Chapter 5 - Quantum Mechanics

5-1: Figure (b) is double-valued, and is not a function at all, and cannot have physical significance. Figure (c) has a discontinuous derivative (a "cusp") in the shown interval. Figure (d) is not finite everywhere in the shown interval. Figure (f) is discontinuous in the shown interval.

5-3: The functions (a) and (b) are both infinite when $\cos x = 0$, at $x = \pm\pi/2$, $\pm 3\pi/2, \ldots, \pm(2n+1)\pi/2$ for any integer n, and neither $\psi = A\sec x$ or $\psi = A\tan x$ could be a solution of Schrödginer's equation for all values of x. The function (c) diverges as $x \to \pm\infty$, and cannot be a solution of Schrödinger's equation for all values of x.

5-5: Both parts involve the integral $\int \cos^4 x\,dx$, evaluated between different limits for the two parts. Of the many ways to find this integral, including consulting tables and using symbolic-manipulation programs, a direct algebraic reduction gives

$$\begin{aligned}
\cos^4 x = \left(\cos^2 x\right)^2 &= \left[\frac{1}{2}(1+\cos 2x)\right]^2 \\
&= \frac{1}{4}\left[1 + 2\,\cos 2x + \cos^2(2\,x)\right] \\
&= \frac{1}{4}\left[1 + 2\cos 2x + \frac{1}{2}(1+\cos 4x)\right] \\
&= \frac{3}{8} + \frac{1}{2}\cos 2x + \frac{1}{8}\cos 4x,
\end{aligned}$$

where the identity $\cos^2\theta = \frac{1}{2}(1+\cos 2\theta)$ has been used twice.

(a) The needed normalization condition is

$$\begin{aligned}
\int_{-\pi/2}^{\pi/2} \psi^*\psi\,dx &= A^2 \int_{-\pi/2}^{\pi/2} \cos^4 x\,dx \\
&= A^2\left[\frac{3}{8}\int_{-\pi/2}^{\pi/2} dx + \frac{1}{2}\int_{-\pi/2}^{\pi/2}\cos 2x\,dx + \frac{1}{8}\int_{-\pi/2}^{\pi/2}\cos 4x\,dx\right] = 1.
\end{aligned}$$

The integrals

$$\int_{-\pi/2}^{\pi/2}\cos 2x\,dx = \frac{1}{2}\sin 2x\bigg|_{-\pi/2}^{\pi/2} \qquad \text{and} \qquad \int_{-\pi/2}^{\pi/2}\cos 4x\,dx = \frac{1}{4}\sin 4x\bigg|_{-\pi/2}^{\pi/2}$$

are seen to vanish, and the normalization condition reduces to

$$1 = A^2 \left(\frac{3}{8}\right)\pi, \qquad \text{or} \qquad A = \sqrt{\frac{8}{3\pi}}.$$

(b) Evaluating the same integral between the different limits,

$$\int_0^{\pi/4} \cos^4 x\,dx = \left[\frac{3}{8}\,x + \frac{1}{4}\,\sin 2x + \frac{1}{32}\,\sin 4x\right]_0^{\pi/4} = \frac{3\pi}{32} + \frac{1}{4}.$$

The probability of the particle being found between $x = 0$ and $x = \pi/4$ is the product of this integral and A^2, or

$$A^2\left(\frac{3\pi}{32} + \frac{1}{4}\right) = \frac{8}{3\pi}\left(\frac{3\pi}{32} + \frac{1}{4}\right) = 0.462.$$

5-7: The given wave function satisfies the continuity condition, and is differentiable to all orders with respect to both t and x, but is not normalizable; specifically, $\Psi^*\Psi = A^*A$ is constant in both space and time, and if the particle is to move freely, there can be no limit to its range, and so the integral of $\Psi^*\Psi$ over an infinite region cannot be finite if $A \neq 0$.

A linear superposition of such waves could give a normalizable wave function, corresponding to a real particle. Such a superposition would necessarily have a nonzero Δp, and hence a finite Δx; at the expense of normalizing the wave function, the wave function is composed of different momentum states, and is localized.

