

Chapter 3

Operators

- 3.1** (a) $g = \hat{A}f = (d/dx) \cos(x^2 + 1) = -2x \sin(x^2 + 1)$;
 (b) $\hat{A}f = \hat{5} \sin x = 5 \sin x$;
 (c) $\hat{A}f = \sin^2 x$;
 (d) $\exp(\ln x) = e^{\ln x} = x$;
 (e) $(d^2/dx^2) \ln 3x = (d/dx) 3[1/(3x)] = -1/x^2$;
 (f) $(d^2/dx^2 + 3x d/dx)(4x^3) = 24x + 36x^3$;
 (g) $(\partial/\partial y)[\sin(xy^2)] = 2xy \cos(xy^2)$.
- 3.2** (a) Operator; (b) function; (c) function; (d) operator; (e) operator; (f) function.
- 3.3** $\hat{A} = 3x^2 \cdot + 2x(d/dx)$.
- 3.4** $\hat{1}, (d/dx), (d^2/dx^2)$.
- 3.5** (a) Some possibilities are $(4/x) \times$ and d/dx .
 (b) $(x/2) \times, (1/4)(\quad)^2$.
 (c) $(1/x^2) \times, (4x)^{-1} d/dx, (1/12) d^2/dx^2$.
- 3.6** To prove that two operators are equal, we must show that they give the same result when they operate on an arbitrary function. In this case, we must show that $(\hat{A} + \hat{B})f$ equals $(\hat{B} + \hat{A})f$. Using the definition (3.2) of addition of operators, we have $(\hat{A} + \hat{B})f = \hat{A}f + \hat{B}f$ and $(\hat{B} + \hat{A})f = \hat{B}f + \hat{A}f = \hat{A}f + \hat{B}f$, which completes the proof.
- 3.7** We have $(\hat{A} + \hat{B})f = \hat{C}f$ for all functions f , so $\hat{A}f + \hat{B}f = \hat{C}f$ and $\hat{A}f = \hat{C}f - \hat{B}f$. Hence $\hat{A} = \hat{C} - \hat{B}$.
- 3.8** (a) $(d^2/dx^2)x^2x^3 = (d/dx)5x^4 = 20x^3$;
 (b) $x^2(d^2/dx^2)x^3 = x^2(6x) = 6x^3$;
 (c) $(d^2/dx^2)[x^2 f(x)] = (d/dx)(2xf + x^2 f') = 2f + 4xf' + x^2 f''$;

(d) $x^2(d^2/dx^2)f = x^2 f''$.

3.9 $\hat{A}\hat{B}f = x^3(d/dx)f = x^3 f'$, so $\hat{A}\hat{B} = x^3 d/dx$. Also $\hat{B}\hat{A}f = (d/dx)(x^3 f) = 3x^2 f + x^3 f'$, so $\hat{B}\hat{A} = 3x^2 \cdot + x^3 d/dx$

3.10 $[(\hat{A}\hat{B})\hat{C}]f = (\hat{A}\hat{B})(\hat{C}f) = \hat{A}[\hat{B}(\hat{C}f)]$, where (3.3) was used twice; first with \hat{A} and \hat{B} in (3.3) replaced by $\hat{A}\hat{B}$ and \hat{C} , respectively, and then with f in (3.3) replaced with the function $\hat{C}f$. Also, $[\hat{A}(\hat{B}\hat{C})]f = \hat{A}[(\hat{B}\hat{C})f] = \hat{A}[\hat{B}(\hat{C}f)]$, which equals $[(\hat{A}\hat{B})\hat{C}]f$.

