize** This part of the example is a substitution problem in which we apply a quantum approach to a macroscopic object.

Use Equation 41.14 for the  $n = 1$  state:

Use Equation (1) to find the speed:

This speed is so small that the object can be considered to be at rest, which is what one would expect for the minimum speed of a macroscopic object.

WHAT IF? What if a sharp line drive is hit so that the baseball is moving with a speed of 150 m/s? What is the quantum number of the state in which the baseball now resides?

**Answer** We expect the quantum number to be very large because the baseball is a macroscopic object. *continued*

$$
E_1 = \frac{h^2}{8m_eL^2}(1)^2 = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(9.11 \times 10^{-31} \text{ kg})(2.00 \times 10^{-10} \text{ m})^2}
$$
  
= 1.51 × 10<sup>-18</sup> J = 9.42 eV  

$$
E_2 = (2)^2 E_1 = 4(9.42 \text{ eV}) = 37.7 \text{ eV}
$$

 $\sqrt{2K}$ 

$$
E_3 = (3)^2 E_1 = 9(9.42 \text{ eV}) = 84.8 \text{ eV}
$$

$$
K = \frac{1}{2}m_e u^2 \rightarrow u = \sqrt{\frac{2K}{m_e}}
$$
  
(1) 
$$
u = \sqrt{\frac{2E_n}{m_e}}
$$

 $m_e$ 

$$
-\frac{2(1.51 \times 10^{-18} \text{J})}{2(1.51 \times 10^{-18} \text{J})}
$$

$$
u = \sqrt{\frac{2(1.51 \times 10^{-18} \text{ J})}{9.11 \times 10^{-31} \text{ kg}}} = 1.82 \times 10^6 \text{ m/s}
$$

$$
E_1 = \frac{h^2}{8mL^2}(1)^2 = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(0.500 \text{ kg})(100 \text{ m})^2} = 1.10 \times 10^{-71} \text{ J}
$$

 $\frac{2(1.10\times 10^{-71}\,\mathrm{J})}{0.500\,\mathrm{kg}} = \, 6.63\times 10^{-36}\,\mathrm{m/s}$ 

**41.2** *cont.*

Evaluate the kinetic energy of the baseball: <sup>1</sup>

 $\frac{1}{2}mu^2 = \frac{1}{2}(0.500 \text{ kg})(150 \text{ m/s})^2 = 5.62 \times 10^3 \text{ J}$ 

$$
n = \sqrt{\frac{8mL^2E_n}{h^2}} = \sqrt{\frac{8(0.500 \text{ kg})(100 \text{ m})^2(5.62 \times 10^3 \text{ J})}{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}} = 2.26 \times 10^{37}
$$

From Equation 41.14, calculate the quantum number *n*:

This result is a tremendously large quantum number. As the baseball pushes air out of the way, hits the ground, and rolls to a stop, it moves through more than  $10^{37}$  quantum states. These states are so close together in energy that we cannot observe the transitions from one state to the next. Rather, we see what appears to be a smooth variation in the speed of the ball. The quantum nature of the universe is simply not evident in the motion of macroscopic objects.

### *Example* **41.3 The Expectation Values for the Particle in a Box**

A particle of mass *m* is confined to a one-dimensional box between  $x = 0$  and  $x = L$ . Find the expectation value of the position *x* of the particle in the state characterized by quantum number *n.*

#### **SOLUTION**

**Conceptualize** Active Figure 41.4b shows that the probability for the particle to be at a given location varies with position within the box. Can you predict what the expectation value of *x* will be from the symmetry of the wave functions?

**Categorize** The statement of the example categorizes the problem for us: we focus on a quantum particle in a box and on the calculation of its expectation value of *x.* 

**Analyze** In Equation 41.8, the integration from  $-\infty$  to  $\infty$  reduces to the limits 0 to *L* because  $\psi = 0$  everywhere except in the box.

Substitute Equation 41.13 into Equation 41.8 to find the expectation value for *x:*

 $\langle x \rangle =$  $\infty$  $\oint_{-\infty}^{\infty}$  \*  $x \psi_n dx = \int_{-\infty}^{\infty}$ *L*  $\alpha$ <sup>x</sup>  $\vee$ 2  $\left(\frac{n\pi x}{L}\right)^2 dx$  $=\frac{2}{L}\int$ *L*  $\int_{0}^{L} x \sin^2 \left( \frac{n \pi x}{L} \right) dx$  $x \sin \left(2 \frac{n \pi x}{L}\right)$  $\cos\left(2\frac{n\pi x}{L}\right)$ *L*

 $4\frac{n\pi}{L}$ 

 $\overline{\phantom{0}}$ 

 $8\left(\frac{n\pi}{L}\right)$ 

 $\frac{1}{2}$ 

0

Evaluate the integral by consulting an integral table or by mathematical integration:8

**Finalize** This result shows that the expectation value of *x* is at the center of the box for all values of *n*, which you would expect from the symmetry of the square of the wave functions (the probability density) about the center (Active Fig. 41.4b).

 $\langle x \rangle = \frac{2}{L} \left| \begin{array}{c} x^2 \ 4 \end{array} \right|$ 

 $=\frac{2}{L}$ 

 $\left[\frac{L^2}{4}\right] = \frac{L}{2}$ 

The  $n = 2$  wave function in Active Figure 41.4b has a value of zero at the midpoint of the box. Can the expectation value of the particle be at a position at which the particle has zero probability of existing? Remember that the expectation value is the *average* position. Therefore, the particle is as likely to be found to the right of the midpoint as to the left, so its average position is at the midpoint even though its probability of being there is zero. As an analogy, consider a group of students for whom the average final examination score is 50%. There is no requirement that some student achieve a score of exactly 50% for the average of all students to be 50%.

<sup>&</sup>lt;sup>8</sup>To integrate this function, first replace  $\sin^2(n\pi x/L)$  with  $\frac{1}{2}(1 - \cos 2n\pi x/L)$  (refer to Table B.3 in Appendix B), which allows  $\langle x \rangle$  to be expressed as two integrals. The second integral can then be evaluated by partial integration (Section B.7 in Appendix B).

#### **Boundary Conditions on Particles in General**

The discussion of the particle in a box is very similar to the discussion in Chapter 18 of standing waves on strings:

- Because the ends of the string must be nodes, the wave functions for allowed waves must be zero at the boundaries of the string. Because the particle in a box cannot exist outside the box, the allowed wave functions for the particle must be zero at the boundaries.
- The boundary conditions on the string waves lead to quantized wavelengths and frequencies of the waves. The boundary conditions on the wave function for the particle in a box lead to quantized wavelengths and frequencies of the particle.

 In quantum mechanics, it is very common for particles to be subject to boundary conditions. We therefore introduce a new analysis model, the **quantum particle under boundary conditions.** In many ways, this model is similar to the waves under boundary conditions model studied in Section 18.3. In fact, the allowed wavelengths for the wave function of a particle in a box (Eq. 41.11) are identical in form to the allowed wavelengths for mechanical waves on a string fixed at both ends (Eq. 18.4).

 The quantum particle under boundary conditions model *differs* in some ways from the waves under boundary conditions model:

- In most cases of quantum particles, the wave function is *not* a simple sinusoidal function like the wave function for waves on strings. Furthermore, the wave function for a quantum particle may be a complex function.
- For a quantum particle, frequency is related to energy through  $E = hf$ , so the quantized frequencies lead to quantized energies.
- There may be no stationary "nodes" associated with the wave function of a quantum particle under boundary conditions. Systems more complicated than the particle in a box have more complicated wave functions, and some boundary conditions may not lead to zeroes of the wave function at fixed points.

In general,

an interaction of a quantum particle with its environment represents one or more boundary conditions, and, if the interaction restricts the particle to a finite region of space, results in quantization of the energy of the system.

 Boundary conditions on quantum wave functions are related to the coordinates describing the problem. For the particle in a box, the wave function must be zero at two values of *x.* In the case of a three-dimensional system such as the hydrogen atom we shall discuss in Chapter 42, the problem is best presented in *spherical coordinates.* These coordinates, an extension of the plane polar coordinates introduced in Section 3.1, consist of a radial coordinate *r* and two angular coordinates. The generation of the wave function and application of the boundary conditions for the hydrogen atom are beyond the scope of this book. We shall, however, examine the behavior of some of the hydrogen-atom wave functions in Chapter 42.

 Boundary conditions on wave functions that exist for all values of *x* require that the wave function approach zero as  $x \to \infty$  (so that the wave function can be normalized) and remain finite as  $x \rightarrow 0$ . One boundary condition on any angular parts of wave functions is that adding  $2\pi$  radians to the angle must return the wave function to the same value because an addition of  $2\pi$  results in the same angular position.

*Quick Quiz* **41.4** Which of the following exhibit quantized energy levels? **(a)** an atom in a crystal **(b)** an electron and a proton in a hydrogen atom **(c)** a proton in the nucleus of a heavy atom **(d)** all of the above **(e)** none of the above

### 41.3 The Schrödinger Equation

In Section 34.3, we discussed a wave equation for electromagnetic radiation that follows from Maxwell's equations. The waves associated with particles also satisfy a wave equation. The wave equation for material particles is different from that associated with photons because material particles have a nonzero rest energy. The appropriate wave equation was developed by Schrödinger in 1926. In analyzing the behavior of a quantum system, the approach is to determine a solution to this equation and then apply the appropriate boundary conditions to the solution. This process yields the allowed wave functions and energy levels of the system under consideration. Proper manipulation of the wave function then enables one to calculate all measurable features of the system.