5-9: It's crucial to realize that the expectation value $\langle px\rangle$ is found from the combined operator $\hat{p}\,\hat{x}$, which, when operating on the wave function $\Psi(x,\,t)$, corresponds to "multiply by x, differentiate with respect to x and multiply by $\hbar/i$," whereas the operator $\hat{x}\,\hat{p}$ corresponds to "differentiate with respect to x, multiply by $\hbar/i$ and multiply by x." Using these operators,

$$(\hat{p}\hat{x})\,\Psi = \hat{p}\,(\hat{x}\,\Psi) = \frac{\hbar}{i}\frac{\partial}{\partial x}\,(x\,\Psi) = \frac{\hbar}{i}\left[\Psi + x\,\frac{\partial}{\partial x}\psi\right],$$

where the product rule for partial differentiation has been used. Also,

$$(\hat{x}\,\hat{p})\,\Psi = \hat{x}\,(\hat{p}\,\Psi) = x\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\right) = \frac{\hbar}{i}\left[x\,\frac{\partial}{\partial x}\Psi\right].$$

Thus
$$(\hat{p}\,\hat{x} - \hat{x}\,\hat{p})\,\Psi = \frac{\hbar}{i}\,\Psi,$$

and
$$\langle px - xp\rangle = \int_{-\infty}^{\infty} \Psi^*\frac{\hbar}{i}\Psi\,dx = \frac{\hbar}{i}\int_{-\infty}^{\infty} \Psi^*\Psi\,dx = \frac{\hbar}{i}$$

for $\Psi(x,\,t)$ normalized.

5-11: Using $\lambda\,\nu = v_p$ in Equation (3.5), and using ψ instead of y,

$$\psi = A\,\cos\left(2\pi\left(t - \frac{x}{v_p}\right)\right) = A\,\cos\left(2\pi\,\nu\,t - 2\pi\frac{x}{\lambda}\right).$$

Differentiating twice with respect to x using the chain rule for partial differentiation (similar to Example 5.1),

$$\frac{\partial\psi}{\partial x} = -A\,\sin\left(2\pi\,\nu\,t - 2\pi\frac{x}{\lambda}\right)\left(-\frac{2\pi}{\lambda}\right) = \frac{2\pi}{\lambda}\,A\,\sin\left(2\pi\,\nu\,t - 2\pi\frac{x}{\lambda}\right),$$

$$\frac{\partial^2\psi}{\partial^2 x} = \frac{2\pi}{\lambda}\,A\,\cos\left(2\pi\,\nu\,t - 2\pi\frac{x}{\lambda}\right)\left(-\frac{2\pi}{\lambda}\right) = -\left(\frac{2\pi}{\lambda}\right)^2\,A\,\cos\left(2\pi\,\nu\,t - 2\pi\frac{x}{\lambda}\right)$$
$$= -\left(\frac{2\pi}{\lambda}\right)^2\,\psi.$$

The kinetic energy of a nonrelativistic particle is

$$\mathrm{KE} = E - U = \frac{p^2}{2m} = \left(\frac{h}{\lambda}\right)^2\frac{1}{2m}, \qquad \text{so that}$$

$$\frac{1}{\lambda^2} = \frac{2m}{h^2}\,(E - U).$$

Substituting the above expression relating $\dfrac{\partial^2\psi}{\partial^2 x}$ and $\left(1/\lambda^2\right)\,\psi$,

$$\frac{\partial^2\psi}{\partial^2 x} = -\left(\frac{2\pi}{\lambda}\right)^2\,\psi = -\frac{8\pi^2\,m}{h^2}\,(E - U)\,\psi = -\frac{2m}{\hbar^2}\,(E - U)\,\psi,$$

which is Equation (5.32).

5-13: The wave function must vanish at $x = 0$, where $V \to \infty$. As the potential energy increases with x, the particle's kinetic energy must decrease, and so the wavelength increases. The amplitude increases as the wavelength increases because a larger wavelength means a smaller momentum (indicated as well by the lower kinetic energy), and the particle is more likely to be found where the momentum has a lower magnitude. The wave function vanishes again where the potential $V \to \infty$; this condition would determine the allowed energies.

5-15: The necessary integrals are of the form

$$\int_{-\infty}^{\infty} \psi_n \, \psi_m \, dx = \frac{2}{L} \int_0^L \sin \frac{n\,\pi\,x}{L} \, \sin \frac{m\,\pi\,x}{L} \, dx$$

for integers n, m, with $n \neq m$ *and* $n \neq -m$. (A more general orthogonality relation would involve the integral of $\psi_n^* \psi_m$, but as the eigenfunctions in this problem are real, the distinction need not be made.)

