6-20 The Schrödinger equation, after rearrangement, is  $\frac{d^2\psi}{dx^2} = \left(\frac{2m}{\hbar^2}\right) \{U(x) - E\}\psi(x)$ . In the well interior, U(x) = 0 and solutions to this equation are  $\sin kx$  and  $\cos kx$ , where  $k^2 = \frac{2mE}{\hbar^2}$ . The waves symmetric about the midpoint of the well (x = 0) are described by

$$\psi(x) = A\cos kx \qquad -L < x < +L$$

In the region outside the well, U(x) = U, and the independent solutions to the wave equation are  $e^{\pm \alpha x}$  with  $\alpha^2 = \left(\frac{2m}{\hbar^2}\right)(U-E)$ .

(a) The growing exponentials must be discarded to keep the wave from diverging at infinity. Thus, the waves in the exterior region, which are symmetric about the midpoint of the well are given by

$$\psi(x) = Ce^{-\alpha|x|} \qquad x > L \text{ or } x < -L.$$

At x = L continuity of  $\psi$  requires  $A \cos kL = Ce^{-\alpha L}$ . For the slope to be continuous here, we also must require  $-Ak \sin kL = -Ce^{-\alpha L}$ . Dividing the two equations gives the desired restriction on the allowed energies:  $k \tan kL = \alpha$ .

(b) The dependence on *E* (or *k*) is made more explicit by noting that  $k^2 + \alpha^2 = \frac{2mU}{\hbar^2}$ , which allows the energy condition to be written  $k \tan kL = \left\{\frac{2mU}{\hbar^2} - k^2\right\}^{1/2}$ . Multiplying by *L*, squaring the result, and using  $\tan^2 \theta + 1 = \sec^2 \theta$  gives  $(kL)^2 \sec^2 (kL) = \frac{2mUL^2}{\hbar^2}$ from which the desired form follows immediately,  $k \sec(kL) = \frac{\sqrt{2mU}}{\hbar}$ . The ground state is the symmetric waveform having the lowest energy. For electrons in a well of height U = 5 eV and width 2L = 0.2 nm, we calculate

$$\frac{2mUL^2}{\hbar^2} = \frac{(2)(511 \times 10^3 \text{ eV}/c^2)(5 \text{ eV})(0.1 \text{ nm})^2}{(197.3 \text{ eV} \cdot \text{nm}/c)^2} = 1.3127.$$

With this value, the equation for  $\theta = kL$ 

$$\frac{\theta}{\cos\theta} = (1.3127)^{1/2} = 1.1457$$

can be solved numerically employing methods of varying sophistication. The simplest of these is trial and error, which gives  $\theta = 0.799$  From this, we find k = 7.99 nm<sup>-1</sup>, and an energy

$$E = \frac{\hbar^2 k^2}{2m} = \frac{(197.3 \text{ eV} \cdot \text{nm/c})^2 (7.99 \text{ nm}^{-1})^2}{2(511 \times 10^3 \text{ eV/c}^2)} = 2.432 \text{ eV}.$$

6-21 *n* = 4



Note that the n = 4 wavefunction has three nodes and is antisymmetric about the midpoint of the well.

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6-23 Inside the well, the particle is free and the Schrödinger waveform is trigonometric with wavenumber  $k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$ :

 $\psi(x) = A \sin kx + B \cos kx$   $0 \le x \le L$ .

The infinite wall at x = 0 requires  $\psi(0) = B = 0$ . Beyond x = L, U(x) = U and the Schrödinger equation  $\frac{d^2\psi}{dx^2} = \left(\frac{2m}{\hbar^2}\right) \{U - E\} \psi(x)$ , which has exponential solutions for E < U

$$\psi(x) = Ce^{-\alpha x} + De^{+\alpha x}, \qquad x > L$$

where  $\alpha = \left[\frac{2m(U-E)}{\hbar^2}\right]^{1/2}$ . To keep  $\psi$  bounded at  $x = \infty$  we must take D = 0. At x = L, continuity of  $\psi$  and  $\frac{d\psi}{dx}$  demands

