# **Chapter 2**

# Linear motion and the harmonic oscillator

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# Exercises

**2.1** For the energy in (a) use E = eV.

 $k = p/\hbar[\text{eqn } 2.7] = 9.48 \times 10^{31} \text{ m}^{-1}$ ; hence

$$\psi(x) = A \exp\{9.48i \times 10^{31} (x/m)\}$$

**Exercise:** What value of V is needed to accelerate an electron so that its wavelength is

equal to its Compton wavelength?

**2.2** In each case  $|\underline{\psi}(x)|^2 = A^2$ , a constant  $(A^2 = 1/L; L \to \infty)$ 

**2.3** Substituting eqn 2.5 for  $\psi$  in eqn 2.4 yields:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(A\mathrm{e}^{\mathrm{i}kx}+B\mathrm{e}^{-\mathrm{i}kx}\right)=\frac{\hbar^2k^2}{2m}\left(A\mathrm{e}^{\mathrm{i}kx}+B\mathrm{e}^{-\mathrm{i}kx}\right)$$

confirming that the wavefunction is an eigenfunction with eigenvalue  $\hbar^2 k^2/2m$ . The

relation between k and E given in eqn 2.5 then follows. Similar substitution of eqn 2.6 for  $\psi$  in eqn 2.4 yields:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}(C\mathrm{cos}kx + D\mathrm{sin}kx) = \frac{\hbar^2k^2}{2m}(C\mathrm{cos}kx + D\mathrm{sin}kx)$$

and the wavefunction is seen to satisfy eqn 2.4.

**2.4** The flux density for the wavefunction  $A \sin kx$  is, using eqn 2.11,

$$J_x(A\sin kx) = \frac{1}{2m} \left( \frac{\hbar k}{i} A^* \sin kx A \cos kx + \frac{\hbar k}{-i} A \sin kx A^* \cos kx \right) = 0$$

**2.5** Use the expression as given in the *brief illustration* in Section 2.7 for the penetration depth  $1/\kappa$ :

$$\frac{1}{\kappa} = \frac{\hbar}{\{2m(V-E)\}^{1/2}}$$
$$= \frac{1.055 \times 10^{-34} \text{ Js}}{\{2 \times 9.109 \times 10^{-31} \text{ kg} \times (2.0 \text{ eV} - E) \times 1.602 \times 10^{-19} \text{ J/eV}\}^{1/2}}$$
$$= 4.0 \times 10^{-10} \text{ m}$$

Solving for the kinetic energy yields E = 1.76 eV.

- 2.6 The transmission probability is given in eqn 2.26. Using the Worksheet entitled Equation
  - 2.26 on the text's website and setting

$$m = m_{\rm e} (\text{so that } m/m_{\rm e}=1)$$
  

$$E = V_0 = 2.0 \text{ eV} (\text{so that } E/E_{\rm h} = V_0/E_{\rm h} = 0.073499)$$
  

$$\beta = 1.0 \times 10^{10} \text{ m}^{-1} (\text{so that } \beta/(1/a_0) = 0.529177)$$
  
yields  $T = \underline{6.361 \times 10^{-1}}$ .

2.7  $\psi_4 = (2/L)^{1/2} \sin(4\pi x/L) = 0$  when  $x = 0, \frac{1}{4}L, \frac{1}{2}L, \frac{3}{4}L, L$ , of which the central three are nodes.

**Exercise:** Repeat the question for n = 6.

**2.8** To show that the n = 1 and n = 2 wavefunctions for a particle in a box are

orthogonal, we must evaluate the integral

$$\int_{0}^{L} \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) dx = 0$$

The integral can be evaluated using mathematical software or standard integration tables and does indeed vanish.

