EXAMPLE 41.1 An electron in a box

An electron is confined to a rigid box. What is the length of the box if the energy difference between the first and second states is 3.0 eV?

MODEL Model the electron as a particle in a rigid one-dimensional box of length L.

SOLVE The first two quantum states, with $n = 1$ and $n = 2$, have energies E_1 and $E_2 = 4E_1$. Thus the energy difference between the states is

$$\Delta E = 3E_1 = \frac{3h^2}{8mL^2} = 3.0\text{ eV} = 4.8 \times 10^{-19}\text{ J}$$

The length of the box for which $\Delta E = 3.0$ eV is

$$L = \sqrt{\frac{3h^2}{8m\Delta E}} = 6.14 \times 10^{-10}\text{ m} = 0.614\text{ nm}$$

ASSESS The expression for E_1 is in SI units, so energies must be in J, not eV.

Solve III: Normalize the Wave Functions

We can determine the constant A by requiring the wave functions to be normalized. The normalization condition, which we found in Chapter 40, is

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

This is the mathematical statement that the particle must be *somewhere* on the x-axis. The integration limits extend to $\pm\infty$, but here we need to integrate only from 0 to L because the wave function is zero outside the box. Thus

$$\int_0^L |\psi_n(x)|^2 dx = A_n^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \qquad (41.24)$$

or

$$A_n = \left[\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx\right]^{-1/2} \qquad (41.25)$$

We placed a subscript n on A_n because it is possible that the normalization constant is different for each wave function in the family. This is a standard integral. We will leave it as a homework problem for you to show that its value, for any n, is

$$A_n = \sqrt{\frac{2}{L}} \qquad n = 1, 2, 3, \ldots \qquad (41.26)$$

We now have a complete solution to the problem. The normalized wave function for the particle in quantum state n is

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & 0 \le x \le L \\ 0 & x < 0 \text{ and } x > L \end{cases} \qquad (41.27)$$

41.4 A Particle in a Rigid Box: Interpreting the Solution

Our solution to the quantum-mechanical problem of a particle in a box tells us that:

1. The particle must have energy $E_n = n^2E_1$, where $n = 1, 2, 3, \ldots$ is the quantum number. $E_1 = h^2/8mL^2$ is the energy of the $n = 1$ ground state.
2. The wave function for a particle in quantum state n is

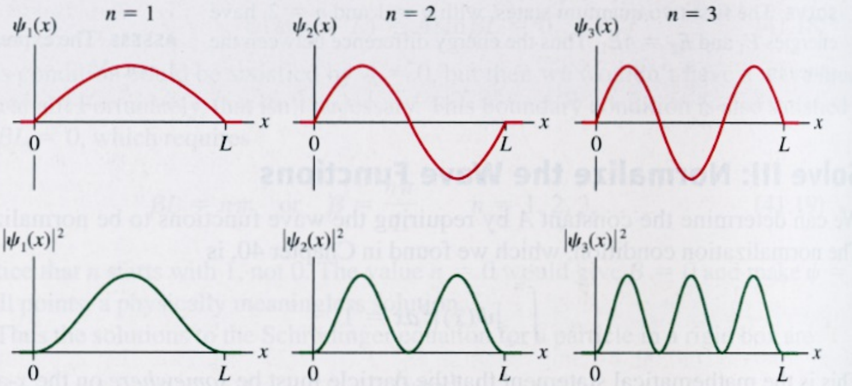
$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & 0 \le x \le L \\ 0 & x < 0 \text{ and } x > L \end{cases}$$

These are the stationary states of the system.

3. The probability density for finding the particle at position x inside the box is

$$P_n(x) = |\psi_n(x)|^2 = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right) \tag{41.28}$$

FIGURE 41.7 Wave functions and probability densities for a particle in a rigid box of length L.

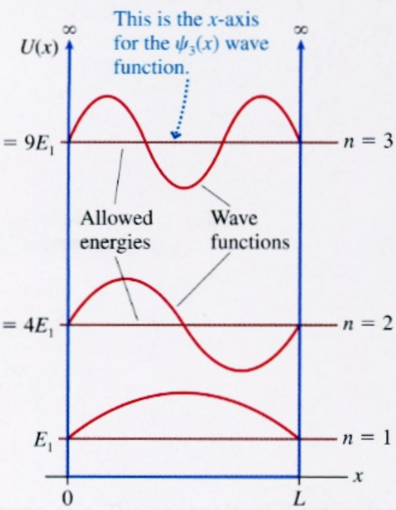


A graphical presentation will make these results more meaningful. **FIGURE 41.7** shows the wave functions $\psi(x)$ and the probability densities $P(x) = |\psi(x)|^2$ for quantum states $n = 1$ to 3. Notice that the wave functions go to zero at the boundaries and thus are continuous with $\psi = 0$ outside the box.