$$A\sin kL = Ce^{-\alpha L}$$
$$kA\cos kL = -\alpha Ce^{-\alpha L}$$

Dividing one by the other gives an equation for the allowed particle energies:  $k \cot kL = -\alpha$ . The dependence on *E* (or *k*) is made more explicit by noting that  $k^2 + \alpha^2 = \frac{2mU}{\hbar^2}$ , which allows the energy condition to be written  $k \cot kL = -\left[\left(\frac{2mU}{\hbar^2}\right) - k^2\right]^{1/2}$ . Multiplying by *L*, squaring the result, and using  $\cot^2 \theta + 1 = \csc^2 \theta$  gives  $(kL)^2 \csc^2 (kL) = \frac{2mUL^2}{\hbar^2}$  from which we obtain  $\frac{kL}{\sin kL} = \left(\frac{2mUL^2}{\hbar^2}\right)^{1/2}$ . Since  $\frac{\theta}{\sin \theta}$  is never smaller than unity for *any* value of  $\theta$ , there can be no bound state energies if  $\frac{2mUL^2}{\hbar^2} < 1$ .

6-24 After rearrangement, the Schrödinger equation is  $\frac{d^2\psi}{dx^2} = \left(\frac{2m}{\hbar^2}\right) \{U(x) - E\}\psi(x)$  with  $U(x) = \frac{1}{2}m\omega^2 x^2$  for the quantum oscillator. Differentiating  $\psi(x) = Cxe^{-\alpha x^2}$  gives

$$\frac{d\psi}{dx} = -2\alpha \, x\psi(x) + C^{-\alpha x^2}$$

and

$$\frac{d^2\psi}{dx^2} = -\frac{2\alpha x d\psi}{dx} - 2\alpha \psi(x) - (2\alpha x)Ce^{-\alpha x^2} = (2\alpha x)^2 \psi(x) - 6\alpha \psi(x)$$

Therefore, for  $\psi(x)$  to be a solution requires  $(2\alpha x)^2 - 6\alpha = \frac{2m}{\hbar^2} \{U(x) - E\} = \left(\frac{m\omega}{\hbar}\right)^2 x^2 - \frac{2mE}{\hbar^2}$ . Equating coefficients of like terms gives  $2\alpha = \frac{m\omega}{\hbar}$  and  $6\alpha = \frac{2mE}{\hbar^2}$ . Thus,  $\alpha = \frac{m\omega}{2\hbar}$  and  $E = \frac{3\alpha \hbar^2}{m} = \frac{3}{2}\hbar\omega$ . The normalization integral is  $1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 2C^2 \int x^2 e^{-2\alpha x^2} dx$  where the second step follows from the symmetry of the integrand about x = 0. Identifying *a* with  $2\alpha$  in the integral of Problem 6-32 gives  $1 = 2C^2 \left(\frac{1}{8\alpha}\right) \left(\frac{\pi}{2\alpha}\right)^{1/2}$  or  $C = \left(\frac{32\alpha^3}{\pi}\right)^{1/4}$ . 6-25 At its limits of vibration  $x = \pm A$  the classical oscillator has all its energy in potential form:  $E = \frac{1}{2}m\omega^2 A^2$  or  $A = \left(\frac{2E}{m\omega^2}\right)^{1/2}$ . If the energy is quantized as  $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ , then the  $\Gamma(2n+1)\hbar \eta^{1/2}$ 

corresponding amplitudes are 
$$A_n = \left[\frac{(2n+1)\hbar}{m\omega}\right]^{q}$$

6-26  $P_c(x)dx$  is proportional to the time that the particle spends in the interval dx. This time dt is inversely related to its speed v as  $dt = \frac{dx}{v}$ , so that  $P_c(x)dx = Cdt$  or  $P_c(x) = \frac{C}{v}$ . But the speed of the oscillator varies with its position in such a way as to keep the total energy constant:

$$E = \frac{1}{2}mv^2 + \frac{1}{2}m\omega^2 x^2$$
 or  $v^2 = \frac{2E}{m} - \omega^2 x^2$ .