 The Schrödinger equation as it applies to a particle of mass *m* confined to moving along the *x* axis and interacting with its environment through a potential energy function  $U(x)$  is

**Time-independent** X **Schrödinger equation**

*Erwin Schrödinger* Austrian Theoretical Physicist (1887–1961)

Schrödinger is best known as one of the creators of quantum mechanics. His approach to quantum mechanics was demonstrated to be mathematically equivalent to the more abstract matrix mechanics developed by Heisenberg. Schrödinger also produced important papers in the fields of statistical mechanics, color vision, and general relativity.<br> **Ericin Schrödinger**<br> **Austrian Theoretical Physicist**<br>
(1887–1961)<br>
Schrödinger is best known as one of the cre-<br>
ators of quantum mechanics. His approach<br>
to be mathemati

$$
-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U\psi = E\psi
$$
 (41.15)

where  $E$  is a constant equal to the total energy of the system (the particle and its environment). Because this equation is independent of time, it is commonly referred to as the **time-independent Schrödinger equation.** (We shall not discuss the time-dependent Schrödinger equation in this book.)

 The Schrödinger equation is consistent with the principle of conservation of mechanical energy of a system. Problem 44 shows, both for a free particle and a particle in a box, that the first term in the Schrödinger equation reduces to the kinetic energy of the particle multiplied by the wave function. Therefore, Equation 41.15 indicates that the total energy of the system is the sum of the kinetic energy and the potential energy and that the total energy is a constant:  $K + U = E =$ constant.

 In principle, if the potential energy function *U* for a system is known, one can solve Equation 41.15 and obtain the wave functions and energies for the allowed states of the system. In addition, in many cases, the wave function  $\psi$  must satisfy boundary conditions. Therefore, once we have a preliminary solution to the Schrödinger equation, we impose the following conditions to find the exact solution and the allowed energies:

- $\psi$  must be normalizable. That is, Equation 41.7 must be satisfied.
- $\psi$  must go to 0 as  $x \to \pm \infty$  and remain finite as  $x \to 0$ .
- $\bullet \psi$  must be continuous in *x* and be single-valued everywhere; solutions to Equation 41.15 in different regions must join smoothly at the boundaries between the regions.
- $\bullet$   $d\psi/dx$  must be finite, continuous, and single-valued everywhere for finite values of *U*. If  $d\psi/dx$  were not continuous, we would not be able to evaluate the factor  $d^2\psi/dx^2$  in Equation 41.15 at the point of discontinuity.

 The task of solving the Schrödinger equation may be very difficult, depending on the form of the potential energy function. As it turns out, the Schrödinger equa-



tion is extremely successful in explaining the behavior of atomic and nuclear systems, whereas classical physics fails to explain this behavior. Furthermore, when quantum mechanics is applied to macroscopic objects, the results agree with classical physics.

#### **The Particle in a Box Revisited**

To see how the quantum particle under boundary conditions model is applied to a problem, let's return to our particle in a one-dimensional box of length *L* (see Fig. 41.3) and analyze it with the Schrödinger equation. Figure 41.3b is the potentialenergy diagram that describes this problem. Potential-energy diagrams are a useful representation for understanding and solving problems with the Schrödinger equation.

 Because of the shape of the curve in Figure 41.3b, the particle in a box is sometimes said to be in a **square well,**9 where a **well** is an upward-facing region of the curve in a potential-energy diagram. (A downward-facing region is called a *barrier,* which we investigate in Section 41.5.) Figure 41.3b shows an infinite square well.

In the region  $0 \le x \le L$ , where  $U = 0$ , we can express the Schrödinger equation in the form

$$
\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi
$$
\n(41.16)

where

$$
k = \frac{\sqrt{2mE}}{\hbar}
$$

The solution to Equation 41.16 is a function  $\psi$  whose second derivative is the negative of the same function multiplied by a constant  $k^2$ . Both the sine and cosine functions satisfy this requirement. Therefore, the most general solution to the equation is a linear combination of both solutions:

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

where *A* and *B* are constants that are determined by the boundary and normalization conditions.

The first boundary condition on the wave function is that  $\psi(0) = 0$ :

$$
\psi(0) = A \sin 0 + B \cos 0 = 0 + B = 0
$$

which means that  $B = 0$ . Therefore, our solution reduces to

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

The second boundary condition,  $\psi(L) = 0$ , when applied to the reduced solution gives

$$
\psi(L) = A \sin kL = 0
$$

This equation could be satisfied by setting  $A = 0$ , but that would mean that  $\psi = 0$ everywhere, which is not a valid wave function. The boundary condition is satisfied if kL is an integral multiple of  $\pi$ , that is, if  $kL = n\pi$ , where *n* is an integer. Substituting  $k = \sqrt{2mE}/\hbar$  into this expression gives

$$
kL = \frac{\sqrt{2mE}}{\hbar}L = n\pi
$$

9It is called a square well even if it has a rectangular shape in a potential-energy diagram.

### **Pitfall Prevention 41.3**

#### **Potential Wells**

A potential well such as that in Figure 41.3b is a graphical representation of energy, not a pictorial representation, so you would not see this shape if you were able to observe the situation. A particle moves *only horizontally* at a fixed vertical position in a potential-energy diagram, representing the conserved energy of the system of the particle and its environment.

If the total energy *E* of the particle–well system is less than *U*, the particle is trapped in the well.



**Figure 41.6** Potential-energy diagram of a well of finite height *U* and length *L.*

Each value of the integer *n* corresponds to a quantized energy that we call *En*. Solving for the allowed energies *En* gives

$$
E_n = \left(\frac{h^2}{8mL^2}\right)n^2\tag{41.17}
$$

which are identical to the allowed energies in Equation 41.14.

 Substituting the values of *k* in the wave function, the allowed wave functions  $\psi_n(x)$  are given by

$$
\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right) \tag{41.18}
$$

which is the wave function (Eq. 41.12) used in our initial discussion of the particle in a box.

### 41.4 A Particle in a Well of Finite Height

Now consider a particle in a *finite* potential well, that is, a system having a potential energy that is zero when the particle is in the region  $0 \leq x \leq L$  and a finite value *U* when the particle is outside this region as in Figure 41.6. Classically, if the total energy *E* of the system is less than *U,* the particle is permanently bound in the potential well. If the particle were outside the well, its kinetic energy would have to be negative, which is an impossibility. According to quantum mechanics, however, a finite probability exists that the particle can be found outside the well even if  $E \leq U$ . That is, the wave function  $\psi$  is generally nonzero outside the well—regions I and III in Figure 41.6—so the probability density  $|\psi|^2$  is also nonzero in these regions. Although this notion may be uncomfortable to accept, the uncertainty principle indicates that the energy of the system is uncertain. This uncertainty allows the particle to be outside the well as long as the apparent violation of conservation of energy does not exist in any measurable way.

In region II, where  $U = 0$ , the allowed wave functions are again sinusoidal because they represent solutions of Equation 41.16. The boundary conditions, however, no longer require that  $\psi$  be zero at the ends of the well, as was the case with the infinite square well.

The Schrödinger equation for regions I and III may be written

$$
\frac{d^2\psi}{dx^2} = \frac{2m(U-E)}{\hbar^2}\psi
$$
\n(41.19)

Because  $U > E$ , the coefficient of  $\psi$  on the right-hand side is necessarily positive. Therefore, we can express Equation 41.19 as

$$
\frac{d^2\psi}{dx^2} = C^2\psi
$$
\n(41.20)

where  $C^2 = 2m(U - E)/\hbar^2$  is a positive constant in regions I and III. As you can verify by substitution, the general solution of Equation 41.20 is

$$
\psi = Ae^{Cx} + Be^{-Cx} \tag{41.21}
$$

where *A* and *B* are constants.

 We can use this general solution as a starting point for determining the appropriate solution for regions I and III. The solution must remain finite as  $x \to \pm \infty$ . Therefore, in region I, where  $x < 0$ , the function  $\psi$  cannot contain the term  $Be^{-Cx}$ . This requirement is handled by taking  $B = 0$  in this region to avoid an infinite value for  $\psi$  for large negative values of *x*. Likewise, in region III, where  $x > L$ , the function  $\psi$  cannot contain the term  $Ae^{Cx}$ . This requirement is handled by taking



#### **ACTIVE FIGURE 41.7**

The first three allowed states for a particle in a potential well of finite height. The states are shown superimposed on the potential energy function of Figure 41.6. The wave functions and probability densities are plotted vertically from separate axes that are offset vertically for clarity. The positions of these axes on the potential energy function suggest the relative energies of the states.

 $A = 0$  in this region to avoid an infinite value for  $\psi$  for large positive *x* values. Hence, the solutions in regions I and III are

$$
\psi_{\rm I} = A e^{Cx} \qquad \text{for } x < 0
$$

$$
\psi_{\rm III} = B e^{-Cx} \qquad \text{for } x > L
$$

In region II, the wave function is sinusoidal and has the general form

$$
\psi_{\text{II}}(x) = F \sin kx + G \cos kx
$$

where *F* and *G* are constants.

 These results show that the wave functions outside the potential well (where classical physics forbids the presence of the particle) decay exponentially with distance. At large negative *x* values,  $\psi_{\text{I}}$  approaches zero; at large positive *x* values,  $\psi_{\text{III}}$ approaches zero. These functions, together with the sinusoidal solution in region II, are shown in Active Figure 41.7a for the first three energy states. In evaluating the complete wave function, we impose the following boundary conditions:

$$
\psi_{\text{I}} = \psi_{\text{II}}
$$
 and  $\frac{d\psi_{\text{I}}}{dx} = \frac{d\psi_{\text{II}}}{dx}$  at  $x = 0$   
 $\psi_{\text{II}} = \psi_{\text{III}}$  and  $\frac{d\psi_{\text{II}}}{dx} = \frac{d\psi_{\text{III}}}{dx}$  at  $x = L$ 

 These four boundary conditions and the normalization condition (Eq. 41.7) are sufficient to determine the four constants *A, B, F,* and *G* and the allowed values of the energy *E.* Active Figure 41.7b plots the probability densities for these states. In each case, the wave functions inside and outside the potential well join smoothly at the boundaries.