3.11 (a) $(\hat{A} + \hat{B})^2 f = (\hat{A} + \hat{B})(\hat{A} + \hat{B})f = (\hat{A} + \hat{B})(\hat{A}f + \hat{B}f) = \hat{A}(\hat{A}f + \hat{B}f) + \hat{B}(\hat{A}f + \hat{B}f)$ (Eq. 1), where the definitions of the product and the sum of operators were used. If we interchange \hat{A} and \hat{B} in this result, we get $(\hat{B} + \hat{A})^2 f = \hat{B}(\hat{B}f + \hat{A}f) + \hat{A}(\hat{B}f + \hat{A}f)$. Since $\hat{A}f + \hat{B}f = \hat{B}f + \hat{A}f$, we see that $(\hat{A} + \hat{B})^2 f = (\hat{B} + \hat{A})^2 f$.

(b) If \hat{A} and \hat{B} are linear, Eq. 1 becomes $(\hat{A} + \hat{B})^2 f = \hat{A}^2 f + \hat{A}\hat{B}f + \hat{B}\hat{A}f + \hat{B}^2 f$. If $\hat{A}\hat{B} = \hat{B}\hat{A}$, then $(\hat{A} + \hat{B})^2 f = \hat{A}^2 f + 2\hat{A}\hat{B}f + \hat{B}^2 f$.

3.12 $[\hat{A}, \hat{B}]f = (\hat{A}\hat{B} - \hat{B}\hat{A})f = \hat{A}\hat{B}f - \hat{B}\hat{A}f$ and $[\hat{B}, \hat{A}]f = (\hat{B}\hat{A} - \hat{A}\hat{B})f = \hat{B}\hat{A}f - \hat{A}\hat{B}f = -[\hat{A}, \hat{B}]f$.

3.13 (a) $[\sin z, d/dz]f(z) = (\sin z)(d/dz)f(z) - (d/dz)[(\sin z)f(z)] = (\sin z)f' - (\cos z)f - (\sin z)f' = -(\cos z)f$, so $[\sin z, d/dz] = -\cos z$.

(b) $[d^2/dx^2, ax^2 + bx + c]f = (d^2/dx^2)[(ax^2 + bx + c)f] - (ax^2 + bx + c)(d^2/dx^2)f = (d/dx)[(2ax + b)f + (ax^2 + bx + c)f'] - (ax^2 + bx + c)f'' = 2af + 2(2ax + b)f' + (ax^2 + bx + c)f'' - (ax^2 + bx + c)f'' = 2af + (4ax + 2b)f'$, so $[d^2/dx^2, ax^2 + bx + c] = 2a + (4ax + 2b)(d/dx)$.

(c) $[d/dx, d^2/dx^2]f = (d/dx)(d^2/dx^2)f - (d^2/dx^2)(d/dx)f = f''' - f''' = 0 \cdot f$ so $[d/dx, d^2/dx^2] = 0$.

3.14 (a) Linear; (b) nonlinear; (c) linear; (d) nonlinear; (e) linear.

3.15 $[A_n(x)d^{(n)}/dx^{(n)} + A_{n-1}(x)d^{(n-1)}/dx^{(n-1)} + \dots + A_1(x)d/dx + A_0(x)]y(x) = g(x)$

3.16 Given: $\hat{A}(f + g) = \hat{A}f + \hat{A}g$, $\hat{A}(cf) = c\hat{A}f$, $\hat{B}(f + g) = \hat{B}f + \hat{B}g$, $\hat{B}(cf) = c(\hat{B}f)$.
 Prove: $\hat{A}\hat{B}(f + g) = \hat{A}\hat{B}f + \hat{A}\hat{B}g$, $\hat{A}\hat{B}(cf) = c\hat{A}\hat{B}f$.
 Use of the given equations gives $\hat{A}\hat{B}(f + g) = \hat{A}(\hat{B}f + \hat{B}g) = \hat{A}(\hat{B}f) + \hat{A}(\hat{B}g) = \hat{A}\hat{B}f + \hat{A}\hat{B}g$, since $\hat{B}f$ and $\hat{B}g$ are functions; also, $\hat{A}\hat{B}(cf) = \hat{A}(c\hat{B}f) = c\hat{A}(\hat{B}f) = c\hat{A}\hat{B}f$.