Such integrals are tabulated, or may be found from symbolic-manipulation programs. As an example, the Maple commands that show this result are:

```
>assume(n, integer); additionally(m,integer);
>int(sin(n*Pi*x/L)*sin(m*Pi*x/L),x=0..L);
>int(sin(n*Pi*x/L)*sin(n*Pi*x/L),x=0..L);
```

To do the integrals directly, a convenient identity to use is

$$\sin\alpha \, \sin\beta = \frac{1}{2} \left[\cos(\alpha - \beta) - \cos(\alpha + \beta)\right],$$

as may be verified by expanding the cosines of the sum and difference of α and β. To show orthogongality, the stipulation $n \neq m$ means that $\alpha \neq \beta$ and $\alpha \neq -\beta$, and the integrals are of the form

$$\begin{aligned}
\int_{-\infty}^{\infty} \psi_n \, \psi_m \, dx &= \frac{1}{L} \int_0^L \left[\cos \frac{(n-m)\,\pi\,x}{L} - \cos \frac{(n+m)\,\pi\,x}{L} \right] dx \\
&= \frac{1}{L} \left[\frac{L}{(n-m)\,\pi} \, \sin \frac{(n-m)\,\pi\,x}{L} - \frac{L}{(n+m)\,\pi} \, \sin \frac{(n+m)\,\pi\,x}{L} \right]_0^L \\
&= 0,
\end{aligned}$$

where $\sin(n-m)\pi = \sin(n-m)\pi = \sin 0 = 0$ has been used.

5-17: Using Equation (5.46), the expectation value $\langle x^2 \rangle$ is

$$\langle x^2 \rangle_n = \frac{2}{L} \int_0^L x^2 \, \sin^2 \left(\frac{n\,\pi\,x}{L} \right) \, dx.$$

Those with access to sybolic-manipulation programs will be able to find the needed definite integral almost immediately. For instance, a possible Maple command is:

```
>assume(n, integer):
  simplify((2/L)*int(x^2*sin(n*Pi*x/L)*sin(n*Pi*x/L),x=0..L));
```

See the end of this chapter for an alternate analytic technique for evaluating this inegral using *Leibniz's Rule.* From either a table or repeated integration by parts, the indefinite integral is

$$\int x^2 \sin^2 \frac{n\,\pi\,x}{L}\,dx = \left(\frac{L}{n\,\pi}\right)^3 \int u^3 \sin u\,du$$
$$= \left(\frac{L}{n\,\pi}\right)^3 \left[\frac{u^3}{6} - \frac{u^2}{4}\sin 2u - \frac{u}{4}\cos 2u + \frac{1}{8}\sin 2u\right],$$

where the substitution $u = \left(\frac{n\,\pi}{L}\right) x$ has been made.

This form makes evaluation of the definite integral a bit simpler; when $x = 0$ $u = 0$, and when $x = L$ $u = n\pi$. Each of the terms in the integral vanish at $u = 0$, and the terms with $\sin 2u$ vanish at $u = n\,\pi$, $\cos 2u = \cos 2\,n\,\pi = 1$, and so the result is

$$\left\langle x^2 \right\rangle_n = \frac{2}{L}\left(\frac{L}{n\,\pi}\right)^3 \left[\frac{(n\,\pi)^3}{6} - \frac{n\,\pi}{4}\right] = L^2\left[\frac{1}{3} - \frac{1}{2\,n^2\,\pi^2}\right].$$

As a check, note that

$$\lim_{n\to\infty} \left\langle x^2 \right\rangle_n = \frac{L^2}{3},$$

which is the expectation value of $\left\langle x^2 \right\rangle$ in the classical limit, for which the probability distribution is independent of position in the box.

5-19: This is a special case of the probability that such a particle is between x_1 and x_2, as found in Example 5.4. With $x_1 = 0$ and $x_2 = L$,

$$P_{0L} = \left[\frac{x}{L} - \frac{1}{2\,n\,\pi}\sin\frac{2\,n\,\pi\,x}{L}\right]_0^L = \frac{1}{n}.$$

5-21: The normalization constant, assuming A to be real, is given by

$$\int \psi^*\psi\,dV = 1 = \int \psi^*\psi\,dx\,dy\,dz$$
$$= A^2\left(\int_0^L \sin^2\frac{n_x\,\pi\,x}{L}\,dx\right)\left(\int_0^L \sin^2\frac{n_y\,\pi\,y}{L}\,dy\right)\left(\int_0^L \sin^2\frac{n_z\,\pi\,z}{L}\,dz\right).$$

Each integral above is equal to $\frac{L}{2}$ (from calculations identical to Equation (5.43)). The result is

$$A^2\left(\frac{L}{2}\right)^3 = 1 \qquad \text{or} \qquad A = \left(\frac{2}{L}\right)^{3/2}.$$