 The notion of trapping particles in potential wells is used in the burgeoning field of **nanotechnology,** which refers to the design and application of devices having dimensions ranging from 1 to 100 nm. The fabrication of these devices often involves manipulating single atoms or small groups of atoms to form very tiny structures or mechanisms.

 One area of nanotechnology of interest to researchers is the **quantum dot,** a small region that is grown in a silicon crystal and acts as a potential well. This region can trap electrons into states with quantized energies. The wave functions for a particle in a quantum dot look similar to those in Active Figure 41.7a if *L* is on the order of nanometers. The storage of binary information using quantum dots is The wave function is sinusoidal in regions I and III, but is exponentially decaying in region II.



**Figure 41.8** Wave function  $\psi$  for a particle incident from the left on a barrier of height *U* and width *L.* The wave function is plotted vertically from an axis positioned at the energy of the particle.

#### **Pitfall Prevention 41.4**

#### **"Height" on an Energy Diagram**

The word *height* (as in *barrier height*) refers to an energy in discussions of barriers in potential-energy diagrams. For example, we might say the height of the barrier is 10 eV. On the other hand, the barrier *width* refers to the traditional usage of such a word and is an actual physical length measurement between the locations of the two vertical sides of the barrier.

an active field of research. A simple binary scheme would involve associating a one with a quantum dot containing an electron and a zero with an empty dot. Other schemes involve cells of multiple dots such that arrangements of electrons among the dots correspond to ones and zeroes. Several research laboratories are studying the properties and potential applications of quantum dots. Information should be forthcoming from these laboratories at a steady rate in the next few years.

### 41.5 Tunneling Through a Potential Energy Barrier

Consider the potential energy function shown in Figure 41.8. In this situation, the potential energy has a constant value of *U* in the region of width *L* and is zero in all other regions.10 A potential energy function of this shape is called a **square barrier,** and *U* is called the **barrier height.** A very interesting and peculiar phenomenon occurs when a moving particle encounters such a barrier of finite height and width. Suppose a particle of energy  $E \leq U$  is incident on the barrier from the left (Fig. 41.8). Classically, the particle is reflected by the barrier. If the particle were located in region II, its kinetic energy would be negative, which is not classically allowed. Consequently, region II and therefore region III are both classically *forbidden* to the particle incident from the left. According to quantum mechanics, however, all regions are accessible to the particle, regardless of its energy. (Although all regions are accessible, the probability of the particle being in a classically forbidden region is very low.) According to the uncertainty principle, the particle could be within the barrier as long as the time interval during which it is in the barrier is short and consistent with Equation 40.24. If the barrier is relatively narrow, this short time interval can allow the particle to pass through the barrier.

 Let's approach this situation using a mathematical representation. The Schrödinger equation has valid solutions in all three regions. The solutions in regions I and III are sinusoidal like Equation 41.12. In region II, the solution is exponential like Equation 41.21. Applying the boundary conditions that the wave functions in the three regions and their derivatives must join smoothly at the boundaries, a full solution, such as the one represented by the curve in Figure 41.8, can be found. Because the probability of locating the particle is proportional to  $|\psi|^2$ , the probability of finding the particle beyond the barrier in region III is nonzero. This result is in complete disagreement with classical physics. The movement of the particle to the far side of the barrier is called **tunneling** or **barrier penetration.**

 The probability of tunneling can be described with a **transmission coefficient** *T* and a **reflection coefficient** *R.* The transmission coefficient represents the probability that the particle penetrates to the other side of the barrier, and the reflection coefficient is the probability that the particle is reflected by the barrier. Because the incident particle is either reflected or transmitted, we require that  $T + R = 1$ . An approximate expression for the transmission coefficient that is obtained in the case of  $T \ll 1$  (a very wide barrier or a very high barrier, that is,  $U \gg E$ ) is

$$
T \approx e^{-2CL} \tag{41.22}
$$

where

$$
C = \frac{\sqrt{2m(U-E)}}{\hbar}
$$
 (41.23)

This quantum model of barrier penetration and specifically Equation 41.22 show that *T* can be nonzero. That the phenomenon of tunneling is observed experimentally provides further confidence in the principles of quantum physics.

10It is common in physics to refer to *L* as the *length* of a well but the *width* of a barrier.

*Quick Quiz* **41.5** Which of the following changes would increase the probability of transmission of a particle through a potential barrier? (You may choose more than one answer.) **(a)** decreasing the width of the barrier **(b)** increasing the width of the barrier **(c)** decreasing the height of the barrier **(d)** increasing the height of the barrier **(e)** decreasing the kinetic energy of the incident particle **(f)** increasing the kinetic energy of the incident particle

*Example* **41.4 Transmission Coefficient for an Electron**

A 30-eV electron is incident on a square barrier of height 40 eV.

**(A)** What is the probability that the electron tunnels through the barrier if its width is 1.0 nm?

#### **SOLUTION**

**Conceptualize** Because the particle energy is smaller than the height of the potential barrier, we expect the electron to reflect from the barrier with a probability of 100% according to classical physics. Because of the tunneling phenomenon, however, there is a finite probability that the particle can appear on the other side of the barrier.

**Categorize** We evaluate the probability using an equation developed in this section, so we categorize this example as a substitution problem.

Evaluate the quantity 
$$
U - E
$$
 that  
appears in Equation 41.23:  

$$
U - E = 40 \text{ eV} - 30 \text{ eV} = 10 \text{ eV} \left( \frac{1.6 \times 10^{-19} \text{ J}}{1 \text{ eV}} \right) = 1.6 \times 10^{-18} \text{ J}
$$
  
Evaluate the quantity 2*CL* using Equa-  
tion 41.23:  
From Equation 41.22, find the proba-  
bility of tunneling through the barrier:  
(B) What is the probability that the electron tunnels through the barrier if its width is 0.10 nm?  
**SOLUTION**

In this case, the width *L* in Equation (1) is one-tenth as large, so evaluate the new value of 2*CL*:  $2CL = (0.1)(32.4) = 3.24$ 

From Equation 41.22, find the new probability of tunneling through the barrier:  $T \approx e^{-2CL} = e^{-3.24} = 0.039$ 

In part (A), the electron has approximately 1 chance in  $10^{14}$  of tunneling through the barrier. In part (B), however, the electron has a much higher probability (3.9%) of penetrating the barrier. Therefore, reducing the width of the barrier by only one order of magnitude increases the probability of tunneling by about 12 orders of magnitude!

### 41.6 Applications of Tunneling

As we have seen, tunneling is a quantum phenomenon, a manifestation of the wave nature of matter. Many examples exist (on the atomic and nuclear scales) for which tunneling is very important.

The alpha particle can tunnel through the barrier and escape from the nucleus even though its energy is lower than the height of the well.



**Figure 41.9** The potential well for an alpha particle in a nucleus.

#### **Alpha Decay**

One form of radioactive decay is the emission of alpha particles (the nuclei of helium atoms) by unstable, heavy nuclei (Chapter 44). To escape from the nucleus, an alpha particle must penetrate a barrier whose height is several times larger than the energy of the nucleus–alpha particle system as shown in Figure 41.9. The barrier results from a combination of the attractive nuclear force (discussed in Chapter 44) and the Coulomb repulsion (discussed in Chapter 23) between the alpha particle and the rest of the nucleus. Occasionally, an alpha particle tunnels through the barrier, which explains the basic mechanism for this type of decay and the large variations in the mean lifetimes of various radioactive nuclei.

 Figure 41.8 shows the wave function of a particle tunneling through a barrier in one dimension. A similar wave function having spherical symmetry describes the barrier penetration of an alpha particle leaving a radioactive nucleus. The wave function exists both inside and outside the nucleus, and its amplitude is constant in time. In this way, the wave function correctly describes the small but constant probability that the nucleus will decay. The moment of decay cannot be predicted. In general, quantum mechanics implies that the future is indeterminate. This feature is in contrast to classical mechanics, from which the trajectory of an object can be calculated to arbitrarily high precision from precise knowledge of its initial position and velocity and of the forces exerted on it. Do not think that the future is undetermined simply because we have incomplete information about the present. The wave function contains all the information about the state of a system. Sometimes precise predictions can be made, such as the energy of a bound system, but sometimes only probabilities can be calculated about the future. The fundamental laws of nature are probabilistic. Therefore, it appears that Einstein's famous statement about quantum mechanics, "God does not roll dice," was wrong.

 A radiation detector can be used to show that a nucleus decays by emitting a particle at a particular moment and in a particular direction. To point out the contrast between this experimental result and the wave function describing it, Schrödinger imagined a box containing a cat, a radioactive sample, a radiation counter, and a vial of poison. When a nucleus in the sample decays, the counter triggers the administration of lethal poison to the cat. Quantum mechanics correctly predicts the probability of finding the cat dead when the box is opened. Before the box is opened, does the cat have a wave function describing it as fractionally dead, with some chance of being alive?

 This question is under continuing investigation, never with actual cats but sometimes with interference experiments building upon the experiment described in Section 40.7. Does the act of measurement change the system from a probabilistic to a definite state? When a particle emitted by a radioactive nucleus is detected at one particular location, does the wave function describing the particle drop instantaneously to zero everywhere else in the Universe? (Einstein called such a state change a "spooky action at a distance.") Is there a fundamental difference between a quantum system and a macroscopic system? The answers to these questions are unknown.