**2.9** The wavefunction for a particle in a geometrically square two-dimensional box of length *L* is given by (see eqn 2.35)

$$\psi_{n_1n_2}(x, y) = \frac{2}{L} \sin\left(\frac{n_1\pi x}{L}\right) \sin\left(\frac{n_2\pi y}{L}\right)$$

- (a) Nodes correspond to points where the wavefunction passes through zero. For (i)  $n_1 = 2, n_2 = 1$ , this occurs at points (x,y) such that  $\underline{x = L/2}$ . For (ii)  $n_1 = 3, n_2 = 2$ , this occurs at points (x,y) such that  $\underline{x = L/3 \text{ or } 2L/3}$  and at points (x,y) such that  $\underline{y} = \underline{L/2}$ .
- (b) Maxima in the probability densities occur where  $\psi^2$  is maximized. For (i)  $n_1 = 2$ ,  $n_2 = 1$ , this occurs at points (x,y) such that  $\underline{x = L/4 \text{ or } 3L/4}$  and  $\underline{y = L/2}$ . For (ii)  $n_1$   $= 3, n_2 = 2$ , this occurs at points (x,y) such that  $\underline{x = L/6, L/2 \text{ or } 5L/6}$  and  $\underline{y = L/4 \text{ or}}$  $\underline{3L/4}$ .
- **2.10** The energy of a particle in a three-dimensional cubic box is given by:

$$E_{n_1n_2n_3} = \frac{h^2}{8m} \left( \frac{n_1^2}{L^2} + \frac{n_2^2}{L^2} + \frac{n_3^2}{L^2} \right) \qquad n_1 = 1, 2, \dots \quad n_2 = 1, 2, \dots \quad n_3 = 1, 2, \dots$$

The lowest energy level corresponds to  $(n_1 = n_2 = n_3 = 1)$  and equals  $3h^2/8mL^2$ . Three times this energy, that is  $9h^2/8mL^2$ , can be achieved with the following sets of

quantum numbers:

$$(n_1 = 2, n_2 = 2, n_3 = 1)$$
  
 $(n_1 = 2, n_2 = 1, n_3 = 2)$   
 $(n_1 = 1, n_2 = 2, n_3 = 2)$ 

Therefore the degeneracy of the energy level is  $\underline{3}$ .

2.11 The harmonic oscillator wavefunction is given in eqn 2.41. Nodes correspond to those points x such that the Hermite polynomial  $H_{\nu}(\alpha x)$  vanishes. Using Table 2.1, we seek values of  $z = \alpha x$  such that  $4z^2 - 2 = 0$ . This equation is satisfied by

$$z = \pm \sqrt{\frac{1}{2}}$$

and therefore  $x = \underline{\alpha}/\sqrt{2}$  and  $x = \underline{-\alpha}/\sqrt{2}$ .

#### 2.12 The energy levels of the harmonic oscillator are given by 2.40. The separation

between neighboring vibrational energy levels v and v+1 is given by

$$\Delta E = \hbar \omega = \hbar \sqrt{\frac{k_f}{m}} = 1.055 \times 10^{-34} \text{Js} \times \sqrt{\frac{275 \text{ Nm}^{-1}}{1.33 \times 10^{-25} \text{kg}}} = 4.797 \times 10^{-21} \text{J}$$

Equating this with the photon energy  $hc/\lambda$  yields a wavelength of  $4.14 \times 10^{-5}$  m and a corresponding wavenumber of  $1/(4.14 \times 10^{-3} \text{ cm}) = 241 \text{ cm}^{-1}$ .

# Problems

**2.1** See Fig. 2.1.



Figure 2.1: The wavefunction in the presence of various potentials.

**Exercise:** Sketch the general form of the wavefunction for a potential with two parabolic wells separated and surrounded by regions of constant potential.

**2.4** From eqns 2.12 and 2.13,

$$\Psi(x, t) = \int g(k)\Psi_k(x, t)dk = AB \int_{k-\frac{1}{2}\Delta k}^{k+\frac{1}{2}\Delta k} \exp\left\{ikx - ik^2\hbar t/2m\right\}dk$$
$$\Psi(x, 0) = AB \int_{k-\frac{1}{2}\Delta k}^{k+\frac{1}{2}\Delta k} \exp\left\{ikx\right\}dk$$
$$= (AB/ix)\left\{e^{i(k+\frac{1}{2}\Delta k)x} - e^{i(k-\frac{1}{2}\Delta k)x}\right\}$$
$$= (ABe^{ikx}/ix)\left\{e^{\frac{1}{2}i\Delta kx} - e^{-\frac{1}{2}i\Delta kx}\right\} = 2AB(e^{ikx}\sin\frac{1}{2}\Delta kx)/x$$

$$|\Psi(x, 0)|^2 = 4A^2B^2\{\sin(\frac{1}{2}\Delta kx)/x\}^2$$

For normalization (to unity), write AB = N; then

$$\int |\Psi|^2 d\tau = 4N^2 \int_{-\infty}^{\infty} \{\sin(\frac{1}{2}\Delta kx) / x\}^2 dx = 2N^2 \Delta k \int_{-\infty}^{\infty} (\sin z / z)^2 dz \ [z = \frac{1}{2}\Delta kx]$$
$$= 2N^2 \Delta k\pi = 1; \text{ hence } N = (2\Delta k\pi)^{-1/2}$$