Writing *E* in terms of the classical amplitude as  $E = \frac{1}{2}m\omega^2 A^2$  gives  $v = \omega (A^2 - x^2)^{1/2}$  and  $P_c(x) = \frac{C}{\omega} (A^2 - x^2)^{-1/2}$ . The constant *C* is a normalizing factor chosen to ensure a total probability of one:

$$1 = \int_{-A}^{A} P_{c}(x) dx = \frac{C}{\omega} \int_{-A}^{A} \left(A^{2} - x^{2}\right)^{-1/2} dx.$$

The integral is evaluated with the trigonometric substitution  $x = A \sin \theta$  (so that  $dx = A \cos \theta d\theta$ ) to get  $1 = \frac{C}{\omega} \int_{-\pi/2}^{\pi/2} d\theta = \frac{\pi C}{\omega}$ . Thus,  $\frac{C}{\omega}$  is just  $\frac{1}{\pi}$  and  $P_c(x) = \frac{1/\pi}{(A^2 - x^2)^{1/2}}$  for a classical oscillator with amplitude of vibration equal to A.

6-32 The probability density for this case is  $|\psi_0(x)|^2 = C_0^2 e^{-ax^2}$  with  $C_0 = \left(\frac{a}{\pi}\right)^{1/4}$  and  $a = \frac{m\omega}{\hbar}$ . For the calculation of the average position  $\langle x \rangle = \int_{-\infty}^{\infty} x |\psi_0(x)|^2 dx$  we note that the integrand is an odd function, so that the integral over the negative half-axis x < 0 exactly cancels that over the positive half-axis (x > 0), leaving  $\langle x \rangle = 0$ . For the calculation of  $\langle x^2 \rangle$ , however, the integrand  $x^2 |\psi_0|^2$  is symmetric, and the two half-axes contribute equally, giving

$$\langle x^2 \rangle = 2C_0^2 \int_0^\infty x^2 e^{-ax^2} dx = 2C_0^2 \left(\frac{1}{4a}\right) \left(\frac{\pi}{a}\right)^{1/2}$$

Substituting for  $C_0$  and a gives  $\langle x^2 \rangle = \frac{1}{2a} = \frac{\hbar}{2m\omega}$  and  $\Delta x = (\langle x^2 \rangle - \langle x \rangle^2)^{1/2} = (\frac{\hbar}{2m\omega})^{1/2}$ .

- 6-33 (a) Since there is no preference for motion in the leftward sense vs. the rightward sense, a particle would spend equal time moving left as moving right, suggesting  $\langle p_x \rangle = 0$ .
  - (b) To find  $\langle p_x^2 \rangle$  we express the average energy as the sum of its kinetic and potential energy contributions:  $\langle E \rangle = \left\langle \frac{p_x^2}{2m} \right\rangle + \langle U \rangle = \frac{\langle p_x^2 \rangle}{2m} + \langle U \rangle$ . But energy is sharp in the oscillator ground state, so that  $\langle E \rangle = E_0 = \frac{1}{2}\hbar\omega$ . Furthermore, remembering that  $U(x) = \frac{1}{2}m\omega^2 x^2$  for the quantum oscillator, and using  $\langle x^2 \rangle = \frac{\hbar}{2m\omega}$  from Problem 6-32, gives  $\langle U \rangle = \frac{1}{2}m\omega^2 \langle x^2 \rangle = \frac{1}{4}\hbar\omega$ . Then  $\langle p_x^2 \rangle = 2m(E_0 \langle U \rangle) = 2m\left(\frac{\hbar\omega}{4}\right) = \frac{m\hbar\omega}{2}$ .

