

6-2 (a) Normalization requires

$$1 = \int_{-\infty}^{\infty} |\psi|^2 dx = A^2 \int_{-\frac{L}{4}}^{\frac{L}{4}} \cos^2 \left(\frac{2\pi x}{L} \right) dx = \left(\frac{A^2}{2} \right) \int_{-\frac{L}{4}}^{\frac{L}{4}} \left(1 + \cos \left(\frac{4\pi x}{L} \right) \right) dx$$

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

(b)
$$P = \int_0^{\frac{L}{8}} |\psi|^2 dx = A^2 \int_0^{\frac{L}{8}} \cos^2 \left(\frac{2\pi x}{L} \right) dx = \left(\frac{4}{L} \right) \left(\frac{1}{2} \right) \int_0^{\frac{L}{8}} \left(1 + \cos \left(\frac{4\pi x}{L} \right) \right) dx$$
$$= \left(\frac{2}{L} \right) \left(\frac{L}{8} \right) + \left(\frac{2}{L} \right) \left(\frac{L}{4\pi} \right) \sin \left(\frac{4\pi x}{L} \right) \Big|_0^{\frac{L}{8}} = \frac{1}{4} + \frac{1}{2\pi} = 0.409$$

6-4 The time development of Ψ is given by Equation 6.8 or

$$\Psi(x, t) = \int a(k) e^{i\{kx - \omega(k)t\}} dk = \left(\frac{C\alpha}{\sqrt{\pi}} \right) \int_{-\infty}^{\infty} e^{\{ikx - i\omega(k)t - \alpha^2 k^2\}} dk,$$

with $\omega(k) = \frac{\hbar k^2}{2m}$ for a free particle of mass m . As in Example 6.3, the integral may be reduced to a recognizable form by completing the square in the exponent. Since $\omega(k)t = \left(\frac{\hbar t}{2m} \right) k^2$, we group this term together with $\alpha^2 k^2$ by introducing $\beta^2 = \alpha^2 + \frac{i\hbar t}{2m}$ to get

$$ikx - \omega(k)t - \alpha^2 k^2 = -\left(\beta k - \frac{ix}{2\beta} \right)^2 - \frac{x^2}{4\beta^2}.$$

Then, changing variables to $z = \beta k - \frac{ix}{2\beta}$ gives

$$\Psi(x, t) = \left(\frac{C\alpha}{\beta\sqrt{\pi}} \right) e^{-x^2/4\beta^2} \int_{-\infty}^{\infty} e^{-z^2} dz = \left(\frac{C\alpha}{\beta} \right) e^{-x^2/4\beta^2}.$$

To interpret this result, we must recognize that β is complex and separate real and imaginary parts. Thus, $|\beta^2|^2 = \left| \alpha^2 + \frac{i\hbar t}{2m} \right|^2 = \alpha^4 + \left(\frac{\hbar t}{2m} \right)^2$ and the exponent for Ψ is

$$\frac{x^2}{4\beta^2} = \frac{x^2 \left(\alpha^2 - \frac{i\hbar t}{2m} \right)}{4|\beta^2|^2} = \frac{x^2}{4 \left[\alpha^2 + \left(\frac{\hbar t}{2m} \right)^2 \right]} + (\text{imaginary terms})$$

then

$$|\Psi(x, t)| = \frac{C\alpha}{\left(\alpha^4 + \left(\frac{\hbar t}{2m} \right)^2 \right)^{1/4}} e^{\{-x^2/[4(\alpha^2 + (\hbar t/2m)^2)]\}}.$$

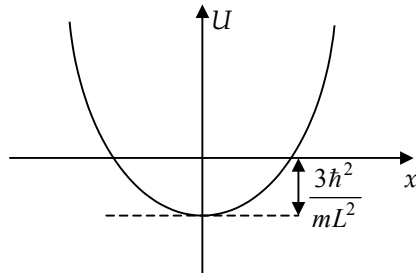
We see that apart from a phase factor, $\Psi(x, t)$ is still a gaussian but with amplitude diminished by $\frac{\alpha}{\left(\alpha^4 + \left(\frac{\hbar t}{2m}\right)^2\right)^{1/4}}$ and a width $\Delta x(t) = \left(\alpha^2 + \left(\frac{\hbar t}{2m\alpha}\right)^2\right)^{1/2}$ where $\alpha = \Delta x(0)$ is the initial width.

- 6-5 (a) Solving the Schrödinger equation for U with $E=0$ gives

$$U = \left(\frac{\hbar^2}{2m}\right) \frac{\left(\frac{d^2\psi}{dx^2}\right)}{\psi}.$$

If $\psi = Ae^{-x^2/L^2}$ then $\frac{d^2\psi}{dx^2} = (4Ax^3 - 6AxL^2)\left(\frac{1}{L^4}\right)e^{-x^2/L^2}$, $U = \left(\frac{\hbar^2}{2mL^2}\right)\left(\frac{4x^2}{L^2} - 6\right)$.