#### **Nuclear Fusion**

The basic reaction that powers the Sun and, indirectly, almost everything else in the solar system is fusion, which we shall study in Chapter 45. In one step of the process that occurs at the core of the Sun, protons must approach one another to within such a small distance that they fuse and form a deuterium nucleus. (See Section 45.4.) According to classical physics, these protons cannot overcome and penetrate the barrier caused by their mutual electrical repulsion. Quantum mechanically, however, the protons are able to tunnel through the barrier and fuse together.

#### **Scanning Tunneling Microscopes**

The scanning tunneling microscope (STM) enables scientists to obtain highly detailed images of surfaces at resolutions comparable to the size of a *single atom.* Figure 41.10, showing the surface of a piece of graphite, demonstrates what STMs can do. What makes this image so remarkable is that its resolution is approximately 0.2 nm. For an optical microscope, the resolution is limited by the wavelength of the light used to make the image. Therefore, an optical microscope has a resolution no better than 200 nm, about half the wavelength of visible light, and so could never show the detail displayed in Figure 41.10.

 Scanning tunneling microscopes achieve such high resolution by using the basic idea shown in Figure 41.11. An electrically conducting probe with a very sharp tip is brought near the surface to be studied. The empty space between tip and surface represents the "barrier" we have been discussing, and the tip and surface are the two walls of the "potential well." Because electrons obey quantum rules rather than Newtonian rules, they can "tunnel" across the barrier of empty space. If a voltage is applied between surface and tip, electrons in the atoms of the surface material can tunnel preferentially from surface to tip to produce a tunneling current. In this way, the tip samples the distribution of electrons immediately above the surface.

 In the empty space between tip and surface, the electron wave function falls off exponentially (see region II in Fig. 41.8 and Example 41.4). For tip-to-surface distances  $z > 1$  nm (that is, beyond a few atomic diameters), essentially no tunneling takes place. This exponential behavior causes the current of electrons tunneling from surface to tip to depend very strongly on *z.* By monitoring the tunneling current as the tip is scanned over the surface, scientists obtain a sensitive measure of the topography of the electron distribution on the surface. The result of this scan is used to make images like that in Figure 41.10. In this way, the STM can measure the height of surface features to within 0.001 nm, approximately 1/100 of an atomic diameter!

 You can appreciate the sensitivity of STMs by examining Figure 41.10. Of the six carbon atoms in each ring, three appear lower than the other three. In fact, all six atoms are at the same height, but all have slightly different electron distributions. The three atoms that appear lower are bonded to other carbon atoms directly beneath them in the underlying atomic layer; as a result, their electron distributions, which are responsible for the bonding, extend downward beneath the surface. The atoms in the surface layer that appear higher do not lie directly over subsurface atoms and hence are not bonded to any underlying atoms. For these higher-appearing atoms, the electron distribution extends upward into the space above the surface. Because STMs map the topography of the electron distribution, this extra electron density makes these atoms appear higher in Figure 41.10.

 The STM has one serious limitation: Its operation depends on the electrical conductivity of the sample and the tip. Unfortunately, most materials are not electrically conductive at their surfaces. Even metals, which are usually excellent electrical conductors, are covered with nonconductive oxides. A newer microscope, the atomic force microscope, or AFM, overcomes this limitation.

#### **Resonant Tunneling Devices**

Let's expand on the quantum-dot discussion in Section 41.4 by exploring the **resonant tunneling device.** Active Figure 41.12a on page 1238 shows the physical construction of such a device. The island of gallium arsenide in the center is a quantum dot located between two barriers formed from the thin extensions of aluminum arsenide. Active Figure 41.12b shows both the potential barriers encountered by The contours seen here represent the ring-like arrangement of individual carbon atoms on the crystal surface.



**Figure 41.10** The surface of graphite as "viewed" with a scanning tunneling microscope. This type of microscope enables scientists to see details with a lateral resolution of about 0.2 nm and a vertical resolution of 0.001 nm.



**Figure 41.11** Schematic view of a scanning tunneling microscope. A scan of the tip over the sample can reveal surface contours down to the atomic level. An STM image is composed of a series of scans displaced laterally from one another. (Based on a drawing from P. K. Hansma, V. B. Elings, O. Marti, and C. Bracker, *Science* **242:** 209, 1988.  $\odot$  1988 by the AAAS.)

#### **ACTIVE FIGURE 41.12**

(a) The physical structure of a resonant tunneling device. (b) A potential-energy diagram showing the double barrier representing the walls of the quantum dot. (c) A voltage is applied across the device.



electrons incident from the left and the quantized energy levels in the quantum dot. This situation differs from the one shown in Figure 41.8 in that there are quantized energy levels on the right of the first barrier. In Figure 41.8, an electron that tunnels through the barrier is considered a free particle and can have any energy. In contrast, the second barrier in Active Figure 41.12b imposes boundary conditions on the particle and quantizes its energy in the quantum dot. In Active Figure 41.12b, as the electron with the energy shown encounters the first barrier, it has no matching energy levels available on the right side of the barrier, which greatly reduces the probability of tunneling.

 Active Figure 41.12c shows the effect of applying a voltage: the potential decreases with position as we move to the right across the device. The deformation of the potential barrier results in an energy level in the quantum dot coinciding with the energy of the incident electrons. This "resonance" of energies gives the device its name. When the voltage is applied, the probability of tunneling increases tremendously and the device carries current. In this manner, the device can be used as a very fast switch on a nanotechnological scale.

#### **Resonant Tunneling Transistors**

Figure 41.13a shows the addition of a gate electrode at the top of the resonant tunneling device over the quantum dot. This electrode turns the device into a **resonant tunneling transistor.** The basic function of a transistor is amplification, converting a small varying voltage into a large varying voltage. Figure 41.13b, representing the potential-energy diagram for the tunneling transistor, has a slope at the bottom of the quantum dot due to the differing voltages at the source and drain electrodes. In this configuration, there is no resonance between the electron energies outside the quantum dot and the quantized energies within the dot. By applying a small voltage to the gate electrode as in Figure 41.13c, the quantized energies can be brought into resonance with the electron energy outside the well and resonant tunneling occurs. The resulting current causes a voltage across an external resistor that is much larger than that of the gate voltage; hence, the device amplifies the input signal to the gate electrode.



Figure 41.13 (a) A resonant tunneling transistor. (b) A potential-energy diagram showing the double barrier representing the walls of the quantum dot. (c) A voltage is applied to the gate electrode.

### 41.7 The Simple Harmonic Oscillator

Consider a particle that is subject to a linear restoring force  $F = -kx$ , where *k* is a constant and *x* is the position of the particle relative to equilibrium ( $x = 0$ ). The classical motion of a particle subject to such a force is simple harmonic motion, which was discussed in Chapter 15. The potential energy of the system is, from Equation 15.20,

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

where the angular frequency of vibration is  $\omega = \sqrt{k/m}$ . Classically, if the particle is displaced from its equilibrium position and released, it oscillates between the points  $x = -A$  and  $x = A$ , where *A* is the amplitude of the motion. Furthermore, its total energy *E* is, from Equation 15.21,

$$
E = K + U = \frac{1}{2}kA^2 = \frac{1}{2}m\omega^2A^2
$$

In the classical model, any value of *E* is allowed, including  $E = 0$ , which is the total energy when the particle is at rest at  $x = 0$ .

 Let's investigate how the simple harmonic oscillator is treated from a quantum point of view. The Schrödinger equation for this problem is obtained by substituting  $U = \frac{1}{2} m \omega^2 x^2$  into Equation 41.15:

$$
-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi
$$
 (41.24)

The mathematical technique for solving this equation is beyond the level of this book; nonetheless, it is instructive to guess at a solution. We take as our guess the following wave function:

$$
\psi = Be^{-Cx^2} \tag{41.25}
$$

Substituting this function into Equation 41.24 shows that it is a satisfactory solution to the Schrödinger equation, provided that

$$
C = \frac{m\omega}{2\hbar} \quad \text{and} \quad E = \frac{1}{2}\hbar\omega
$$

It turns out that the solution we have guessed corresponds to the ground state of the system, which has an energy  $\frac{1}{2}\hbar\omega$ . Because  $C = m\omega/2\hbar$ , it follows from Equation 41.25 that the wave function for this state is

$$
\psi = Be^{-(m\omega/2\hbar)x^2}
$$
\n(41.26)

where *B* is a constant to be determined from the normalization condition. This result is but one solution to Equation 41.24. The remaining solutions that describe the excited states are more complicated, but all solutions include the exponential factor  $e^{-Cx^2}$ .

 The energy levels of a harmonic oscillator are quantized as we would expect because the oscillating particle is bound to stay near  $x = 0$ . The energy of a state having an arbitrary quantum number *n* is

$$
E_n = (n + \frac{1}{2})\hbar\omega \qquad n = 0, 1, 2, \dots
$$
 (41.27)

The state  $n = 0$  corresponds to the ground state, whose energy is  $E_0 = \frac{1}{2}\hbar\omega$ ; the state  $n = 1$  corresponds to the first excited state, whose energy is  $E_1 = \frac{3}{2}\hbar\omega$ ; and so on. The energy-level diagram for this system is shown in Figure 41.14. The separations between adjacent levels are equal and given by

$$
\Delta E = \hbar \omega \tag{41.28}
$$

 Notice that the energy levels for the harmonic oscillator in Figure 41.14 are equally spaced, just as Planck proposed for the oscillators in the walls of the cavity that was used in the model for blackbody radiation in Section 40.1. Planck's Equation 40.4 for the energy levels of the oscillators differs from Equation 41.27 only in the term  $\frac{1}{2}$  added to *n*. This additional term does not affect the energy emitted in a transition, given by Equation 40.5, which is equivalent to Equation 41.28. That Planck generated these concepts without the benefit of the Schrödinger equation is testimony to his genius.