(c) 
$$\Delta p_x = \left(\left\langle p_x^2 \right\rangle - \left\langle p_x \right\rangle^2\right)^{1/2} = \left(\frac{m\hbar\omega}{2}\right)^{1/2}$$

6-34 From Problems 6-32 and 6-33, we have  $\Delta x = \left(\frac{\hbar}{2m\omega}\right)^{1/2}$  and  $\Delta p_x = \left(\frac{m\hbar\omega}{2}\right)^{1/2}$ . Thus,  $\Delta x \Delta p_x = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left(\frac{m\hbar\omega}{2}\right)^{1/2} = \frac{\hbar}{2}$  for the oscillator ground state. This is the minimum uncertainty product permitted by the uncertainty principle, and is realized only for the ground state of the quantum oscillator.

6-35 Applying the momentum operator  $[p_x] = \left(\frac{\hbar}{i}\right) \frac{d}{dx}$  to each of the candidate functions yields

(a) 
$$[p_x]{A\sin(kx)} = \left(\frac{\hbar}{i}\right)k\{A\cos(kx)\}$$

(b) 
$$[p_x] \{A\sin(kx) - A\cos(kx)\} = \left(\frac{\hbar}{i}\right) k \{A\cos(kx) + A\sin(kx)\}$$

(c) 
$$[p_x] \{A\cos(kx) + iA\sin(kx)\} = \left(\frac{\hbar}{i}\right)k\{-A\sin(kx) + iA\cos(kx)\}$$

(d) 
$$[p_x]\left\{e^{ik(x-a)}\right\} = \left(\frac{\hbar}{i}\right)ik\left\{e^{ik(x-a)}\right\}$$

In case (c), the result is a multiple of the original function, since

$$-A\sin(kx) + iA\cos(kx) = i\{A\cos(kx) + iA\sin(kx)\}$$

The multiple is  $\left(\frac{\hbar}{i}\right)(ik) = \hbar k$  and is the eigenvalue. Likewise for (d), the operation  $[p_x]$  returns the original function with the multiplier  $\hbar k$ . Thus, (c) and (d) are eigenfunctions of  $[p_x]$  with eigenvalue  $\hbar k$ , whereas (a) and (b) are not eigenfunctions of this operator.

## 6-37 (a) Normalization requires

$$1 = \int_{-\infty}^{\infty} |\Psi|^2 dx = C^2 \int_{-\infty}^{\infty} \{\psi_1^* + \psi_2^*\} \{\psi_1 + \psi_2\} dx$$
$$= C^2 \{\int |\psi_1|^2 dx + \int |\psi_2|^2 dx + \int \psi_2^* \psi_1 dx + \int \psi_1^* \psi_2 dx\}$$

The first two integrals on the right are unity, while the last two are, in fact, the same integral since  $\psi_1$  and  $\psi_2$  are both real. Using the waveforms for the infinite square well, we find

$$\int \psi_2 \psi_1 dx = \frac{2}{L} \int_0^L \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi x}{L}\right) dx = \frac{1}{L} \int_0^L \left\{\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right\} dx$$

where, in writing the last line, we have used the trigonometric exponential identities of sine and cosine. Both of the integrals remaining are readily evaluated, and are zero. Thus,  $1 = C^2 \{1+0+0+0\} = 2C^2$ , or  $C = \frac{1}{\sqrt{2}}$ . Since  $\psi_{1,2}$  are stationary states, they develop in time according to their respective energies  $E_{1,2}$  as  $e^{-iE_t/\hbar}$ . Then  $\Psi(x, t) = C \{\psi_1 e^{-iE_1t/\hbar} + \psi_2 e^{-iE_2t/\hbar}\}$ .

(c)  $\Psi(x, t)$  is a stationary state only if it is an eigenfunction of the energy operator  $[E] = i\hbar \frac{\partial}{\partial t}$ . Applying [E] to  $\Psi$  gives

$$[E]\Psi = C\left\{i\hbar\left(\frac{-iE_1}{\hbar}\right)\psi_1 e^{-iE_1t/\hbar} + i\hbar\left(\frac{-iE_2}{\hbar}\right)\psi_2 e^{-iE_2t/\hbar}\right\} = C\left\{E_1\psi_1 e^{-iE_1t/\hbar} + E_2\psi_2 e^{-iE_2t/\hbar}\right\}.$$