Therefore,  $\Psi(x,0) = (2/\Delta k\pi)^{1/2} (e^{ikx} \sin \frac{1}{2} \Delta kx)/x$ 

$$|\Psi(x, 0)|^{2} = (2/\Delta k\pi)(\sin \frac{1}{2}\Delta kx/x)^{2}$$
$$|\Psi(0, 0)|^{2} = (2/\Delta k\pi) \lim_{x \to 0} (\sin \frac{1}{2}\Delta kx/x)^{2} = (2/\Delta k\pi)(\frac{1}{2}\Delta kx/x)^{2}$$

$$= (2/\Delta k\pi)(\Delta k/2)^2 = \Delta k/(2\pi)$$

We seek the value of x for which  $|\Psi(x, 0)|^2 / |\Psi(0, 0)|^2 = \frac{1}{2}$ ; that is

$$\frac{\left\{\sin\left(\frac{1}{2}\Delta kx\right)/x\right\}^2}{\left(\frac{1}{2}\Delta k\right)^2} = \frac{1}{2}$$

or

$$\frac{\sin\frac{1}{2}\Delta kx}{\frac{1}{2}\Delta kx} = \frac{1}{\sqrt{2}}$$

which is satisfied by  $\frac{1}{2}\Delta kx = \pm 1.392$  [solve numerically]. Hence the probability density falls to one half its value at x = 0 when  $x = \pm 2.784/\Delta k$ . From the uncertainty principle  $\Delta p_x \Delta x \ge \frac{1}{2}\hbar$ , so  $\Delta k \Delta x \ge \frac{1}{2}$ , and hence  $\Delta x \ge 0.5/\Delta k$  which is in accord with  $\Delta x \approx 2 \times 2.784/\Delta k$ .

Exercise: Examine the properties of a Gaussian wavepacket in the same way.

2.7 Consider the zones set out in Fig. 2.5; impose the condition of continuity of  $\psi$  and  $\psi'$  at each interface.



Fig 2.5 The zones of potential energy used in Problem 2.7.

$$\psi_{I} = A e^{ikx} + B e^{-ikx}, k^{2} = 2mE/\hbar^{2} \psi_{II} = A' e^{ikx} + B' e^{-ikx}, k'^{2} = 2m(E-V)/\hbar^{2}$$

 $\psi_{\text{III}} = A'' e^{ikx}$  [no particles incident from right]

(1) $A + B = A' + B'$ ,	[from $\psi_{I}(0) = \psi_{II}(0)$ ]
(2) $A'e^{ik'L} + B'e^{-ik'L} = A''e^{ikL}$ ,	[from $\psi_{II}(L) = \psi_{III}(L)$ ]
(3) $kA - kB = k'A' - k'B'$ ,	[from $\psi'_{I}(0) = \psi'_{II}(0)$ ]
(4) $k'A'e^{ik'L} - k'B'e^{-ik'L} = kA''e^{ikL}$	[from $\psi'_{II}(L) = \psi'_{III}(L)$ ]

From (1) and (3):

$$A' = \frac{1}{2}(1+\gamma)A + \frac{1}{2}(1-\gamma)B; B' = \frac{1}{2}(1-\gamma)A + \frac{1}{2}(1+\gamma)B$$

From (2) and (4)

$$A'' = A' e^{i(k'-k)L} + B' e^{-i(k'+k)L}$$
$$\gamma A'' = A' e^{i(k'-k)L} - B' e^{-i(k'+k)L}$$

so

$$\frac{1}{2}(1+\gamma)A'' = A'e^{i(k'-k)L}, \ \frac{1}{2}(1-\gamma)A'' = B'e^{-i(k'+k)L}$$