### *Example* **41.5 Molar Specific Heat of Hydrogen Gas**

In Figure 21.7 (Section 21.4), which shows the molar specific heat of hydrogen as a function of temperature, vibration does not contribute to the molar specific heat at room temperature. Explain why, modeling the hydrogen molecule as a simple harmonic oscillator. The effective spring constant for the bond in the hydrogen molecule is 573 N/m.

#### **SOLUTION**

**Conceptualize** Imagine the only mode of vibration available to a diatomic molecule. This mode (shown in Fig. 21.6c) consists of the two atoms always moving in opposite directions with equal speeds.

**Categorize** We categorize this example as a quantum harmonic oscillator problem, with the molecule modeled as a twoparticle system.

**Analyze** The motion of the particles relative to the center of mass can be analyzed by considering the oscillation of a single particle with reduced mass  $\mu$ . (See Problem 40.)

Use the result of Problem 40 to evaluate the reduced mass of the hydrogen molecule, in which the masses of the two particles are the same:

$$
\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{m^2}{2m} = \frac{1}{2}m
$$



The levels are equally spaced, with separation  $\hbar\omega$ . The ground-

Wave function for the ground **X state of a simple harmonic** 

**oscillator**

**Figure 41.14** Energy-level diagram for a simple harmonic oscillator, superimposed on the potential energy function.

### **41.5** *cont.*

Using Equation 41.28, calculate the energy necessary to excite the molecule from its ground vibrational state to its first excited vibrational state:

Substitute numerical values, noting that *m* is the mass of a hydrogen atom:

Set this energy equal to  $\frac{3}{2}k_{\rm B}T$  from Equation 21.4 and find the temperature at which the average molecular translational kinetic energy is equal to that required to excite the first vibrational state of the molecule:

$$
\Delta E = \hbar \omega = \hbar \sqrt{\frac{k}{\mu}} = \hbar \sqrt{\frac{k}{\frac{1}{2}m}} = \hbar \sqrt{\frac{2k}{m}}
$$

$$
\Delta E = (1.055 \times 10^{-34} \text{ J} \cdot \text{s}) \sqrt{\frac{2(573 \text{ N/m})}{1.67 \times 10^{-27} \text{ kg}}} = 8.74 \times 10^{-20} \text{ J}
$$

$$
\frac{3}{2}k_{\rm B}T = \Delta E
$$
  

$$
T = \frac{2}{3}\left(\frac{\Delta E}{k_{\rm B}}\right) = \frac{2}{3}\left(\frac{8.74 \times 10^{-20} \text{ J}}{1.38 \times 10^{-23} \text{ J/K}}\right) = 4.22 \times 10^3 \text{ K}
$$

**Finalize** The temperature of the gas must be more than 4 000 K for the translational kinetic energy to be comparable to the energy required to excite the first vibrational state. This excitation energy must come from collisions between molecules, so if the molecules do not have sufficient translational kinetic energy, they cannot be excited to the first vibrational state and vibration does not contribute to the molar specific heat. Hence, the curve in Figure 21.7 does not rise to a value corresponding to the contribution of vibration until the hydrogen gas has been raised to thousands of kelvins.

 Figure 21.7 shows that rotational energy levels must be more closely spaced in energy than vibrational levels because they are excited at a lower temperature than the vibrational levels. The translational energy levels are those of a particle in a three-dimensional box, where the box is the container holding the gas. These levels are given by an expression similar to Equation 41.14. Because the box is macroscopic in size, *L* is very large and the energy levels are very close together. In fact, they are so close together that translational energy levels are excited at a fraction of a kelvin.

## *Summary* Definitions

The **wave function**  $\Psi$  for a system is a mathematical function that can be written as a product of a space function  $\psi$  for one particle of the system and a complex time function:

$$
\Psi(\vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2, \vec{\mathbf{r}}_3, \dots, \vec{\mathbf{r}}_j, \dots, t) = \psi(\vec{\mathbf{r}}_j)e^{-i\omega t}
$$
 (41.2)

where  $\omega$  (=  $2\pi f$ ) is the angular frequency of the wave function and  $i = \sqrt{-1}$ . The wave function contains within it all the information that can be known about the particle.

The measured position *x* of a particle, averaged over many trials, is called the **expectation value** of *x* and is defined by

$$
\langle x \rangle \equiv \int_{-\infty}^{\infty} \psi \cdot x \psi \, dx \qquad (41.8)
$$

### Concepts and Principles

In quantum mechanics, a particle in a system can be represented by a wave function  $\psi(x, y, z)$ . The probability per unit volume (or probability density) that a particle will be found at a point is  $|\psi|^2 = \psi^* \psi$ , where  $\psi^*$  is the complex conjugate of  $\psi$ . If the particle is confined to moving along the *x* axis, the probability that it is located in an interval  $dx$  is  $|\psi|^2 dx$ . Furthermore, the sum of all these probabilities over all values of *x* must be 1:

$$
\int_{-\infty}^{\infty} |\psi|^2 \, dx = 1 \tag{41.7}
$$

This expression is called the **normalization condition.**

The wave function for a system must satisfy the **Schrödinger equation.** The time-independent Schrödinger equation for a particle confined to moving along the *x* axis is

$$
-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U\psi = E\psi
$$
 (41.15)

where *U* is the potential energy of the system and *E* is the total energy.

If a particle of mass *m* is confined to moving in a onedimensional box of length *L* whose walls are impenetrable, then  $\psi$  must be zero at the walls and outside the box. The wave functions for this system are given by

$$
\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)
$$
  $n = 1, 2, 3, ...$  (41.12)

where  $A$  is the maximum value of  $\psi$ . The allowed states of a particle in a box have quantized energies given by

$$
E_n = \left(\frac{h^2}{8mL^2}\right)n^2 \quad n = 1, 2, 3, \dots \qquad (41.14)
$$

### Analysis Model for Problem Solving



**Quantum Particle Under Boundary Conditions.** An interaction of a quantum particle with its environment represents one or more boundary conditions. If the interaction restricts the particle to a finite region of space, the energy of the system is quantized. All wave functions must satisfy the following four boundary conditions: (1)  $\psi(x)$  must remain finite as *x* approaches 0, (2)  $\psi(x)$  must approach zero as *x* approaches  $\pm \infty$ , (3)  $\psi(x)$  must be continuous for all values of *x*, and (4)  $d\psi/dx$  must be continuous for all finite values of  $U(x)$ . If the solution to Equation 41.15 is piecewise, conditions (3) and (4) must be applied at the boundaries between regions of *x* in which Equation 41.15 has been solved.

### **Objective Questions** denotes answer available in Student

- **1.** The probability of finding a certain quantum particle in the section of the *x* axis between  $x = 4$  nm and  $x = 7$  nm is 48%. The particle's wave function  $\psi(x)$  is constant over this range. What numerical value can be attributed to  $\psi(x)$ , in units of  $nm^{-1/2}$ ? (a) 0.48 (b) 0.16 (c) 0.12 (d) 0.69 (e) 0.40
- **2.** Is each one of the following statements (a) through (e) true or false for a photon? (a) It is a quantum particle, behaving in some experiments like a classical particle and in some experiments like a classical wave. (b) Its rest energy is zero. (c) It carries energy in its motion. (d) It carries momentum in its motion. (e) Its motion is described by a wave function that has a wavelength and satisfies a wave equation.
- **3.** Is each one of the following statements (a) through (e) true or false for an electron? (a) It is a quantum particle, behaving in some experiments like a classical particle and in some experiments like a classical wave. (b) Its rest energy is zero. (c) It carries energy in its motion. (d) It carries momentum in its motion. (e) Its motion is described by a wave function that has a wavelength and satisfies a wave equation.
- **4.** A quantum particle of mass  $m_1$  is in a square well with infinitely high walls and length 3 nm. Rank the situations (a) through (e) according to the particle's energy from highest to lowest, noting any cases of equality. (a) The particle of mass  $m_1$  is in the ground state of the well. (b) The same particle is in the  $n = 2$  excited state of the same well. (c) A particle with mass  $2m_1$  is in the ground state of the same well. (d) A particle of mass  $m_1$  in the ground state of the same well, and the uncertainty principle has become inoperative; that is, Planck's constant has been reduced to zero. (e) A particle of mass  $m_1$  is in the ground state of a well of length 6 nm.
- **5.** A particle in a rigid box of length *L* is in the first excited state for which  $n = 2$  (Fig. OQ41.5). Where is the particle most likely to be found? (a) At the center of the box. (b) At either end of the box. (c) All points in the box are equally likely. (d) One-fourth of the way from either end of the box. (e) None of those answers is correct.



**Figure OQ41.5**

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- **6.** Two square wells have the same length. Well 1 has walls of finite height, and well 2 has walls of infinite height. Both wells contain identical quantum particles, one in each well. **(i)** Is the wavelength of the ground-state wave function (a) greater for well 1, (b) greater for well 2, or (c) equal for both wells? **(ii)** Is the magnitude of the ground-state momentum (a) greater for well 1, (b) greater for well 2, or (c) equal for both wells? **(iii)** Is the ground-state energy of the particle (a) greater for well 1, (b) greater for well 2, or (c) equal for both wells?
- **7.** A beam of quantum particles with kinetic energy 2.00 eV is reflected from a potential barrier of small width and original height 3.00 eV. How does the fraction of the particles that are reflected change as the barrier height is reduced to 2.01 eV? (a) It increases. (b) It decreases. (c) It stays constant at zero. (d) It stays constant at 1. (e) It stays constant with some other value.
- **8.** Suppose a tunneling current in an electronic device goes through a potential-energy barrier. The tunneling current is small because the width of the barrier is large and the barrier is high. To increase the current most effectively, what should you do? (a) Reduce the width of the barrier. (b) Reduce the height of the barrier. (c) Either choice (a) or choice (b) is equally effective. (d) Neither choice (a) nor choice (b) increases the current.
- **9.** Unlike the idealized diagram of Figure 41.11, a typical tip used for a scanning tunneling microscope is rather jagged on the atomic scale, with several irregularly spaced points. For such a tip, does most of the tunneling current occur between the sample and (a) all the points of the tip equally, (b) the most centrally located point, (c) the point closest to the sample, or (d) the point farthest from the sample?
- **10.** Figure OQ41.10 represents the wave function for a hypothetical quantum particle in a given region. From the choices *a* through *e,* at what value of *x* is the particle most likely to be found?