Since  $E_1 \neq E_2$ , the operations [*E*] does *not* return a multiple of the wavefunction, and so  $\Psi$  is not a stationary state. Nonetheless, we may calculate the average energy for this state as

$$\begin{aligned} \langle E \rangle &= \int \Psi^* [E] \Psi dx = C^2 \int \left\{ \psi_1^* e^{+iE_1t/\hbar} + \psi_2^* e^{+iE_2t/\hbar} \right\} \left\{ E_1 \psi_1 e^{-iE_1t/\hbar} + E_2 \psi_2 e^{-iE_2t/\hbar} \right\} dx \\ &= C^2 \left\{ E_1 \int |\psi_1|^2 dx + E_2 \int |\psi_2|^2 dx \right\} \end{aligned}$$

with the cross terms vanishing as in part (a). Since  $\psi_{1,2}$  are normalized and  $C^2 = \frac{1}{2}$ 

we get finally 
$$\langle E \rangle = \frac{E_1 + E_2}{2}$$

6-38 The average position at any instant is given by

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi|^2 \, dx = C^2 \int_{-\infty}^{\infty} x \left\{ \psi_1^* e^{+iE_1t/\hbar} + \psi_2^* e^{+iE_2t/\hbar} \right\} \left\{ \psi_1 e^{-iE_1t/\hbar} + \psi_2 e^{-iE_2t/\hbar} \right\} dx$$
$$= C^2 \left\{ \int_{-\infty}^{\infty} x |\psi_1|^2 \, dx + \int_{-\infty}^{\infty} x |\psi_2|^2 \, dx + e^{-i\Omega t} \int_{-\infty}^{\infty} x \psi_1^* \psi_2 dx + e^{+i\Omega t} \int_{-\infty}^{\infty} x \psi_2^* \psi_1 dx \right\}$$

where  $\Omega = \frac{E_2 - E_1}{\hbar}$ . The last two integrals on the right are identical, since  $\psi_{1,2}$  are real. Furthermore,  $e^{-i\Omega t} + e^{+i\Omega t} = 2\cos(\Omega t)$  and  $C^2 = \frac{1}{2}$  from Problem 6-37. Thus, the result takes the form  $\langle x \rangle = x_0 + A\cos(\Omega t)$  with definitions given. To evaluate  $x_0$ , we note that  $\langle x \rangle = \frac{L}{2}$  for any stationary state of the well. Therefore,  $x_0 = \frac{1}{2} \left\{ \frac{L}{2} + \frac{L}{2} \right\} = \frac{L}{2} = 0.5$  nm no matter which two stationary states we use in the superposition. To find *A*, we use the ground and first excited state waves of the infinite well to write

$$A = \frac{2}{L} \int_{0}^{L} x \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi x}{L}\right) dx = \frac{1}{L} \int x \left\{ \cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right) \right\} dx.$$

Integrating by parts once, we obtain

$$A = \frac{1}{L} \left(\frac{L}{3\pi}\right) \left\{ 3\sin\left(\frac{\pi x}{L}\right) - \sin\left(\frac{3\pi x}{L}\right) \right\} \Big|_{0}^{L} - \frac{1}{L} \left(\frac{L}{3\pi}\right) \int_{0}^{L} \left\{ 3\sin\left(\frac{\pi x}{L}\right) - \sin\left(\frac{3\pi x}{L}\right) \right\} dx$$
$$= 0 + \frac{1}{L} \left(\frac{L}{3\pi}\right)^{2} \left\{ 9\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right) \right\} \Big|_{0}^{L} = \frac{L}{9\pi^{2}} \left\{ -9 + 1 - 9 + 1 \right\} = -\frac{16L}{9\pi^{2}} = -0.18 \text{ nm}$$