Then

$$A'' e^{ikL} \left\{ (1+\gamma)^2 e^{-ik'L} - (1-\gamma)^2 e^{ik'L} \right\} = 4\gamma A$$
$$A''/A = 2\gamma e^{-ikL} / \{ 2\gamma \cos k'L - i(1+\gamma^2) \sin k'L \}$$

The transmission coefficient (or tunnelling probability) is

$$P = |A''|^2 / |A|^2 = |A''/A|^2$$
$$= \frac{4\gamma^2}{4\gamma^2 + (1-\gamma^2)^2 \sin^2 k'L}, \ \gamma^2 = E/(E-V)$$

**Exercise:** Find the transmission coefficient for a particle incident on a rectangular dip in the potential energy.

**2.10** Use the normalized wavefunctions in eqn 2.31:

$$\psi_n = (2/L)^{1/2} \sin(n\pi x/L); \text{ also use}$$
$$\int \sin^2 ax dx = \frac{1}{2}x - (1/4a) \sin 2ax$$

(a) 
$$P_n = \int_0^{\frac{1}{2}L} \psi_n^2 dx = (2/L) \int_0^{\frac{1}{2}L} \sin^2(n\pi x/L) dx = \frac{1}{2}$$
 for all  $n$   
(b)  $P_n = \int_0^{\frac{1}{4}L} \psi_n^2 dx = (2/L) \int_0^{\frac{1}{4}L} \sin^2(n\pi x/L) dx = \frac{1}{4} \{1 - (2/\pi n) \sin(\frac{1}{2}n\pi)\}$   
 $P_1 = \frac{1}{4} \{1 - (2/\pi)\} = \underline{0.090\ 85}$ 

**(c)** 

$$P_n = \int_{\frac{1}{2}L-\delta x}^{\frac{1}{2}L+\delta x} \psi_n^2 dx = (2/L) \int_{\frac{1}{2}L-\delta x}^{\frac{1}{2}L+\delta x} \sin^2(n\pi x/L) dx$$
$$= (2/L) \{ \delta x - (L/2\pi n) \cos(n\pi) \sin(2n\pi \delta x/L) \}$$
$$= (2/L) \{ \delta x - (-1)^n (L/2\pi n) \sin(2n\pi \delta x/L) \}$$
$$P_1 = (2/L) \{ \delta x + (L/2\pi) \sin(2\pi \delta x/L) \} \approx \underline{4\delta x/L} \text{ when } \delta x/L << 1$$

Note that

$$\lim_{n \to \infty} P_n = (a) \frac{1}{2}, (b) \frac{1}{4}, (c) \frac{2\delta x}{L}$$

the last corresponding to a uniform distribution (the classical limit).

**Exercise:** Find  $P_n$  (and  $P_1$ ) for the particle being in a short region of length  $\delta x$  centred on the general point *x*.

**2.13** Use the wavefunction  $\psi_n = (2/L)^{1/2} \sin(n\pi x/L)$  and the integral

$$\int x \sin^2 ax dx = (1/4a^2) \{ a^2 x^2 - ax \sin(2ax) - \frac{1}{2}\cos(2ax) \}$$

$$\langle x \rangle_n = \int_0^L x \psi_n^2 dx = (2/L) \int_0^L x \sin^2(n\pi x/L) dx$$
$$= (L/2n^2 \pi^2) \{ n^2 \pi^2 - n\pi \sin(2n\pi) - \frac{1}{2} [\cos(2n\pi) - 1] \} = \frac{1}{2} L$$

The result is also obvious, by symmetry.

**Exercise:** Evaluate  $\langle x \rangle$  when the particle is in the normalized mixed state  $\psi_1 \cos \beta + \psi_2 \sin \beta$ . Account for its dependence on the parameter  $\beta$ .

## **2.16** Refer to Fig. 2.8. Consider the case E < V.



Figure 2.8: The zones of potential energy used in Problem 2.16.