- (b) $U(x)$ is a parabola centered at $x=0$ with $U(0) = \frac{-3\hbar^2}{mL^2} < 0$:



- 6-7 Since the particle is confined to the box, Δx can be no larger than L , the box length. With $n = 0$, the particle energy $E_n = \frac{n^2 h^2}{8mL^2}$ is also zero. Since the energy is all kinetic, this implies $\langle p_x^2 \rangle = 0$. But $\langle p_x \rangle = 0$ is expected for a particle that spends equal time moving left as right, giving $\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = 0$. Thus, for this case $\Delta p_x \Delta x = 0$, in violation of the uncertainty principle.

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

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

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

This is the gamma ray region of the electromagnetic spectrum.

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

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

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

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

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

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

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

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

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

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

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

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

$$(b) \quad \text{Electron in the same box:}$$

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

$$(c) \quad \text{The electron has a much higher energy because it is much less massive.}$$

$$6-15 \quad (a) \quad U = \left(\frac{e^2}{4\pi \epsilon_0 d} \right) \left[-1 + \frac{1}{2} - \frac{1}{3} + \left(-1 + \frac{1}{2} \right) + (-1) \right] = \frac{(-7/3)e^2}{4\pi \epsilon_0 d} = \frac{(-7/3)ke^2}{d}$$

$$(b) \quad K = 2E_1 = \frac{2h^2}{8m \times 9d^2} = \frac{h^2}{36md^2}$$

$$(c) \quad E = U + K \text{ and } \frac{dE}{dd} = 0 \text{ for a minimum } \left[\frac{(+7/3)e^2k}{d^2} \right] - \frac{h^2}{18md^3} = 0$$

$$d = \frac{3h^2}{(7)(18ke^2m)} \text{ or } d = \frac{h^2}{42mke^2}$$

$$d = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{(42)(9.11 \times 10^{-31} \text{ kg})(9 \times 10^9 \text{ N} \cdot \text{m}^2 \cdot \text{C}^{-2})(1.6 \times 10^{-19} \text{ C})^2} = 0.5 \times 10^{-10} \text{ m} = 0.050 \text{ nm}$$

(d) Since the lithium spacing is a , where $Na^3 = V$ and the density is $\frac{Nm}{V}$ where m is the mass of one atom, we get

$$a = \left(\frac{Vm}{Nm} \right)^{1/3} = \left(\frac{m}{\text{density}} \right)^{1/3} = \left(1.66 \times 10^{-27} \text{ kg} \times \frac{7}{530 \text{ kg/m}^3} \right)^{1/3} \text{ m} = 2.8 \times 10^{-10} \text{ m} \\ = 0.28 \text{ nm}$$

(2.8 times larger than $2d$)

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

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

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

$$P = \int_0^{L/3} |\psi|^2 dx = \left(\frac{2}{L}\right)^{L/3} \int_0^{L/3} \sin^2\left(\frac{\pi x}{L}\right) dx = \frac{2}{\pi} \int_0^{\pi/3} \sin^2 \phi d\phi = \frac{2}{\pi} \left[\frac{\phi}{6} - \frac{(3)^{1/2}}{8} \right] = 0.1955.$$

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

$$\begin{aligned} P &= \frac{2}{L} \int_0^{L/3} \sin^2\left(\frac{100\pi x}{L}\right) dx = \frac{2}{L} \left(\frac{L}{100\pi}\right) \int_0^{100\pi/3} \sin^2 \phi d\phi = \frac{1}{50\pi} \left[\frac{100\pi}{6} - \frac{1}{4} \sin\left(\frac{200\pi}{3}\right) \right] \\ &= \frac{1}{3} - \left[\frac{1}{200\pi} \right] \sin\left(\frac{2\pi}{3}\right) = \frac{1}{3} - \frac{\sqrt{3}}{400\pi} = 0.3319 \end{aligned}$$

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

- 6-17 (a) The wavefunctions and probability densities are the same as those shown in the two lower curves in Figure 6.16 of the text.

- (b) $P_1 = \int_{1.5 \text{ \AA}}^{3.5 \text{ \AA}} |\psi|^2 dx = \frac{2}{10 \text{ \AA}} \int_{1.5 \text{ \AA}}^{3.5 \text{ \AA}} \sin^2\left(\frac{\pi x}{10}\right) dx$

$$\frac{1}{5} \left[\frac{x}{2} - \frac{5}{4\pi} \sin\left(\frac{\pi x}{5}\right) \right]_{1.5}^{3.5}$$

In the above result we used $\int \sin^2 ax dx = \frac{x}{2} - \frac{1}{4a} \sin(2ax)$. Therefore,

$$\begin{aligned} P_1 &= \frac{1}{10} \left[x - \frac{5}{\pi} \sin\left(\frac{\pi x}{5}\right) \right]_{1.5}^{3.5} = \frac{1}{10} \left\{ 3.5 - \frac{5}{\pi} \sin\left[\frac{\pi(3.5)}{5}\right] - 1.5 + \frac{5}{\pi} \sin\left[\frac{\pi(1.5)}{5}\right] \right\} \\ &= \frac{1}{10} \left[2.0 + \frac{5}{\pi} (\sin 0.3\pi - \sin 0.7\pi) \right] = \frac{1}{10} [2.00 + 0.0] = 0.200 \end{aligned}$$