5-23: (a) For the wave function of Problem 5-21, Equation (5.33) must be used to find the energy. Before substitution into Equation (5.33), it is convenient and useful to note that for this wave function

$$\frac{\partial^2\psi}{\partial^2 x} = -\frac{n_x^2\,\pi^2}{L^2}\,\psi, \qquad \frac{\partial^2\psi}{\partial^2 y} = -\frac{n_y^2\,\pi^2}{L^2}\,\psi, \qquad \frac{\partial^2\psi}{\partial^2 x} = -\frac{n_z^2\,\pi^2}{L^2}\,\psi.$$

Then, substitution into Equation (5.33) gives

$$-\frac{\pi^2}{L^2}\left(n_x^2 + n_y^2 + n_z^2\right)\psi + \frac{2\,m}{\hbar^2}\,E\psi = 0,$$

and so the energies are

$$E_{n_x,\,n_y,\,n_z} = \frac{\pi^2\,\hbar^2}{2\,m\,L^2}\left(n_x^2 + n_y^2 + n_z^2\right).$$

(b) The lowest energy occurs when $n_x = n_y = n_z = 1$ (see Problem 5-22). None of the integers n_x, n_y or n_z can be zero, as that would mean $\psi = 0$ identically. The minimum energy is then

$$E_{\text{min}} = \frac{3\,\pi^2\hbar^2}{2\,m\,L^2},$$

which is three times the ground-state energy of a particle in a one-dimensional box of length L (Equation (5.40) with $n = 1$).

5-25: Solving Equation (5.60) for k_2,

$$k_2 = \frac{1}{2L}\,\ln\frac{1}{T} = \frac{1}{2\,(0.200\times 10^{-9}\ \text{m})}\,\ln(100) = 1.1513\times 10^{10}\ \text{m}^{-1},$$

keeping extra significant figures. Equation (5.86), from the Appendix, may be solved for the energy E, but a more direct expression is

$$\begin{aligned} E &= U - \text{KE} = U - \frac{p^2}{2\,m} = U - \frac{(\hbar\,k_2)^2}{2\,m} \\ &= 6.00\ \text{eV} - \frac{\left(\left(1.055\times 10^{-34}\ \text{J}\cdot\text{s}\right)\left(1.1513\times 10^{10}\ \text{m}^{-1}\right)\right)^2}{2\,(9.1095\times 10^{-31}\ \text{kg})\,(1.602\times 10^{-19}\ \text{J/eV})} \\ &= 0.949\ \text{eV}. \end{aligned}$$

As the potential is given to the nearest 0.01 eV, the electron energy would be known to this precision, or 0.95 eV.

Special Integrals for Harmonic Oscillators

Many problems in this section involve improper definite integrals of the form

$$\int_{-\infty}^{\infty} y^{2n}\, e^{-\beta y^2}\, dy$$

for n a nonnegative integer and $\beta > 0$. Integrals of this form are well-known and tabulated, and may be found by use of symbolic-manipulation programs. The general result is used, but not given explicitly, in Equation (5.72). An outline of several methods for finding such integrals is given at the end of the solutions to Chapter 5 in this manual.

By exhibiting Equation (5.72) as a set of normalized wave functions, integrals of the above form may be found. That is, by using $H_n(y)$ as given in Table 5.2,

$$\begin{aligned}
\psi_0^*\psi_0 &= \sqrt{\frac{2\,m\,\nu}{\hbar}}\, e^{-y^2} \\
\psi_1^*\psi_1 &= \sqrt{\frac{2\,m\,\nu}{\hbar}}\frac{1}{2}\,(2\,y)^2\, e^{-y^2} \\
\psi_2^*\psi_2 &= \sqrt{\frac{2\,m\,\nu}{\hbar}}\frac{1}{8}\,\left(4\,y^2-2\right)^2\, e^{-y^2}.
\end{aligned}$$

From these expressions it can be seen, for instance, that

$$1 = \int_{-\infty}^{\infty} \psi_0^*\psi_0\, dx = \sqrt{\frac{2\,m\,\nu}{\hbar}}\sqrt{\frac{\hbar}{2\pi\,m\,\nu}}\,\int_{-\infty}^{\infty} e^{-y^2}\, dy,$$

so that

$$\int_{-\infty}^{\infty} e^{-y^2}\, dy = \sqrt{\pi},$$

where Equation (5.67) has been used to relate x and y, and hence dx and dy.