$\psi_1 = A e^{-\kappa x} + B e^{\kappa x},$	$\kappa^2 = 2m(V-E)/\hbar^2$
$\psi_{\rm II} = A' {\rm e}^{{\rm i}kx} + B' {\rm e}^{-{\rm i}kx},$	$k^2 = 2mE/\hbar^2$
$\psi_{\rm III} = A'' {\rm e}^{-\kappa \alpha} + B'' {\rm e}^{\kappa \alpha},$	$\kappa^2 = 2m(V-E)/\hbar^2$

Because  $\psi < \infty$  everywhere, A = 0, B'' = 0 [consider  $x \to -\infty$  and  $x \to \infty$  respectively]. At the interfaces of the zones:

$$\psi'_{II}(0)/\psi_{II}(0) = -\kappa(A - B)/(A + B) = \kappa \quad [A = 0]$$
  
$$\psi'_{II}(0)/\psi_{II}(0) = ik(A' - B')/(A' + B')$$
  
$$\psi'_{II}(L)/\psi_{II}(L) = ik(A'e^{ikL} - B'e^{-ikL})/(A'e^{ikL} + B'e^{-ikL})$$
  
$$\psi'_{III}(L)/\psi_{III}(L) = -\kappa(A''e^{-\kappa L} - B''e^{\kappa L})/(A''e^{-\kappa L} + B''e^{\kappa L}) = -\kappa \quad [B'' = 0]$$

Because  $\psi'/\psi$  is continuous at each boundary,

$$(A' - B')/(A' + B') = \kappa/ik = -i\kappa/k = -i\gamma \quad [\gamma = \kappa/k]$$
$$(A'e^{ikL} - B'e^{-ikL})/(A'e^{ikL} + B'e^{-ikL}) = -\kappa/ik = i\kappa/k = i\gamma$$

This pair of equations solves to

$$(1 + i\gamma)A' = (1 - i\gamma)B', \quad (1 - i\gamma)A'e^{ikL} = (1 + i\gamma)B'e^{-ikL}$$

It follows that

$$(1 - \gamma^2) \sin kL - 2\gamma \cos kL = 0, \text{ or } \tan kL = 2\gamma/(1 - \gamma^2)$$

Then, since

$$\tan kL = 2 \tan(\frac{1}{2}kL)/[1 - \tan^2(\frac{1}{2}kL)], \quad \tan(\frac{1}{2}kL) = \gamma$$

Consequently,

$$\cos(\frac{1}{2}kL) = 1/(1+\gamma^2)^{1/2} = \hbar k/(2mV)^{1/2}$$

Therefore,

$$kL = 2 \arccos{\{\hbar k/(2mV)^{1/2}\}} + n\pi, \quad n = 0, 1, \dots$$

But  $\arccos z = \frac{1}{2}\pi - \arcsin z$ , so

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$$kL + 2 \arcsin{\hbar k/(2mV)^{1/2}} = n\pi, \quad n = 1, 2, \dots$$

Solve this equation for *k* by plotting y = kL and

square-well solutions.

$$y = n\pi - 2 \arcsin(\hbar^2 k^2 / 2mV)^{1/2}$$
 for  $n = 1, 2, ...$ 

and finding the values of k at which the two lines coincide, and then form  $E_n = \hbar^2 k^2/2m$ for each value of n. This procedure is illustrated in Fig. 2.9 for the special case  $V = 225\hbar^2/2mL^2$ , so, with kL = z, y = z and  $y = n\pi - 2 \arcsin z/15$ ,  $E_n = z_n^2 (\hbar^2/2mL^2)$  with  $z_n$  the intersection value of n. (Because E < V, z < 15.) We find z = 2.9, 5.9, 8.8, 11.7 for n = 1, 2, 3, 4; hence  $E/(\hbar^2/2mL^2) = 8.4, 35, 77, 137$  for n = 1, 2, 3, 4. When V is large in the sense  $2mV >> \hbar^2k^2$ ,  $\arcsin(\hbar^2k^2/2mV)^{1/2} \approx 0$ . Hence the equation to solve is  $kL \approx n\pi$ . Consequently  $E_n \approx n^2h^2/8mL^2$  in accord with the infinitely deep



Figure 2.9: The determination of allowed energies.

**Exercise:** First consider the special case  $V = 6\hbar^2/2mL^2$ , and find the allowed solutions. Then repeat the calculation for an unsymmetrical well in which the potential energy rises to *V* on the left and to 4*V* on the right.