- (c) $P_2 = \frac{1}{5} \int_{1.5}^{3.5} \sin^2\left(\frac{\pi x}{5}\right) dx = \frac{1}{5} \left[\frac{x}{2} - \frac{5}{4\pi} \sin(0.4\pi x) \right]_{1.5}^{3.5} = \frac{1}{10} \left[x - \frac{5}{2\pi} \sin(0.4\pi x) \right]_{1.5}^{3.5}$
 $= \frac{1}{10} \{ 2.0 + (0.798) \{ \sin[0.4\pi(1.5)] - \sin[0.4\pi(3.5)] \} \} = 0.351$

(d) Using $E = \frac{n^2 h^2}{8mL^2}$ we find $E_1 = 0.377 \text{ eV}$ and $E_2 = 1.51 \text{ eV}$.

6-28 A particle within the well is subject to no forces and, hence, moves with uniform speed, spending equal time in all parts of the well. Thus, for such a particle the probability density is *uniform*. That is, $P_c(x) = \text{constant}$. The constant is fixed by requiring the integrated

probability to be unity, that is, $1 = \int_0^L P_c(x) dx = CL$ or $C = \frac{1}{L}$. To find $\langle x \rangle$ we weight the

possible particle positions according to the probability density P_c to get

$\langle x \rangle = \int_0^L x P_c(x) dx = \frac{1}{L} \left(\frac{x^2}{2} \right) \Big|_0^L = \frac{L}{2}$. Similarly, $\langle x^2 \rangle$ is found by weighting the possible values of

x^2 with P_c :

$$\langle x^2 \rangle = \int_0^L x^2 P_c(x) dx = \frac{1}{L} \left(\frac{x^3}{3} \right) \Big|_0^L = \frac{L^2}{3}.$$

The classical and quantum results for $\langle x \rangle$ agree exactly; for $\langle x^2 \rangle$ the quantum prediction is smaller by an amount $\frac{L^2}{2(n\pi)^2}$ which, however, goes to zero in the limit of large quantum numbers n , where classical and quantum results must coincide (correspondence principle).

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 $x = \ln 2$ nm. Thus, the most likely position is at $x_p = \ln 2$ nm = 0.693 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

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

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

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.

- 6-30 The possible particle positions within the box are weighted according to the probability density $|\psi|^2 = \frac{2}{L} \sin^2 \left(\frac{n\pi x}{L} \right)$. The position is calculated as $\langle x \rangle = \int_0^L x |\psi|^2 dx = \frac{2}{L} \int_0^L x \sin^2 \left(\frac{n\pi x}{L} \right) dx$. Making the change of variable $\theta = \frac{n\pi x}{L}$ (so that $d\theta = \frac{\pi dx}{L}$) gives $\langle x \rangle = \frac{2L}{\pi^2} \int_0^{\pi} \theta \sin^2 n\theta d\theta$. Using the trigonometric identity $2 \sin^2 \theta = 1 - \cos 2\theta$, we get $\langle x \rangle = \frac{L}{\pi^2} \left\{ \int_0^{\pi} \theta d\theta - \int_0^{\pi} \theta \cos 2n\theta d\theta \right\}$. An integration by parts shows that the second integral vanishes, while the first integrates to $\frac{\pi^2}{2}$. Thus, $\langle x \rangle = \frac{L}{2}$, independent of n . For the computation of $\langle x^2 \rangle$, there is an extra factor of x in the integrand. After changing variables to $\theta = \frac{\pi x}{L}$ we get $\langle x^2 \rangle = \frac{L^2}{\pi^3} \left\{ \int_0^{\pi} \theta^2 d\theta - \int_0^{\pi} \theta^2 \cos 2n\theta d\theta \right\}$. The first integral evaluates to $\frac{\pi^3}{3}$, the second may be integrated by parts twice to get

$$\int_0^{\pi} \theta^2 \cos 2n\theta d\theta = -\frac{1}{n} \int_0^{\pi} \theta \sin 2n\theta d\theta = \left(\frac{1}{2n^2} \right) \theta \cos 2n\theta \Big|_0^{\pi} = \frac{\pi}{2n^2}.$$

$$\text{Then } \langle x^2 \rangle = \frac{L^2}{\pi^3} \left\{ \frac{\pi^3}{3} - \frac{\pi}{2n^2} \right\} = \frac{L^2}{3} - \frac{L^2}{2(n\pi)^2}.$$

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 $\Delta x = (\langle x^2 \rangle - \langle x \rangle^2)^{1/2} = \left(\frac{x_0^2}{2}\right)^{1/2} = \frac{x_0}{\sqrt{2}}$. 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 .