For electrons in this well we have the energies

 $E_1 = \frac{h^2}{8mL^2} = \frac{(1.24 \text{ keV} \cdot \text{nm/c})^2}{8(511 \text{ keV/c}^2)(1 \text{ nm})^2} = 0.376 \text{ eV} \text{ and } E_2 = (2)^2 E_1 = 1.50 \text{ eV}.$  The period of oscillation is  $T = \frac{2\pi}{\Omega}$ , or

$$T = \frac{h}{E_2 - E_1} = \frac{4.136 \times 10^{-15} \text{ eV} \cdot \text{s}}{1.124 \text{ eV}} = 3.68 \times 10^{-15} \text{ s}.$$

A classical electron with (kinetic) energy 
$$\frac{E_1 + E_2}{2} = 0.94 \text{ eV}$$
 would have speed  
 $v = \left(\frac{2E}{m}\right)^{1/2} = (1.92 \times 10^{-3})c$ 

and would require 
$$\frac{2L}{v} = 3.47 \times 10^{-15}$$
 s to shuttle back and forth in the well one time, a distance  $2L = 2$  nm.

7-2 (a) To the left of the step the particle is free with kinetic energy *E* and corresponding wavenumber  $k_1 = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$ :

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad x \le 0$$

To the right of the step the kinetic energy is reduced to E - U and the wavenumber is now  $k_2 = \left[\frac{2m(E-U)}{\hbar^2}\right]^{1/2}$ 

 $\psi(x) = Ce^{ik_2x} + De^{-ik_2x} \qquad x \ge 0$ 

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with D = 0 for waves incident on the step from the left. At x = 0 both  $\psi$  and  $\frac{d\psi}{dx}$ must be continuous:  $\psi(0) = A + B = C$ 

$$\left. \frac{d\psi}{dx} \right|_0 = ik_1 \left( A - B \right) = ik_2 C \; .$$

(b) Eliminating C gives 
$$A + B = \frac{k_1}{k_2}(A - B)$$
 or  $A\left(\frac{k_1}{k_2} - 1\right) = B\left(\frac{k_1}{k_2} + 1\right)$ . Thus,

$$R = \left|\frac{B}{A}\right|^2 = \frac{(k_1/k_2 - 1)^2}{(k_1/k_2 + 1)^2} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$
$$T = 1 - R = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

- As  $E \rightarrow U$ ,  $k_2 \rightarrow 0$ , and  $R \rightarrow 1$ ,  $T \rightarrow 0$  (no transmission), in agreement with the (C) result for any energy E < U. For  $E \rightarrow \infty$ ,  $k_1 \rightarrow k_2$  and  $R \rightarrow 0$ ,  $T \rightarrow 1$  (perfect transmission) suggesting correctly that very energetic particles do not see the step and so are unaffected by it.
- 7-3 With E = 25 MeV and U = 20 MeV, the ratio of wavenumber is  $\frac{k_1}{k_2} = \left(\frac{E}{E-U}\right)^{1/2} = \left(\frac{25}{25-20}\right)^{1/2} = \sqrt{5} = 2.236$ . Then from Problem 7-2  $R = \frac{\left(\sqrt{5}-1\right)^2}{\left(\sqrt{5}+1\right)^2} = 0.146$  and

T = 1 - R = 0.854. Thus, 14.6% of the incoming particles would be reflected and 85.4% would be transmitted. For electrons with the same energy, the transparency and reflectivity of the step are unchanged.

## 7-4 The reflection coefficient for this case is given in Problem 7-2 as

$$R = \left|\frac{B}{A}\right|^2 = \frac{(k_1/k_2 - 1)^2}{(k_1/k_2 + 1)^2} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}.$$

The wavenumbers are those for electrons with kinetic energies E = 54.0 eV and E - U = 54.0 eV + 10.0 eV = 64.0 eV:

$$\frac{k_1}{k_2} = \left(\frac{E}{E-U}\right)^{1/2} = \left(\frac{54 \text{ eV}}{64 \text{ eV}}\right)^{1/2} = 0.9186.$$

Then,  $R = \frac{(0.9186-1)^2}{(0.9186+1)^2} = 1.80 \times 10^{-3}$  is the fraction of the incident beam that is reflected at the

boundary.