**2.19 (a)** 
$$E_{n_1n_2} = \frac{h^2}{8m} \left( \frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} \right) = \frac{h^2}{8mL_2^2} \left( \frac{n_1^2}{\lambda^2} + n_2^2 \right)$$

where  $\lambda = L_1/L_2$ . Therefore, if  $\lambda$  is an integer, the states  $(n_1, n_2)$  and  $(\lambda n_2, n_1/\lambda)$  are degenerate.

(b) The states related by the relation in (a) are doubly degenerate.

### 2.22 The Schrödinger equation is

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

Substitute  $y = (m\omega/\hbar)^{1/2}x$  with  $\omega^2 = k_f/m$ ; then  $\psi'' - y^2\psi = -\lambda\psi$ , with  $\lambda = E/\frac{1}{2}\hbar\omega$  and

 $\psi'' = \mathrm{d}^2 \psi/\mathrm{d} y^2.$ 

Substitute eqn 2.41:  $\psi = N_v H_v e^{-y^{2/2}}$ :

$$(d^2/dy^2)(H_v e^{-y^2/2}) - y^2 H_v e^{-y^2/2} = -\lambda H_v e^{-y^2/2}$$

Use

$$(d^{2}/dy^{2})(H_{v}e^{-y^{2}/2}) = (H_{v}'' - 2yH_{v}' - H_{v} + y^{2}H_{v})e^{-y^{2}/2}$$
$$= (2yH_{v}' - 2vH_{v} - 2yH_{v}' - H_{v} + y^{2}H_{v})e^{-y^{2}/2} \quad [given]$$
$$= \{y^{2}H_{v} - (2v+1)H_{v}\}e^{-y^{2}/2}$$

Then

$$\{y^2 H_v - (2v+1)H_v - y^2 H_v\} e^{-y^2/2} = -\lambda H_v e^{-y^2/2}$$

so  $\lambda = 2v + 1$ , or  $E = \frac{1}{2}(2v+1)\hbar\omega = (v + \frac{1}{2})\hbar\omega$ , as required.

2.25 (a)

$$\langle v+1|x|v\rangle = N_{v+1}N_v\alpha^{-2}\int_{-\infty}^{\infty}H_{v+1}(y)yH_v(y)e^{-y^2}dy \quad [y=\alpha x]$$

$$= \alpha^{-2}N_{v+1}N_v\int_{-\infty}^{\infty}H_{v+1}\{\frac{1}{2}H_{v+1}+vH_{v-1}\}e^{-y^2}dy \quad [\text{Table 2.1}]$$

$$= \frac{1}{2}\alpha^{-2}N_{v+1}N_v\int_{-\infty}^{\infty}H_{v+1}^2e^{-y^2}dy \quad [\text{orthogonality}]$$

$$= \frac{1}{2}\alpha^{-2}N_{v+1}N_v\pi^{1/2}2^{v+1}(v+1)!$$

$$= \frac{\pi^{1/2}2^{v+1}(v+1)!}{2\pi^{1/2}\alpha\{2^{v}2^{v+1}v!(v+1)!\}^{1/2}} = \frac{1}{\sqrt{2}\alpha}(v+1)^{1/2}$$

**(b)** 

$$\langle v + 2 | x^{2} | v \rangle = N_{v+2} N_{v} \alpha^{-3} \int_{-\infty}^{\infty} H_{v+2} y^{2} H_{v} e^{-y^{2}} dy$$

$$= \alpha^{-3} N_{v+2} N_{v} \int_{-\infty}^{\infty} H_{v+2} y \{ \frac{1}{2} H_{v+1} + v H_{v-1} \} e^{-y^{2}} dy$$

$$= \alpha^{-3} N_{v+2} N_{v} \int_{-\infty}^{\infty} H_{v+2} \{ \frac{1}{4} H_{v+2} + \frac{1}{2} v H_{v} + \frac{1}{2} v H_{v} + v^{2} H_{v-2} \} e^{-y^{2}} dy$$

$$= \frac{1}{4} \alpha^{-3} N_{v+2} N_{v} \int_{-\infty}^{\infty} H_{v+2}^{2} e^{-y^{2}} dy \quad \text{[orthogonality]}$$

$$= \frac{1}{4} \alpha^{-3} N_{v+2} N_{v} \pi^{1/2} 2^{v+2} (v+2)! \quad \text{[Table 2.1]}$$

$$= \frac{\alpha^{-3} \pi^{1/2} 2^{v+2} (v+2)! v! \alpha^{-2} \pi \}^{1/2}}{4 \{ 2^{v+2} 2^{v} (v+2)! v! \alpha^{-2} \pi \}^{1/2}} = \frac{1}{2} \alpha^{-2} \{ (v+2)(v+1) \}^{1/2}$$

