

6-6

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

$$\frac{\partial \psi}{\partial x} = -kA \sin kx + kB \cos kx$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 A \cos kx - k^2 B \sin kx$$

$$\left(\frac{-2m}{\hbar^2}\right)(E - U)\psi = \left(\frac{-2mE}{\hbar^2}\right)(A \cos kx + B \sin kx)$$

The Schrödinger equation is satisfied if $\frac{\partial^2 \psi}{\partial x^2} = \left(\frac{-2m}{\hbar^2}\right)(E - U)\psi$ or

$$-k^2(A \cos kx + B \sin kx) = \left(\frac{-2mE}{\hbar^2}\right)(A \cos kx + B \sin kx).$$

Therefore $E = \frac{\hbar^2 k^2}{2m}$.

6-9 $E_n = \frac{n^2 \hbar^2}{8mL^2}$, so $\Delta E = E_2 - E_1 = \frac{3\hbar^2}{8mL^2}$

$$\Delta E = (3) \frac{(1240 \text{ eV nm}/c)^2}{8(938.28 \times 10^6 \text{ eV}/c^2)(10^{-5} \text{ nm})^2} = 6.14 \text{ MeV}$$

$$\lambda = \frac{hc}{\Delta E} = \frac{1240 \text{ eV nm}}{6.14 \times 10^6 \text{ eV}} = 2.02 \times 10^{-4} \text{ nm}$$

This is the gamma ray region of the electromagnetic spectrum.

6-10 $E_n = \frac{n^2 \hbar^2}{8mL^2}$

$$\frac{\hbar^2}{8mL^2} = \frac{(6.63 \times 10^{-34} \text{ Js})^2}{8(9.11 \times 10^{-31} \text{ kg})(10^{-10} \text{ m})^2} = 6.03 \times 10^{-18} \text{ J} = 37.7 \text{ eV}$$

(a) $E_1 = 37.7 \text{ eV}$
 $E_2 = 37.7 \times 2^2 = 151 \text{ eV}$
 $E_3 = 37.7 \times 3^2 = 339 \text{ eV}$
 $E_4 = 37.7 \times 4^2 = 603 \text{ eV}$

(b) $hf = \frac{hc}{\lambda} = E_{n_i} - E_{n_f}$

$$\lambda = \frac{hc}{E_{n_i} - E_{n_f}} = \frac{1240 \text{ eV} \cdot \text{nm}}{E_{n_i} - E_{n_f}}$$

For $n_i = 4$, $n_f = 1$, $E_{n_i} - E_{n_f} = 603 \text{ eV} - 37.7 \text{ eV} = 565 \text{ eV}$, $\lambda = 2.19 \text{ nm}$

$n_i = 4$, $n_f = 2$, $\lambda = 2.75 \text{ nm}$

$n_i = 4$, $n_f = 3$, $\lambda = 4.70 \text{ nm}$

$n_i = 3$, $n_f = 1$, $\lambda = 4.12 \text{ nm}$

$n_i = 3$, $n_f = 2$, $\lambda = 6.59 \text{ nm}$

$n_i = 2$, $n_f = 1$, $\lambda = 10.9 \text{ nm}$

- 6-11 In the present case, the box is displaced from $(0, L)$ by $\frac{L}{2}$. Accordingly, we may obtain the wavefunctions by replacing x with $x - \frac{L}{2}$ in the wavefunctions of Equation 6.18. Using

$$\sin\left[\left(\frac{n\pi}{L}\right)\left(x - \frac{L}{2}\right)\right] = \sin\left[\left(\frac{n\pi x}{L}\right) - \frac{n\pi}{2}\right] = \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi}{2}\right) - \cos\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi}{2}\right)$$

we get for $-\frac{L}{2} \leq x \leq \frac{L}{2}$

$$\psi_1(x) = \left(\frac{2}{L}\right)^{1/2} \cos\left(\frac{\pi x}{L}\right); P_1(x) = \left(\frac{2}{L}\right) \cos^2\left(\frac{\pi x}{L}\right)$$

$$\psi_2(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{2\pi x}{L}\right); P_2(x) = \left(\frac{2}{L}\right) \sin^2\left(\frac{2\pi x}{L}\right)$$

$$\psi_3(x) = \left(\frac{2}{L}\right)^{1/2} \cos\left(\frac{3\pi x}{L}\right); P_3(x) = \left(\frac{2}{L}\right) \cos^2\left(\frac{3\pi x}{L}\right)$$

6-12 $\Delta E = \frac{hc}{\lambda} = \left(\frac{h^2}{8mL^2}\right)[2^2 - 1^2]$ and $L = \left[\frac{(3/8)h\lambda}{mc}\right]^{1/2} = 7.93 \times 10^{-10} \text{ m} = 7.93 \text{ \AA}$.