The wave functions $\psi(x)$ for a particle in a rigid box are analogous to standing waves on a string that is tied at both ends. You can see that **$\psi_n(x)$ has $(n - 1)$ nodes (zeros), excluding the ends, and n antinodes (maxima and minima).** This is a general result for any wave function, not just for a particle in a rigid box.

FIGURE 41.8 shows another way in which energies and wave functions are shown graphically in quantum mechanics. First, the graph shows the potential-energy function $U(x)$ of the particle. Second, the allowed energies are shown as horizontal lines (total energy lines) across the potential-energy graph. These are labeled with the quantum number n and the energy E_n. Third—and this is a bit tricky—the wave function for each n is drawn *as if* the energy line were the zero of the y-axis. That is, the graph of $\psi_n(x)$ is drawn on top of the E_n energy line. This allows energies and wave functions to be displayed simultaneously, but it does *not* imply that ψ_2 is in any sense "above" ψ_1. Both oscillate sinusoidally about zero, as Figure 41.7 shows.

FIGURE 41.8 An alternative way to show the potential-energy diagram, the energies, and the wave functions.



EXAMPLE 41.2 Energy levels and quantum jumps

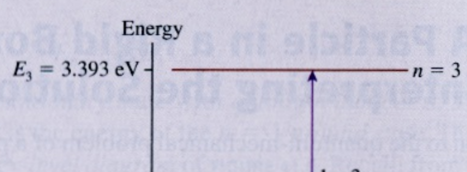
A semiconductor device known as a *quantum-well device* is designed to "trap" electrons in a 1.0-nm-wide region. Treat this as a one-dimensional problem.

a. What are the energies of the first three quantum states?
b. What wavelengths of light can these electrons absorb?

MODEL Model an electron in a quantum-well device as a particle confined in a rigid box of length $L = 1.0$ nm.

VISUALIZE **FIGURE 41.9** shows the first three energy levels and the transitions by which an electron in the ground state can absorb a photon.

FIGURE 41.9 Energy levels and quantum jumps for an electron in a quantum-well device.



SOLVE a. The particle's mass is $m = m_e = 9.11 \times 10^{-31}$ kg. The allowed energies, in both J and eV, are

$$E_1 = \frac{h^2}{8mL^2} = 6.03 \times 10^{-20}\ \text{J} = 0.377\ \text{eV}$$

$$E_2 = 4E_1 = 1.508\ \text{eV}$$

$$E_3 = 9E_1 = 3.393\ \text{eV}$$

b. An electron spends most of its time in the $n = 1$ ground state. According to Bohr's model of stationary states, the electron can absorb a photon of light and undergo a transition, or quantum jump, to $n = 2$ or $n = 3$ if the light has frequency $f = \Delta E/h$. The wavelengths, given by $\lambda = c/f = hc/\Delta E$, are

$$\lambda_{1\to 2} = \frac{hc}{E_2 - E_1} = 1098\ \text{nm}$$

$$\lambda_{1\to 3} = \frac{hc}{E_3 - E_1} = 411\ \text{nm}$$

ASSESS In practice, various complications usually make the $1 \to 3$ transition unobservable. But quantum-well devices do indeed exhibit strong absorption and emission at the $\lambda_{1\to 2}$ wavelength. In this example, which is typical of quantum-well devices, the wavelength is in the near-infrared portion of the spectrum. Devices such as these are used to construct the semiconductor lasers used in CD players and laser printers.

NOTE ▶ The wavelengths of light emitted or absorbed by a quantum system are determined by the *difference* between two allowed energies. Quantum jumps involve two stationary states. ◀

Zero-Point Motion

The lowest energy state in Example 41.2, the ground state, has E_1 =0.38 eV. There is no stationary state having $E = 0$. Unlike a classical particle, **a quantum particle in a box cannot be at rest!** No matter how much its energy is reduced, such as by cooling it toward absolute zero, it cannot have energy less than E_1.

The particle motion associated with energy E_1, called the **zero-point motion,** is a consequence of Heisenberg's uncertainty principle. Because the particle is somewhere in the box, its position uncertainty is $\Delta x = L$. If the particle were at rest in the box, we would know that its velocity and momentum are exactly zero with *no* uncertainty: $\Delta p_x = 0$. But then $\Delta x \Delta p_x = 0$ would violate the Heisenberg uncertainty principle. One of the conclusions that follows from the uncertainty principle is that **a confined particle cannot be at rest.**

Although the particle's position and velocity are uncertain, the particle's energy in each state can be calculated with a high degree of precision. This distinction between a precise energy and uncertain position and velocity seems strange, but it is just our old friend the standing wave. In order to *have* a stationary state at all, the de Broglie waves have to form standing waves. Only for very precise frequencies, and thus precise energies, can the standing-wave pattern appear.