Similarly,

$$1 = \int_{-\infty}^{\infty} \psi_1^*\psi_1\, dx = \sqrt{\frac{2\,m\,\nu}{\hbar}}\sqrt{\frac{\hbar}{2\pi\,m\,\nu}}\,\int_{-\infty}^{\infty} y^2\, e^{-y^2}\, dy,$$

so that

$$\int_{-\infty}^{\infty} y^2\, e^{-y^2}\, dy = \frac{\sqrt{\pi}}{2}.$$

To continue the process with ψ_2,

$$\begin{aligned}
1 &= \frac{1}{\sqrt{\pi}}\frac{1}{8}\left[16\int_{-\infty}^{\infty} y^4\, e^{-y^2}\, dy - 16\int_{-\infty}^{\infty} y^2\, e^{-y^2}\, dy + 4\int_{-\infty}^{\infty} e^{-y^2}\, dy\right] \\
&= 2\int_{-\infty}^{\infty} y^4\, e^{-y^2}\, dy - 1 + \frac{1}{2},
\end{aligned}$$

so that

$$\int_{-\infty}^{\infty} y^4\, e^{-y^2}\, dy = \frac{3}{4}\sqrt{\pi}$$

5-27: If a particle in a harmonic-oscillator potential had zero energy, the particle would have to be at rest at the position of the potential minimum. The uncertainty principle dictates that such a particle would have an infinite uncertainty in momentum, and hence an infinite uncertainty in energy. This contradiction implies that the zero-point energy of a harmonic oscillator cannot be zero.

5-29: When the classical amplitude of motion is A, the energy of the oscillator is

$$\frac{1}{2}\,k\,A^2 = \frac{1}{2}\,h\,\nu, \qquad \text{so} \qquad A = \sqrt{\frac{h\,\nu}{k}}.$$

Using this for x in Equation (5.67) gives

$$y = \sqrt{\frac{2\pi\,m\,\nu}{\hbar}}\sqrt{\frac{h\,\nu}{k}} = 2\pi\sqrt{\frac{m\,\nu^2}{k}} = 1,$$

where Equation (5.64) has been used to relate ν, m and k.

5-31: The expectation values will be of the forms

$$\int_{-\infty}^{\infty} x\,\psi^*\psi\,dx \qquad \text{and} \qquad \int_{-\infty}^{\infty} x^2\,\psi^*\psi\,dx.$$

It is far more convenient to use the dimensionless variable y as defined in Equation (5.67). The necessary integrals will be proportional to

$$\int_{-\infty}^{\infty} y\,e^{-y^2}\,dy, \quad \int_{-\infty}^{\infty} y^2\,e^{-y^2}\,dy, \quad \int_{-\infty}^{\infty} y^3\,e^{-y^2}\,dy \quad \text{and} \quad \int_{-\infty}^{\infty} y^4\,e^{-y^2}\,dy.$$

The first and third integrals are seen to be zero (see Example 5.7). The other two integrals may be found from tables, from symbolic-manipulation programs, or by any of the methods outlined at the end of this chapter or in **Special Integrals for Harmonic Oscillators**, preceding the solutions for Section 5.8 problems in this manual. The integrals are

$$\int_{-\infty}^{\infty} y^2\,e^{-y^2}\,dy = \frac{1}{2}\sqrt{\pi}, \qquad \int_{-\infty}^{\infty} y^4\,e^{-y^2}\,dy = \frac{3}{4}\sqrt{\pi}.$$

An immediate result is that $\langle x\rangle = 0$ for the first two states of any harmonic oscillator, and in fact $\langle x\rangle = 0$ for any state of a harmonic oscillator (if $x = 0$ is the minimum of potential energy). A generalization of the above to any case where the potential energy is a symmetric function of x, which gives rise to wave functions that are either symmetric or antisymmetric, leads to $\langle x\rangle = 0$.

To find $\langle x^2 \rangle$ for the first two states, the necessary integrals are

$$\int_{-\infty}^{\infty} x^2\, \psi_0^* \psi_0\, dx = \left(\frac{2\, m\, \nu}{\hbar}\right)^{1/2} \left(\frac{\hbar}{2\pi\, m\, \nu}\right)^{3/2} \int_{-\infty}^{\infty} y^2\, e^{-y^2}\, dy$$
$$= \frac{\hbar}{2\pi^{3/2}\, m\, \nu}\, \frac{\sqrt{\pi}}{2} = \frac{(1/2)h\nu}{4\pi^2\, m\, \nu^2} = \frac{E_0}{k};$$

$$\int_{-\infty}^{\infty} x^2\, \psi_1^* \psi_1\, dx = \left(\frac{2\, m\, \nu}{\hbar}\right)^{1/2} \left(\frac{\hbar}{2\pi\, m\, \nu}\right)^{3/2} \int_{-\infty}^{\infty} 2\, y^4\, e^{-y^2}\, dy$$
$$= \frac{\hbar}{2\pi^{3/2}\, m\, \nu}\, 2\, \frac{3\sqrt{\pi}}{2} = \frac{(3/2)h\nu}{4\pi^2\, m\, \nu^2} = \frac{E_1}{k}.$$

In both of the above integrals,

$$dx = \frac{dx}{dy}\, dy = \sqrt{\frac{\hbar}{2\pi\, m\, \nu}}\, dy$$

has been used, as well as Table 5.2 and Equation (5.64).