**Figure OQ41.10**

### **Conceptual Questions** denotes answer available in Student

- **1.** What is the significance of the wave function  $\psi$ ?
- **2.** Discuss the relationship between ground-state energy and the uncertainty principle.
- **3.** For a quantum particle in a box, the probability density at certain points is zero as seen in Figure CQ41.3. Does this value imply that the particle cannot move across these points? Explain.





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- **4.** How is the Schrödinger equation useful in describing quantum phenomena?
- **5.** Richard Feynman said, "A philosopher once said that 'it is necessary for the very existence of science that the same conditions always produce the same results.' Well, they don't!" In view of what has been discussed in this chapter, present an argument showing that the philosopher's statement is false. How might the statement be reworded to make it true?
- **6.** In quantum mechanics, it is possible for the energy *E* of a particle to be less than the potential energy, but classically this condition is not possible. Explain.
- **7.** Consider the wave functions in Figure CQ41.7. Which of them are not physically significant in the interval shown? For those that are not, state why they fail to qualify.
- **8.** Why are the following wave functions not physically possible for all values of  $x$ ? (a)  $\psi(x) = Ae^x$  (b)  $\psi(x) = A \tan x$





**Problems**

WebAssign The problems found in this chapter may be assigned online in Enhanced WebAssign

**1.** denotes straightforward problem; **2.** denotes intermediate problem; **3.** denotes challenging problem

**1.** full solution available in the Student Solutions Manual/Study Guide

**1.** denotes problems most often assigned in Enhanced WebAssign; these provide students with targeted feedback and either a Master It tutorial or a Watch It solution video.

#### **Section 41.1 The Wave Function**

**1.** M A free electron has a wave function

$$
\psi(x) = A e^{i(5.00 \times 10^{10} x)}
$$

where  $x$  is in meters. Find its (a) de Broglie wavelength, (b) momentum, and (c) kinetic energy in electron volts.

- QC denotes asking for quantitative and conceptual reasoning
- **S** denotes symbolic reasoning problem
- M denotes Master It tutorial available in Enhanced WebAssign
- GP denotes guided problem
- shaded denotes "paired problems" that develop reasoning with symbols and numerical values

**2. S** The wave function for a quantum particle is

$$
\psi(x) = \sqrt{\frac{a}{\pi(x^2 + a^2)}}
$$

for  $a > 0$  and  $-\infty < x < +\infty$ . Determine the probability that the particle is located somewhere between  $x = -a$  and  $x = +a$ .

- **3.** The wave function for a quantum particle is given by  $\psi(x) = Ax$  between  $x = 0$  and  $x = 1.00$ , and  $\psi(x) = 0$  elsewhere. Find (a) the value of the normalization constant *A,* (b) the probability that the particle will be found between  $x = 0.300$  and  $x = 0.400$ , and (c) the expectation value of the particle's position.
- **4.** The wave function for a particle is given by  $\psi(x) = Ae^{-|x|/a}$ , where *A* and *a* are constants. (a) Sketch this function for values of *x* in the interval  $-3a < x < 3a$ . (b) Determine the value of *A.* (c) Find the probability that the particle will be found in the interval  $-a < x < a$ .

#### **Section 41.2 Analysis Model: Quantum Particle Under Boundary Conditions**

- **5.** An electron is confined to a one-dimensional region in which its ground-state  $(n = 1)$  energy is 2.00 eV. (a) What is the length *L* of the region? (b) What energy input is required to promote the electron to its first excited state?
- **6.** An electron that has an energy of approximately 6 eV moves between infinitely high walls 1.00 nm apart. Find (a) the quantum number *n* for the energy state the electron occupies and (b) the precise energy of the electron.
- **7.** An electron is contained in a one-dimensional box of length 0.100 nm. (a) Draw an energy-level diagram for the electron for levels up to  $n = 4$ . (b) Photons are emitted by the electron making downward transitions that could eventually carry it from the  $n = 4$  state to the  $n = 1$  state. Find the wavelengths of all such photons.
- **8.** A 4.00-g particle confined to a box of length *L* has a speed of 1.00 mm/s. (a) What is the classical kinetic energy of the particle? (b) If the energy of the first excited state  $(n = 2)$  is equal to the kinetic energy found in part (a), what is the value of *L*? (c) Is the result found in part (b) realistic? Explain.
- **9.** A ruby laser emits 694.3-nm light. Assume light of this wavelength is due to a transition of an electron in a box from its  $n = 2$  state to its  $n = 1$  state. Find the length of the box.
- 10. **S** A laser emits light of wavelength  $\lambda$ . Assume this light is due to a transition of an electron in a box from its  $n = 2$ state to its  $n = 1$  state. Find the length of the box.
- 11. **QC** The nuclear potential energy that binds protons and neutrons in a nucleus is often approximated by a square well. Imagine a proton confined in an infinitely high square well of length 10.0 fm, a typical nuclear diameter. Assuming the proton makes a transition from the  $n = 2$ state to the ground state, calculate (a) the energy and (b) the wavelength of the emitted photon. (c) Identify the region of the electromagnetic spectrum to which this wavelength belongs.
- 12. **Q C** A proton is confined to move in a one-dimensional box of length 0.200 nm. (a) Find the lowest possible energy

of the proton. (b) **What If?** What is the lowest possible energy of an electron confined to the same box? (c) How do you account for the great difference in your results for parts (a) and (b)?

- **13. QC** (a) Use the quantum-particle-in-a-box model to calculate the first three energy levels of a neutron trapped in an atomic nucleus of diameter 20.0 fm. (b) Explain whether the energy-level differences have a realistic order of magnitude.
- **14.** *Why is the following situation impossible?* A proton is in an infinitely deep potential well of length 1.00 nm. It absorbs a microwave photon of wavelength 6.06 mm and is excited into the next available quantum state.
- **15.** An electron confined to a box absorbs a photon with wavelength  $\lambda$ . As a result, the electron makes a transition from the  $n = 1$  state to the  $n = 3$  state. (a) Find the length of the box. (b) What is the wavelength  $\lambda'$  of the photon emitted when the electron makes a transition from the  $n =$ 3 state to the  $n = 2$  state?
- **16. Q C S** For a quantum particle of mass *m* in the ground state of a square well with length *L* and infinitely high walls, the uncertainty in position is  $\Delta x \approx L$ . (a) Use the uncertainty principle to estimate the uncertainty in its momentum. (b) Because the particle stays inside the box, its average momentum must be zero. Its average squared momentum is then  $\langle p^2 \rangle \approx (\Delta p)^2$ . Estimate the energy of the particle. (c) State how the result of part (b) compares with the actual ground-state energy.
- 17. **S** The wave function for a quantum particle confined to moving in a one-dimensional box located between  $x = 0$ and  $x = L$  is

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

Use the normalization condition on  $\psi$  to show that

$$
A=\sqrt{\frac{2}{L}}
$$

18. **QC** A quantum particle in an infinitely deep square well has a wave function given by

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

for  $0 \le x \le L$  and zero otherwise. (a) Determine the expectation value of *x.* (b) Determine the probability of finding the particle near  $\frac{1}{2}L$  by calculating the probability that the particle lies in the range  $0.490L \le x \le 0.510L$ . (c) **What If?** Determine the probability of finding the particle near  $\frac{1}{4}L$ by calculating the probability that the particle lies in the range  $0.240L \le x \le 0.260L$ . (d) Argue that the result of part (a) does not contradict the results of parts (b) and (c).

 **19.** An electron is trapped in an infinitely deep potential well 0.300 nm in length. (a) If the electron is in its ground state, what is the probability of finding it within 0.100 nm of the left-hand wall? (b) Identify the classical probability of finding the electron in this interval and state how it compares with the answer to part (a). (c) Repeat parts (a) and (b) assuming the particle is in the 99th energy state.

20. **QC** S An electron in an infinitely deep square well has a wave function that is given by

$$
\psi_3(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right)
$$

for  $0 \le x \le L$  and is zero otherwise. (a) What are the most probable positions of the electron? (b) Explain how you identify them.

21. **M** A quantum particle in an infinitely deep square well has a wave function that is given by

$$
\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)
$$

for  $0 \le x \le L$  and is zero otherwise. (a) Determine the probability of finding the particle between  $x = 0$  and  $x = \frac{1}{3}L$ . (b) Use the result of this calculation and a symmetry argument to find the probability of finding the particle between  $x = \frac{1}{3}L$  and  $x = \frac{2}{3}L$ . Do not re-evaluate the integral.

**22.** A quantum particle is in the  $n = 1$  state of an infinitely deep square well with walls at  $x = 0$  and  $x = L$ . Let  $\ell$  be an arbitrary value of *x* between  $x = 0$  and  $x = L$ . (a) Find an expression for the probability, as a function of  $\ell$ , that the particle will be found between  $x = 0$  and  $x = \ell$ . (b) Sketch the probability as a function of the variable  $\ell/L$ . Choose values of  $\ell/L$  ranging from 0 to 1.00 in steps of 0.100. (c) Explain why the probability function must have particular values at  $\ell/L = 0$  and at  $\ell/L = 1$ . (d) Find the value of  $\ell$  for which the probability of finding the particle between  $x = 0$  and  $x = \ell$  is twice the probability of finding the particle between  $x = \ell$  and  $x = L$ . *Suggestion:* Solve the transcendental equation for  $\ell/L$  numerically.