- 6-13 (a) Proton in a box of width $L = 0.200 \text{ nm} = 2 \times 10^{-10} \text{ m}$

$$E_1 = \frac{h^2}{8m_p L^2} = \frac{(6.626 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(1.67 \times 10^{-27} \text{ kg})(2 \times 10^{-10} \text{ m})^2} = 8.22 \times 10^{-22} \text{ J}$$

$$= \frac{8.22 \times 10^{-22} \text{ J}}{1.60 \times 10^{-19} \text{ J/eV}} = 5.13 \times 10^{-3} \text{ eV}$$

- (b) Electron in the same box:

$$E_1 = \frac{h^2}{8m_e L^2} = \frac{(6.626 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(9.11 \times 10^{-31} \text{ kg})(2 \times 10^{-10} \text{ m})^2} = 1.506 \times 10^{-18} \text{ J} = 9.40 \text{ eV}$$

- (c) The electron has a much higher energy because it is much less massive.

6-16 (a) $\psi(x) = A \sin\left(\frac{\pi x}{L}\right)$, $L = 3 \text{ \AA}$. Normalization requires

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

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

$$P = \int_0^{L/3} |\psi|^2 dx = \left(\frac{2}{L}\right)^{1/2} \int_0^{L/3} \sin^2\left(\frac{\pi x}{L}\right) dx = \frac{2}{\pi} \int_0^{\pi/3} \sin^2 \phi d\phi = \frac{2}{\pi} \left[\frac{\phi}{2} - \frac{\sin(2\phi)}{4} \right]_0^{\pi/3} = 0.1955$$

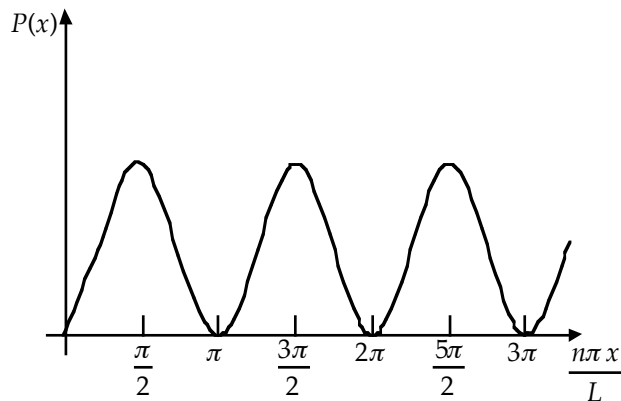
(b) $\psi = A \sin\left(\frac{100\pi x}{L}\right)$, $A = \left(\frac{2}{L}\right)^{1/2}$

$$P = \frac{2}{L} \int_0^{L/3} \sin^2\left(\frac{100\pi x}{L}\right) dx = \frac{2}{L} \left(\frac{L}{100\pi}\right) \int_0^{100\pi/3} \sin^2 \phi d\phi = \frac{1}{50\pi} \left[\frac{100\pi}{2} - \frac{1}{4} \sin\left(\frac{200\pi}{3}\right) \right]$$

$$= \frac{1}{3} - \left[\frac{1}{200\pi} \right] \sin\left(\frac{2\pi}{3}\right) = \frac{1}{3} - \frac{\sqrt{3}}{400\pi} = 0.3319$$

(c) Yes: For large quantum numbers the probability approaches $\frac{1}{3}$.

6-18 Since the wavefunction for a particle in a one-dimension box of width L is given by $\psi_n = A \sin\left(\frac{n\pi x}{L}\right)$ it follows that the probability density is $P(x) = |\psi_n|^2 = A^2 \sin^2\left(\frac{n\pi x}{L}\right)$, which is sketched below:



From this sketch we see that $P(x)$ is a *maximum* when $\frac{n\pi x}{L} = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots = \pi\left(m + \frac{1}{2}\right)$ or when

$$x = \frac{L}{n} \left(m + \frac{1}{2}\right) \quad m = 0, 1, 2, 3, \dots, n.$$

Likewise, $P(x)$ is a *minimum* when $\frac{n\pi x}{L} = 0, \pi, 2\pi, 3\pi, \dots = m\pi$ or when

$$x = \frac{Lm}{n} \quad m = 0, 1, 2, 3, \dots, n$$

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

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

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

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

At $x = L$ continuity of ψ 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 $U = 5 \text{ eV}$ and width $2L = 0.2 \text{ nm}$, 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 $k = 7.99 \text{ nm}^{-1}$, and an energy

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

6-29 (a) Normalization requires

$1 = \int_{-\infty}^{\infty} |\psi|^2 dx = C^2 \int_0^{\infty} e^{-2x} (1 - e^{-x})^2 dx = C^2 \int_0^{\infty} (e^{-2x} - 2e^{-3x} + e^{-4x}) dx$. The integrals are elementary and give $1 = C^2 \left\{ \frac{1}{2} - 2\left(\frac{1}{3}\right) + \frac{1}{4} \right\} = \frac{C^2}{12}$. The proper units for C are those of $(\text{length})^{-1/2}$ thus, normalization requires $C = (12)^{1/2} \text{ nm}^{-1/2}$.

(b) The most likely place for the electron is where the probability $|\psi|^2$ is largest. This is also where ψ itself is largest, and is found by setting the derivative $\frac{d\psi}{dx}$ equal zero:

$$0 = \frac{d\psi}{dx} = C \{-e^{-x} + 2e^{-2x}\} = Ce^{-x} \{2e^{-x} - 1\}.$$

The RHS vanishes when $x = \infty$ (a minimum), and when $2e^{-x} = 1$, or $x = \ln 2 \text{ nm}$. Thus, the most likely position is at $x_p = \ln 2 \text{ nm} = 0.693 \text{ nm}$.

(c) The average position is calculated from

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx = C^2 \int_0^{\infty} x e^{-2x} (1 - e^{-x})^2 dx = C^2 \int_0^{\infty} x (e^{-2x} - 2e^{-3x} + e^{-4x}) dx.$$

The integrals are readily evaluated with the help of the formula $\int_0^{\infty} x e^{-ax} dx = \frac{1}{a^2}$ to

get $\langle x \rangle = C^2 \left\{ \frac{1}{4} - 2\left(\frac{1}{9}\right) + \frac{1}{16} \right\} = C^2 \left\{ \frac{13}{144} \right\}$. Substituting $C^2 = 12 \text{ nm}^{-1}$ gives

$$\langle x \rangle = \frac{13}{12} \text{ nm} = 1.083 \text{ nm}.$$

We see that $\langle x \rangle$ is somewhat greater than the most probable position, since the probability density is skewed in such a way that values of x larger than x_p are weighted more heavily in the calculation of the average.

6-31 The symmetry of $|\psi(x)|^2$ about $x = 0$ can be exploited effectively in the calculation of average values. To find $\langle x \rangle$

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

We notice that the integrand is antisymmetric about $x = 0$ due to the extra factor of x (an odd function). Thus, the contribution from the two half-axes $x > 0$ and $x < 0$ cancel exactly, leaving $\langle x \rangle = 0$. For the calculation of $\langle x^2 \rangle$, however, the integrand is symmetric and the half-axes contribute equally to the value of the integral, giving

$$\langle x \rangle = \int_0^{\infty} x^2 |\psi|^2 dx = 2C^2 \int_0^{\infty} x^2 e^{-2x/x_0} dx.$$

Two integrations by parts show the value of the integral to be $2\left(\frac{x_0}{2}\right)^3$. Upon substituting

for C^2 , we get $\langle x^2 \rangle = 2\left(\frac{1}{x_0}\right)(2)\left(\frac{x_0}{2}\right)^3 = \frac{x_0^2}{2}$ and $\Delta x = \left(\langle x^2 \rangle - \langle x \rangle^2\right)^{1/2} = \left(\frac{x_0^2}{2}\right)^{1/2} = \frac{x_0}{\sqrt{2}}$. In

calculating the probability for the interval $-\Delta x$ to $+\Delta x$ we appeal to symmetry once again to write

$$P = \int_{-\Delta x}^{+\Delta x} |\psi|^2 dx = 2C^2 \int_0^{\Delta x} e^{-2x/x_0} dx = -2C^2 \left(\frac{x_0}{2}\right) e^{-2x/x_0} \Big|_0^{\Delta x} = 1 - e^{-\sqrt{2}} = 0.757$$

or about 75.7% independent of x_0 .