5-33: (a) The zero-point energy would be

$$E_0 = \frac{1}{2}\, h\, \nu = \frac{h}{2\, T} = \frac{4.136 \times 10^{-15}\ \text{eV}\cdot\text{s}}{2\, (1.00\ \text{s})} = 2.07 \times 10^{-15}\ \text{eV},$$

which is not detectable.

(b) The total energy is $E = m\, g\, H$ (here, H is the maximum pendulum height, given as an upper-case letter to distinguish from Planck's constant), and solving Equation (5.70) for n,

$$n = \frac{E}{h\, \nu} - \frac{1}{2} = \frac{m\, g\, H}{h/T}$$
$$= \frac{(1.00 \times 10^{-3}\ \text{kg})\, \left(9.80\ \text{m/s}^2\right)\, (1.00 \times 10^{-3}\ \text{m})\, (1.00\ \text{s})}{(6.626 \times 10^{-34}\ \text{J}\cdot\text{s})} - \frac{1}{2} = 1.48 \times 10^{28}.$$

Equivalently, using the result of part (a) in place of $h\, \nu$,

$$n = \frac{1}{2}\left(\frac{E}{E_0} - 1\right) = \frac{1}{2}\left(\frac{m\, g\, H}{E_0} - 1\right)$$
$$= \frac{1}{2}\left(\frac{(1.00 \times 10^{-3}\ \text{kg})\, \left(9.80\ \text{m/s}^2\right)\, (1.00 \times 10^{-3}\ \text{m})\, (1.00\ \text{s})}{(2.07 \times 10^{-15}\ \text{eV})\, (1.602 \times 10^{-19}\ \text{J/eV})} - 1\right)$$
$$= 1.48 \times 10^{28}.$$

For Problems 34, 35 and 36, it is most convenient to use the wave functions in terms of the dimensionless variable y, as given in Equations (5.67) and (5.72), intead of x. The normalization constants need not be considered in showing that the ψ_n are solutions of Schrödinger's equation as given in Equation (5.69). These exercises reduce to showing that the functions

$$H_n(y)\,e^{-y^2},$$

with $H_n(y)$ as given in Table 5.2, are solutions to Equation (5.69).

A commonly-appearing differentiation is the derivative with respect to y of the product of a polynomial $P(y)$ in y and e^{-y^2};

$$\frac{d}{dy}\left(P(y)\,e^{-y^2}\right) = \left(\frac{d}{dy}P(y) - y\,P(y)\right)\,e^{-y^2}.$$

5-35: The unnormalized wave function is $\psi_2 = \left(2\,y^2 - 1\right)\,e^{-y^2}$, and

$$\frac{d}{dy}\psi_2 = \left(4\,y - 2\,y^3 + y\right)\,e^{-y^2}, \qquad \frac{d^2}{dy^2}\psi_2 = \left(5 - 6\,y^2 - 5\,y^2 + 2\,y^4\right)\,e^{-y^2}.$$

Combining powers of y,

$$\frac{d^2}{dy^2}\psi_2 - y^2\,\psi_2 = \left(5 - 11\,y^2 + 2\,y^4 - 2\,y^4 + y^2\right)\,e^{-y^2} = \left(5 - 10\,y^2\right)\,e^{-y^2} = -5\,\psi_2,$$

and so ψ_2 is a solution to Equation (5.69) with $\alpha = 5$.

5-37: (a) In the notation of the Appendix, the wave function in the two regions has the form

$$\psi_{\rm I} = A\,e^{i\,k_1\,x} + B\,e^{-i\,k_1\,x}, \qquad \psi_{\rm II} = C\,e^{i\,k'\,x} + D\,e^{-i\,k'\,x},$$

where
$$k_1 = \sqrt{\frac{2\,m\,E}{\hbar}}, \qquad k' = \sqrt{\frac{2\,m\,(E-U)}{\hbar}}.$$

The terms corresponding to $e^{-i\,k_1\,x}$ and $e^{-i\,k'\,x}$ represent particles traveling to the left; this is possible in region I, due to reflection at the step at $x = 0$, but not in region II (the reasoning is the same as that which lead to setting $G = 0$ in Equation (5.82)). Therefore, the $e^{-i\,k'\,x}$ term is not physically meaningful, and $D = 0$.