#### **Section 41.3 The Schrödinger Equation**

23. **S** The wave function of a quantum particle of mass *m* is

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

where *A, B,* and *k* are constants. (a) Assuming the particle is free  $(U = 0)$ , show that  $\psi(x)$  is a solution of the Schrödinger equation (Eq. 41.15). (b) Find the corresponding energy *E* of the particle.

- **24.** S Show that the wave function  $\psi = Ae^{i(kx \omega t)}$  is a solution to the Schrödinger equation (Eq. 41.15), where  $k = 2\pi/\lambda$ and  $U = 0$ .
- **25.** A quantum particle of mass *m* moves in a potential well of length 2*L*. Its potential energy is infinite for  $x < -L$  and for  $x > +L$ . In the region  $-L < x < L$ , its potential energy is given by

$$
U(x) = \frac{-\hbar^2 x^2}{mL^2(L^2 - x^2)}
$$

In addition, the particle is in a stationary state that is described by the wave function  $\psi(x) = A(1 - x^2/L^2)$  for  $-L < x < +L$  and by  $\psi(x) = 0$  elsewhere. (a) Determine the energy of the particle in terms of  $\hbar$ ,  $m$ , and  $L$ . (b) Determine the normalization constant *A.* (c) Determine the probability that the particle is located between  $x = -L/3$ and  $x = +L/3$ .

- 26. **S** Consider a quantum particle moving in a onedimensional box for which the walls are at  $x = -L/2$  and  $x = L/2$ . (a) Write the wave functions and probability densities for  $n = 1$ ,  $n = 2$ , and  $n = 3$ . (b) Sketch the wave functions and probability densities.
- 27. **S** In a region of space, a quantum particle with zero total energy has a wave function

$$
\psi(x) = A x e^{-x^2/L^2}
$$

(a) Find the potential energy *U* as a function of *x.* (b) Make a sketch of *U*(*x*) versus *x.*

#### **Section 41.4 A Particle in a Well of Finite Height**

- **28.** Suppose a quantum particle is in its ground state in a box that has infinitely high walls (see Active Fig. 41.4a). Now suppose the left-hand wall is suddenly lowered to a finite height and width. (a) Qualitatively sketch the wave function for the particle a short time later. (b) If the box has a length *L,* what is the wavelength of the wave that penetrates the left-hand wall?
- **29.** Sketch (a) the wave function  $\psi(x)$  and (b) the probability density  $|\psi(x)|^2$  for the  $n = 4$  state of a quantum particle in a finite potential well. (See Active Fig. 41.7.)

#### **Section 41.5 Tunneling Through a Potential Energy Barrier**

**30. M** An electron with kinetic energy  $E = 5.00$  eV is incident on a barrier of width  $L = 0.200$  nm and height  $U = 10.0$  eV (Fig. P41.30). What is the probability that the electron (a) tunnels through the barrier? (b) Is reflected?



**Figure P41.30** Problems 30 and 31.

**31.** An electron having total energy  $E = 4.50$  eV approaches a rectangular energy barrier with  $U = 5.00$  eV and  $L =$ 950 pm as shown in Figure P41.30. Classically, the electron **32.** An electron has a kinetic energy of 12.0 eV. The electron is incident upon a rectangular barrier of height 20.0 eV and width 1.00 nm. If the electron absorbed all the energy of a photon of green light (with wavelength 546 nm) at the instant it reached the barrier, by what factor would the electron's probability of tunneling through the barrier increase?

#### **Section 41.6 Applications of Tunneling**

- **33.** A scanning tunneling microscope (STM) can precisely determine the depths of surface features because the current through its tip is very sensitive to differences in the width of the gap between the tip and the sample surface. Assume the electron wave function falls off exponentially in this direction with a decay length of 0.100 nm, that is, with  $C = 10.0$  nm<sup>-1</sup>. Determine the ratio of the current when the STM tip is 0.500 nm above a surface feature to the current when the tip is 0.515 nm above the surface.
- **34.** The design criterion for a typical scanning tunneling microscope (STM) specifies that it must be able to detect, on the sample below its tip, surface features that differ in height by only 0.002 00 nm. Assuming the electron transmission coefficient is  $e^{-2CL}$  with  $C = 10.0$  nm<sup>-1</sup>, what percentage change in electron transmission must the electronics of the STM be able to detect to achieve this resolution?

#### **Section 41.7 The Simple Harmonic Oscillator**

**35.** Show that Equation 41.26 is a solution of Equation 41.24 with energy  $E = \frac{1}{2}\hbar\omega$ .

**36. S** A one-dimensional harmonic oscillator wave function is

$$
\psi = A x e^{-bx^2}
$$

(a) Show that  $\psi$  satisfies Equation 41.24. (b) Find *b* and the total energy *E.* (c) Is this wave function for the ground state or for the first excited state?

- **37.** A quantum simple harmonic oscillator consists of an electron bound by a restoring force proportional to its position relative to a certain equilibrium point. The proportionality constant is 8.99 N/m. What is the longest wavelength of light that can excite the oscillator?
- **38.** A quantum simple harmonic oscillator consists of a particle of mass *m* bound by a restoring force proportional to its position relative to a certain equilibrium point. The proportionality constant is *k.* What is the longest wavelength of light that can excite the oscillator?
- **39.** (a) Normalize the wave function for the ground state of a simple harmonic oscillator. That is, apply Equation 41.7 to Equation 41.26 and find the required value for the constant  $B$  in terms of  $m$ ,  $\omega$ , and fundamental constants. (b) Determine the probability of finding the oscillator in a narrow interval  $-\delta/2 < x < \delta/2$  around its equilibrium position.
- **40. S** Two particles with masses  $m_1$  and  $m_2$  are joined by a light spring of force constant *k.* They vibrate along a straight line with their center of mass fixed. (a) Show that the total energy

$$
\frac{1}{2}m_1u_1^2 + \frac{1}{2}m_2u_2^2 + \frac{1}{2}kx^2
$$

can be written as  $\frac{1}{2}\mu u^2 + \frac{1}{2}kx^2$ , where  $u = |u_1| + |u_2|$  is the *relative* speed of the particles and  $\mu = m_1 m_2/(m_1 + m_2)$  is the reduced mass of the system. This result demonstrates that the pair of freely vibrating particles can be precisely modeled as a single particle vibrating on one end of a spring that has its other end fixed. (b) Differentiate the equation

$$
\frac{1}{2}\mu u^2 + \frac{1}{2}kx^2 = \text{constant}
$$

with respect to *x.* Proceed to show that the system executes simple harmonic motion. (c) Find its frequency.

**41. S** The total energy of a particle–spring system in which the particle moves with simple harmonic motion along the *x* axis is

$$
E = \frac{p_x^2}{2m} + \frac{kx^2}{2}
$$

where  $p_x$  is the momentum of the quantum particle and  $k$ is the spring constant. (a) Using the uncertainty principle, show that this expression can also be written as

$$
E \ge \frac{p_x^2}{2m} + \frac{k\hbar^2}{8{p_x}^2}
$$

(b) Show that the minimum energy of the harmonic oscillator is

$$
E_{\min} = K + U = \frac{1}{4}\hbar\sqrt{\frac{k}{m}} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}
$$

#### **Additional Problems**

- **42.** A particle in a one-dimensional box of length *L* is in its first excited state, corresponding to  $n = 2$ . Determine the probability of finding the particle between  $x = 0$  and  $x =$ *L*/4.
- **43.** A particle of mass  $2.00 \times 10^{-28}$  kg is confined to a onedimensional box of length  $1.00 \times 10^{-10}$  m. For  $n = 1$ , what are (a) the particle's wavelength, (b) its momentum, and (c) its ground-state energy?
- **44. S** Prove that the first term in the Schrödinger equation,  $-(\hbar^2/2m)(d^2\psi/dx^2)$ , reduces to the kinetic energy of the quantum particle multiplied by the wave function (a) for

a freely moving particle, with the wave function given by Equation 41.4, and (b) for a particle in a box, with the wave function given by Equation 41.13.