**Exercise:** Evaluate  $\langle v + 3 | x^3 | v \rangle$  in the same way.

**2.28** According to classical mechanics, the turning point  $x_{tp}$  occurs when all the energy of the oscillator is potential energy and its kinetic energy is zero. This equality occurs when

$$E = \frac{1}{2}k_{\rm f}x_{\rm tp}^2$$
 or  $x_{\rm tp} = \left(\frac{2{\rm E}}{k_{\rm f}}\right)^{1/2}$ 

Since we are only considering the stretching of the harmonic oscillator beyond the classical turning point, we only choose the positive square root for  $x_{tp}$ . The probability *P* of finding the ground-state harmonic oscillator stretched beyond a displacement  $x_{tp}$  is given by:

$$P = \int_{x_{\rm tp}}^{\infty} \psi_0^2 \,\mathrm{d}x$$

Using eqn 2.41 and the Hermite polynomial  $H_0$  in Table 2.1, we obtain:

$$P = \frac{\alpha}{\pi^{1/2}} \int_{x_{\rm tp}}^{\infty} e^{-\alpha^2 x^2} \, \mathrm{d}x$$

The turning point can be expressed in terms of  $\alpha$ , using (i) the definition of  $\alpha$  in eqn 2.41 and (ii) the ground-state energy  $E = \frac{1}{2}\hbar\omega = \frac{1}{2}\hbar(k_{\rm f}/m)^{1/2}$ . This results in  $x_{\rm tp} = 1/\alpha$ . Now introduce the variable  $y = \alpha x$  so that  $dy = \alpha dx$ ,  $y^2 = \alpha^2 x^2$  and  $y_{\rm tp} = \alpha x_{\rm tp} = 1$ . The above integral then becomes, in terms of the variable y:

$$P = \frac{1}{\pi^{1/2}} \int_{1}^{\infty} e^{-y^2} \, \mathrm{d}y$$

The above integral is related to the error function given in the Problem, and using the value of erf 1 given:

$$P = \frac{1}{\pi^{1/2}} \int_1^\infty e^{-y^2} dy = \frac{1}{2} (1 - \text{erf } 1) = \frac{1}{2} (1 - 0.8427)$$

The probability is  $7.865 \times 10^{-2}$ .

**2.31** The wavefunction  $\psi(x)$  is given as a sum of normalized particle-in-a-box eigenfunctions  $\psi_n(x)$ . Therefore, according to quantum mechanical postulate 3', a single measurement of the energy yields a single outcome which is one of the eigenvalues  $E_n$  (associated

with the eigenfunction  $\psi_n$  appearing in the expansion of  $\psi$ ). The probability of obtaining  $E_n$  is  $|c_n|^2$  where  $c_n$  is the coefficient of  $\psi_n$  in the expansion.

(a) When the energy of the particle is measured, possible outcomes are

$$E_1 = \frac{h^2}{8mL^2}$$
  $E_3 = \frac{9h^2}{8mL^2}$   $E_5 = \frac{25h^2}{8mL^2}$ 

(b) The probability of obtaining each result is

$$|c_1|^2 = (1/3)^2 = 1/9$$
 for  $E_1$   
 $|c_3|^2 = |(i/3)|^2 = 1/9$  for  $E_3$   
 $|c_5|^2 = [-(7/9)^{1/2}]^2 = 7/9$  for  $E_5$ 

(c) The expectation value is the weighted sum of the possible eigenvalues:

$$\frac{1}{9}E_1 + \frac{1}{9}E_3 + \frac{7}{9}E_5 = \frac{185h^2}{72mL^2}$$

**Exercise:** If the linear momentum of the particle described above were measured, what would we expect to find?