(b) The boundary conditions at $x = 0$ are then

$$A + B = C, \qquad i\,k_1\,A - i\,k_1\,B = i\,k'\,C \qquad \text{or} \qquad A - B = \frac{k'}{k_1}\,C.$$

Adding to eliminate B, $2\,A = \left(1 + \dfrac{k'}{k_1}\right)\,C$, so

$$\frac{C}{A} = \frac{2\,k_1}{k_1 + k'}, \qquad \text{and} \qquad \frac{CC^*}{AA^*} = \frac{4\,k_1^2}{(k_1 + k')^2}.$$

(Note that the ratios C/A and C^*/A^* are real in this case.)

(c) The particle speeds are different in the two regions, so Equation (5.83) becomes

$$T = \frac{|\psi_{\rm II}|^2\ v'}{|\psi_{\rm I}|^2\ v_1} = \frac{CC^*}{AA^*}\,\frac{k'}{k_1} = \frac{4\,k_1\,k'}{(k_1 + k')^2} = \frac{4\ (k_1/k')}{((k_1/k') + 1)^2}.$$

For the given situation, $k_1/k' = v_1/v' = 2.00$, so $T = \dfrac{(4)\,(2)}{((2) + 1)^2} = \dfrac{8}{9}$. The transmitted current is $(T)(1.00\ \text{mA}) = 0.889\ \text{mA}$, and the reflected current is 0.111 mA.

As a check on the last result, note that the ratio of the reflected current to the incident current is, in the notation of the Appendix,

$$R = \frac{|\psi_{\rm I+}|^2\ v_1}{|\psi_{\rm I+}|^2\ v_1} = \frac{B\,B^*}{A\,A^*}.$$

Eliminating C from the equations obtained in part (b) from the continuity condition as $x = 0$,

$$A\left(1 - \frac{k'}{k_1}\right) = B\left(1 + \frac{k'}{k_1}\right), \qquad \text{so}$$

$$R = \left(\frac{(k1/k') - 1}{(k_1/k') + 1}\right)^2 = \frac{1}{9} = 1 - T,$$

as expected.

A Further Examination of Integrals for the Harmonic Oscillator

Many problems in this chapter involve improper definite integrals of the form

$$\int_{-\infty}^{\infty} y^{2n}\, e^{-\beta y^2}\, dy$$

for n a nonnegative integer and $\beta > 0$. Integrals of this form are well-known and tabulated, and may be found by use of symbolic-manipulation programs. The general result is used, but not given eyplicitly, in Equation (5.72).

While consulting tables or programs is certainly adequate for most purposes, there is some advantage in seeing how these integrals are obtained.

The starting point is often consideration of the integral

$$\int_{-\infty}^{\infty} e^{-u^2}\, du = \sqrt{\pi},$$

a standard result obtained from the transformation of a double integral from cartesian to polar coordinates; the derivation will not be reproduced here. However, making the substitution $u = \sqrt{\beta}\, y$ leads, after a basic change of variable, to

$$\int_{-\infty}^{\infty} e^{-\beta y^2}\, dy = \sqrt{\frac{\pi}{\beta}}.$$

Integration by parts may be used to obtain a recurrence relation. In the above relation,

$$\int_{-\infty}^{\infty} e^{-u^2}\, du = u\, e^{-u^2}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} u\, d\left(e^{-u^2}\right) = 0 + 2\int_{-\infty}^{\infty} u^2\, e^{-u^2}\, du,$$

or

$$\int_{-\infty}^{\infty} u^2\, e^{-u^2}\, du = \frac{1}{2}\int_{-\infty}^{\infty} e^{-u^2}\, du = \frac{\sqrt{\pi}}{2}.$$

Similarly (skipping the explicit inclusion of the boundary terms),

$$\int_{-\infty}^{\infty} u^2\, e^{-u^2}\, du = \int_{-\infty}^{\infty} e^{-u^2}\, d\left(\frac{u^3}{3}\right) = \frac{1}{3}\int_{-\infty}^{\infty} u^3\, d\left(e^{-u^2}\right) = \frac{2}{3}\int_{-\infty}^{\infty} u^4\, e^{-u^2}\, du,$$

so that

$$\int_{-\infty}^{\infty} u^4\, e^{-u^2}\, du = \frac{3\sqrt{\pi}}{4}.$$

A pattern soon emerges, and it may be seen by induction that

$$\int_{-\infty}^{\infty} u^{2n}\, e^{-u^2}\, du = \frac{(2n-1)(2n-3)\cdots(3)(1)}{2^n}\,\sqrt{\pi}.$$

To see this result using Maple, a possible set of commands are:

```
>assume(n,integer); additionally(n>0):
>f:=u^(2*n)*exp(-u^2);
>int(f,u=-infinity..infinity);
```

However, this result, in terms of a Gamma function, is often not useful. To see the above pattern for small integral values of n, the command (but don't enter linebreaks!)

```
>for m from 1 to 10 do
  int(u^(2*m)*exp(-u^2),u=-infinity..infinity) od;
```

shows the above pattern.