- **45.** Prove that assuming  $n = 0$  for a quantum particle in an infinitely deep potential well leads to a violation of the uncertainty principle  $\Delta p_x \Delta x \geq \hbar/2$ .
- **46.** An electron in an infinitely deep potential well has a ground-state energy of 0.300 eV. (a) Show that the photon emitted in a transition from the  $n = 3$  state to the  $n = 1$ state has a wavelength of 517 nm, which makes it green visible light. (b) Find the wavelength and the spectral region for each of the other five transitions that take place among the four lowest energy levels.
- **47.** Calculate the transmission probability for quantummechanical tunneling in each of the following cases. (a) An electron with an energy deficit of  $U - E = 0.010$  0 eV is incident on a square barrier of width  $L = 0.100$  nm. (b) An electron with an energy deficit of 1.00 eV is incident on the same barrier. (c) An alpha particle (mass  $6.65 \times 10^{-27}$  kg) with an energy deficit of 1.00 MeV is incident on a square barrier of width 1.00 fm. (d) An 8.00-kg bowling ball with an energy deficit of 1.00 J is incident on a square barrier of width 2.00 cm.
- **48.** A marble rolls back and forth across a shoebox at a constant speed of 0.8 m/s. Make an order-of-magnitude estimate of the probability of it escaping through the wall of the box by quantum tunneling. State the quantities you take as data and the values you measure or estimate for them.
- **49.** An atom in an excited state 1.80 eV above the ground state remains in that excited state  $2.00 \mu s$  before moving to the ground state. Find (a) the frequency and (b) the wavelength of the emitted photon. (c) Find the approximate uncertainty in energy of the photon.
- **50. CP** S An electron is confined to move in the *xy* plane in a rectangle whose dimensions are  $L_x$  and  $L_y$ . That is, the electron is trapped in a two-dimensional potential well having lengths of  $L<sub>x</sub>$  and  $L<sub>y</sub>$ . In this situation, the allowed energies of the electron depend on two quantum numbers  $n_x$  and  $n_y$  and are given by

$$
E = \frac{h^2}{8m_e} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right)
$$

Using this information, we wish to find the wavelength of a photon needed to excite the electron from the ground state to the second excited state, assuming  $L_x = L_y = L$ . (a) Using the assumption on the lengths, write an expression for the allowed energies of the electron in terms of the quantum numbers  $n_x$  and  $n_y$ . (b) What values of  $n_x$  and  $n_y$ correspond to the ground state? (c) Find the energy of the ground state. (d) What are the possible values of  $n_x$  and  $n_y$ for the first excited state, that is, the next-highest state in terms of energy? (e) What are the possible values of  $n<sub>x</sub>$  and  $n_{y}$  for the second excited state? (f) Using the values in part (e), what is the energy of the second excited state? (g) What is the energy difference between the ground state and the second excited state? (h) What is the wavelength of a photon that will cause the transition between the ground state and the second excited state?

**51. S** For a quantum particle described by a wave function  $\psi(x)$ , the expectation value of a physical quantity  $f(x)$  associated with the particle is defined by

$$
\langle f(x) \rangle \equiv \int_{-\infty}^{\infty} \psi^* f(x) \psi \ dx
$$

For a particle in an infinitely deep one-dimensional box extending from  $x = 0$  to  $x = L$ , show that

$$
\langle x^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}
$$

**52.** A quantum particle is described by the wave function

$$
\psi(x) = \begin{cases} A \cos\left(\frac{2\pi x}{L}\right) & \text{for } -\frac{L}{4} \le x \le \frac{L}{4} \\ 0 & \text{elsewhere} \end{cases}
$$

(a) Determine the normalization constant *A.* (b) What is the probability that the particle will be found between  $x = 0$  and  $x = L/8$  if its position is measured?

- **53.** A quantum particle of mass *m* is placed in a onedimensional box of length *L.* Assume the box is so small that the particle's motion is relativistic and  $K = p^2/2m$  is not valid. (a) Derive an expression for the kinetic energy levels of the particle. (b) Assume the particle is an electron in a box of length  $L = 1.00 \times 10^{-12}$  m. Find its lowest possible kinetic energy. (c) By what percent is the nonrelativistic equation in error? *Suggestion:* See Equation 39.23.
- **54.** *Why is the following situation impossible?* A particle is in the ground state of an infinite square well of length *L.* A light source is adjusted so that the photons of wavelength  $\lambda$  are absorbed by the particle as it makes a transition to the first excited state. An identical particle is in the ground state of a finite square well of length *L.* The light source sends photons of the same wavelength  $\lambda$  toward this particle. The photons are not absorbed because the allowed energies of the finite square well are different from those of the infinite square well. To cause the photons to be absorbed, you move the light source at a high speed toward the particle in the finite square well. You are able to find a speed at which the Doppler-shifted photons are absorbed as the particle makes a transition to the first excited state.

**55.** A quantum particle has a wave function

$$
\psi(x) = \begin{cases} \sqrt{\frac{2}{a}} e^{-x/a} & \text{for } x > 0\\ 0 & \text{for } x < 0 \end{cases}
$$

(a) Find and sketch the probability density. (b) Find the probability that the particle will be at any point where

 $x < 0$ . (c) Show that  $\psi$  is normalized and then (d) find the probability of finding the particle between  $x = 0$  and  $x = a$ .

- **56.** A two-slit electron diffraction experiment is done with slits of *unequal* widths. When only slit 1 is open, the number of electrons reaching the screen per second is 25.0 times the number of electrons reaching the screen per second when only slit 2 is open. When both slits are open, an interference pattern results in which the destructive interference is not complete. Find the ratio of the probability of an electron arriving at an interference maximum to the probability of an electron arriving at an adjacent interference minimum. *Suggestion:* Use the superposition principle.
- **57. S** The normalized wave functions for the ground state,  $\psi_0(x)$ , and the first excited state,  $\psi_1(x)$ , of a quantum harmonic oscillator are

$$
\psi_0(x) = \left(\frac{a}{\pi}\right)^{1/4} e^{-ax^2/2} \qquad \psi_1(x) = \left(\frac{4a^3}{\pi}\right)^{1/4} x e^{-ax^2/2}
$$

where  $a = m\omega/\hbar$ . A mixed state,  $\psi_{01}(x)$ , is constructed from these states:

$$
\psi_{01}(x) = \frac{1}{\sqrt{2}} [\psi_0(x) + \psi_1(x)]
$$

The symbol  $\langle q \rangle$ <sub>s</sub> denotes the expectation value of the quantity *q* for the state  $\psi_s(x)$ . Calculate the expectation values (a)  $\langle x \rangle_0$ , (b)  $\langle x \rangle_1$ , and (c)  $\langle x \rangle_0$ .

#### **Challenge Problems**

**8C** An electron is represented by the time-independent wave function

$$
\psi(x) = \begin{cases} Ae^{-\alpha x} & \text{for } x > 0\\ Ae^{+\alpha x} & \text{for } x < 0 \end{cases}
$$

(a) Sketch the wave function as a function of *x.* (b) Sketch the probability density representing the likelihood that the electron is found between *x* and  $x + dx$ . (c) Only an infinite value of potential energy could produce the discontinuity in the derivative of the wave function at  $x = 0$ . Aside from this feature, argue that  $\psi(x)$  can be a physically reasonable wave function. (d) Normalize the wave function. (e) Determine the probability of finding the electron somewhere in the range

$$
-\frac{1}{2\alpha} \leq x \leq \frac{1}{2\alpha}
$$

**59.** Particles incident from the left in Figure P41.59 are confronted with a step in potential energy. The step has a height *U* at  $x = 0$ . The particles have energy  $E > U$ . Classically, all the particles would continue moving forward with reduced speed. According to quantum mechanics, however, a fraction of the particles are reflected at the step. (a) Prove that the reflection coefficient *R* for this case is

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

where  $k_1 = 2\pi/\lambda_1$  and  $k_2 = 2\pi/\lambda_2$  are the wave numbers for the incident and transmitted particles, respectively. Proceed as follows. Show that the wave function  $\psi_1 = Ae^{ik_1x}$  +  $Be^{-ik_1x}$  satisfies the Schrödinger equation in region 1, for  $x < 0$ . Here  $Ae^{ik_1x}$  represents the incident beam and  $Be^{-ik_1x}$ represents the reflected particles. Show that  $\psi_2 = Ce^{ik_2x}$ satisfies the Schrödinger equation in region 2, for  $x > 0$ . Impose the boundary conditions  $\psi_1 = \psi_2$  and  $d\psi_1/dx =$  $d\psi_2/dx$ , at  $x = 0$ , to find the relationship between *B* and *A*. Then evaluate  $R = B^2/A^2$ . A particle that has kinetic energy  $E = 7.00$  eV is incident from a region where the potential energy is zero onto one where  $U = 5.00$  eV. Find (b) its probability of being reflected and (c) its probability of being transmitted.



**Figure P41.59**

**60. Q C** Consider a "crystal" consisting of two fixed ions of charge  $+e$  and two electrons as shown in Figure P41.60. (a) Taking into account all the pairs of interactions, find the potential energy of the system as a function of *d.* (b) Assuming the electrons to be restricted to a one-dimensional box of length 3*d,* find the minimum kinetic energy of the two electrons. (c) Find the value of *d* for which the total energy is a minimum. (d) State how this value of *d* compares with the spacing of atoms in lithium, which has a density of  $0.530$  g/cm<sup>3</sup> and a molar mass of 6.94 g/mol.



- **61.** An electron is trapped in a quantum dot. The quantum dot may be modeled as a one-dimensional, rigid-walled box of length 1.00 nm. (a) Taking  $x = 0$  as the left side of the box, calculate the probability of finding the electron between  $x_1 = 0.150$  nm and  $x_2 = 0.350$  nm for the  $n = 1$ state. (b) Repeat part (a) for the  $n = 2$  state. Calculate the energies in electron volts of (c) the  $n = 1$  state and (d) the  $n = 2$  state.
- **62. 8** (a) Find the normalization constant *A* for a wave function made up of the two lowest states of a quantum particle in a box extending from  $x = 0$  to  $x = L$ :

$$
\psi(x) = A \left[ \sin \left( \frac{\pi x}{L} \right) + 4 \sin \left( \frac{2 \pi x}{L} \right) \right]
$$

(b) A particle is described in the space  $-a \le x \le a$  by the wave function

$$
\psi(x) = A \cos\left(\frac{\pi x}{2a}\right) + B \sin\left(\frac{\pi x}{a}\right)
$$

Determine the relationship between the values of *A* and *B* required for normalization.

**63. S** The wave function

$$
\psi(x) = Bxe^{-(m\omega/2\hbar)x^2}
$$

is a solution to the simple harmonic oscillator problem. (a) Find the energy of this state. (b) At what position are you least likely to find the particle? (c) At what positions are you most likely to find the particle? (d) Determine the value of *B* required to normalize the wave function. (e) **What If?** Determine the classical probability of finding the particle in an interval of small length  $\delta$  centered at the position  $x = 2(h/m\omega)^{1/2}$ . (f) What is the actual probability of finding the particle in this interval?