EXAMPLE 41.3 Nuclear energies

Protons and neutrons are tightly bound within the nucleus of an atom. If we use a one-dimensional model of a nucleus, what are the first three energy levels of a neutron in a 10-fm-diameter nucleus (1 fm = 10^{-15} m)?

MODEL Model the nucleus as a one-dimensional box of length L = 10 fm. The neutron is confined within the box.

SOLVE The energy levels, with L = 10 fm and $m = m_n = 1.67 \times 10^{-27}$ kg, are

$$E_1 = \frac{h^2}{8mL^2} = 3.29 \times 10^{-13}\ \text{J} = 2.06\ \text{MeV}$$

$$E_2 = 4E_1 = 8.24\ \text{MeV}$$

$$E_3 = 9E_1 = 18.54\ \text{MeV}$$

ASSESS An electron confined in an atom-size space has energies of a few eV. A neutron confined in a nucleus-size space has energies of a few *million* eV.

EXAMPLE 41.4 The probabilities of locating the particle

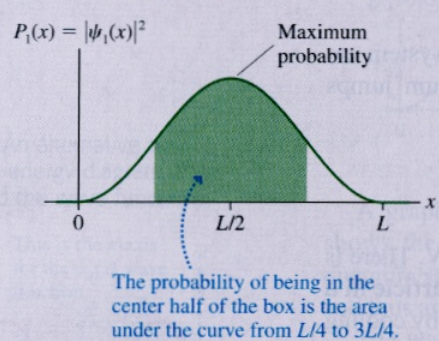
A particle in a rigid box of length L is in its ground state.

a. Where is the particle most likely to be found?
b. What are the probabilities of finding the particle in an interval of width $0.01L$ at $x = 0.00L$, $0.25L$, and $0.50L$?
c. What is the probability of finding the particle in the center half of the box?

MODEL The wave functions for a particle in a rigid box have been determined.

VISUALIZE **FIGURE 41.10** shows the probability density $P_1(x) = |\psi_1(x)|^2$ in the ground state.

FIGURE 41.10 Probability density for a particle in the ground state.



SOLVE a. The particle is most likely to be found at the point where the probability density $P(x)$ is a maximum. You can see from Figure 41.10 that the point of maximum probability for $n = 1$ is $x = L/2$.

b. For a *small* width δx, the probability of finding the particle in δx at position x is

$$\text{Prob(in } \delta x \text{ at } x) = P_1(x)\delta x = |\psi_1(x)|^2 \delta x = \frac{2}{L}\sin^2\left(\frac{\pi x}{L}\right)\delta x$$

The interval $\delta x = 0.01L$ is sufficiently small for this to be valid. The probabilities of finding the particle are

$$\text{Prob(in } 0.01L \text{ at } x = 0.00L) = 0.000 = 0.0\%$$

$$\text{Prob(in } 0.01L \text{ at } x = 0.25L) = 0.010 = 1.0\%$$

$$\text{Prob(in } 0.01L \text{ at } x = 0.50L) = 0.020 = 2.0\%$$

c. The center half of the box stretches from $x = L/4$ to $x = 3L/4$. The probability that the particle is in this interval is the area under the probability-density curve:

$$\text{Prob}\left(\text{in interval } \frac{1}{4}L \text{ to } \frac{3}{4}L\right) = \int_{L/4}^{3L/4} P_1(x)\,dx$$

$$= \frac{2}{L}\int_{L/4}^{3L/4} \sin^2\left(\frac{\pi x}{L}\right)dx$$

$$= \left[\frac{x}{L} - \frac{1}{\pi}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)\right]_{L/4}^{3L/4}$$

$$= \frac{1}{2} + \frac{1}{\pi} = 0.818$$

ASSESS If a particle in a box is in the $n = 1$ ground state, there is an 81.8% chance of finding it in the center half of the box. The probability is greater than 50% because, as you can see in Figure 41.10, the probability density $P_1(x)$ is larger near the center of the box than near the boundaries.

This has been a lengthy presentation of the particle-in-a-box problem. However, it was important that we explore the method of solution completely. Future examples will now go more quickly because many of the issues discussed here will not need to be repeated.

STOP TO THINK 41.2 A particle in a rigid box in the $n = 2$ stationary state is most likely to be found

a. In the center of the box.
b. One-third of the way from either end.
c. One-quarter of the way from either end.
d. It is equally likely to be found at any point in the box.

41.5 The Correspondence Principle

Suppose we confine an electron in a microscopic box, then allow the box to get bigger and bigger. What started out as a quantum-mechanical situation should, when the box becomes macroscopic, eventually look like a classical-physics situation. Similarly, a classical situation such as two charged particles revolving about each other should begin to exhibit quantum behavior as the orbit size becomes smaller and smaller.