Making the same substitution $u = \sqrt{\beta}\, y$ yields

$$\int_{-\infty}^{\infty} y^{2n}\, e^{-\beta y^2}\, dy = \frac{(2n-1)(2n-3)\cdots(3)(1)}{2^n}\sqrt{\frac{\pi}{\beta^{2n+1}}}.$$

Those familiar with *Leibniz's Formula* will recognize that

$$\int_{-\infty}^{\infty} y^{2n}\, e^{-\beta y^2}\, dy = (-1)^n \left(\frac{d^n}{d\beta^n}\right) \int_{-\infty}^{\infty} e^{-\beta y^2}\, dy = (-1)^n \left(\frac{d^n}{d\beta^n}\right)\sqrt{\frac{\pi}{\beta}},$$

the same result obtained by an equivalent and possibly simpler (in terms of calculation) method.

The needed integrals for the first few values of n are:

$n = 1$
$$\int_{-\infty}^{\infty} e^{-\beta y^2}\, dy = \sqrt{\frac{\pi}{\beta}}$$

$n = 2$
$$\int_{-\infty}^{\infty} y^2\, e^{-\beta y^2}\, dy = \frac{1}{2}\sqrt{\frac{\pi}{\beta^3}}$$

$n = 3$
$$\int_{-\infty}^{\infty} y^4\, e^{-\beta y^2}\, dy = \frac{3}{4}\sqrt{\frac{\pi}{\beta^5}}$$

For physics applications, it can never hurt to check the dimensions; if y has dimensions of length, β must have dimensions of $[\text{length}]^{-2}$, and $\int_{-\infty}^{\infty} y^{2n}\, e^{-\beta y^2}\, dy$ must have dimensions of $[\text{length}]^{2n+1}$. In the results presented above, the integral has the same dimensions as $\beta^{-(2n+1)/2}$, and the dimensions are seen to be consistent.

A Further Examination of Integrals related to a Particle in a Box

As an alternative to finding the indefinite integral

$$\left\langle x^2 \right\rangle_n = \frac{2}{L} \int \sin^2\left(\frac{n\,\pi\,x}{L}\right)\,dx,$$

it is interesting to note that the simpler definite integral $\int_0^L \sin^2(n\,\pi\,x/)\,dx$ may be used to find the definite integral $\int_0^L x^2 \sin^2(n\,\pi\,x/)\,dx$ by letting $\alpha = n\,\pi/L$ be a parameter and using *Leibniz's Rule* to differentiate the integral *with respect to* α. That is,

$$\int_0^L \sin^2 \frac{n\,\pi\,x}{L}\,dx = \int_0^L \sin^2 \alpha x\,dx = \frac{L}{2} = \frac{n\,\pi}{2\,\alpha},$$

or

$$\frac{1}{2}\int_0^L (1 - \cos 2\alpha x)\;dx = \frac{n\,\pi}{2\,\alpha}$$

Then, differentiating both sides of this last relation with respect to α twice,

$$-\int_0^L x\,\sin 2\alpha x\,dx = -\frac{n\,\pi}{2\alpha^2}, \qquad -2\int_0^L x^2\,\cos 2\alpha x\,dx = \frac{n\,\pi}{\alpha^3}.$$

(In the two expressions above, there are terms corresponding to, respectively,

$$\frac{dL}{d\alpha}\,L\,\sin 2\alpha L \qquad \text{and} \qquad \frac{dL}{d\alpha}\,\L^2\,\cos 2\alpha L,$$

but thes both vanish.)

Using $\cos 2\alpha x = 1 - 2\sin^2 \alpha x$ gives

$$-2\int_0^L \left(1 - 2\,\sin^2 \alpha x\right)\;dx = -\frac{2}{3}\,L^3 + 4\int_0^L x^2\,\sin^2 \frac{n\,\pi\,x}{L}\,dx = \frac{n\,\pi}{\alpha^3} = \frac{L^3}{n^2\,\pi^2},$$

from which the previous result is obtatined,

$$\frac{2}{L}\int_0^L x^2\,\sin^2 \frac{n\,\pi\,x}{L}\,dx = L^2\left[\frac{1}{3} - \frac{1}{2\,n^2\,\pi^2}\right].$$