3.17 We have

$$\begin{aligned} \hat{A}(\hat{B} + \hat{C})f &= \hat{A}(\hat{B}f + \hat{C}f) && \text{(defn. of sum of ops. } \hat{B} \text{ and } \hat{C}) \\ &= \hat{A}(\hat{B}f) + \hat{A}(\hat{C}f) && \text{(linearity of } \hat{A}) \\ &= \hat{A}\hat{B}f + \hat{A}\hat{C}f && \text{(defn. of op. prod.)} \\ &= (\hat{A}\hat{B} + \hat{A}\hat{C})f && \text{(defn. of sum of ops. } \hat{A}\hat{B} \text{ and } \hat{A}\hat{C}) \end{aligned}$$

Hence $\hat{A}(\hat{B} + \hat{C}) = \hat{A}\hat{B} + \hat{A}\hat{C}$.

3.18 (a) Using first (3.9) and then (3.10), we have $\hat{A}(bf + cg) = \hat{A}(bf) + \hat{A}(cg) = b\hat{A}f + c\hat{A}g$.
 (b) Setting $b = 1$ and $c = 1$ in (3.94), we get (3.9). Setting $c = 0$ in (3.94), we get (3.10).

3.19 (a) Complex conjugation, since $(f + g)^* = f^* + g^*$ but $(cf)^* = c^*f^* \neq cf^*$.

(b) $(\)^{-1}(d/dx)(\)^{-1}$, since $(\)^{-1}(d/dx)(\)^{-1}cf = (\)^{-1}(d/dx)c^{-1}f^{-1} = (\)^{-1}[c^{-1}(-f^{-2})f'] = -cf^2/f'$ and $c(\)^{-1}(d/dx)(\)^{-1}f = c(\)^{-1}(d/dx)f^{-1} = -c(\)^{-1}(f^{-2}f') = -cf^2/f'$, but $(\)^{-1}(d/dx)(\)^{-1}(f + g) = (\)^{-1}(d/dx)(f + g)^{-1} = -(\)^{-1}[(f + g)^{-2}(f' + g')] = -(f + g)^2(f' + g')^{-1} \neq (\)^{-1}(d/dx)(\)^{-1}f + (\)^{-1}(d/dx)(\)^{-1}g = -f^2/f' - g^2/g'$.

3.20 (a) This is always true since it is the definition of the sum of operators.

(b) Only true if \hat{A} is linear.

(c) Not generally true; for example, it is false for differentiation and integration. It is true if \hat{A} is multiplication by a function.

(d) Not generally true. Only true if the operators commute.

(e) Not generally true.

(f) Not generally true.

(g) True, since $fg = gf$.

(h) True, since $\hat{B}g$ is a function.

3.21 (a) $\hat{T}_h[f(x) + g(x)] = f(x + h) + g(x + h) = \hat{T}_h f(x) + \hat{T}_h g(x)$.

Also, $\hat{T}_h[cf(x)] = cf(x + h) = c\hat{T}_h f(x)$. So \hat{T}_h is linear.

$$(b) (\hat{T}_1 \hat{T}_1 - 3\hat{T}_1 + 2)x^2 = (x+2)^2 - 3(x+1)^2 + 2x^2 = -2x + 1.$$

3.22 $e^{\hat{D}} f(x) = (1 + \hat{D} + \hat{D}^2/2! + \hat{D}^3/3! + \dots) f(x) = f(x) + f'(x) + f''(x)/2! + f'''(x)/3! + \dots$.
 $\hat{T}_1 f(x) = f(x+1)$. The Taylor series (4.85) in Prob. 4.1 with x changed to z gives
 $f(z) = f(a) + f'(a)(z-a)/1! + f''(a)(z-a)^2/2! + \dots$. Letting $h \equiv z-a$, the Taylor series becomes
 $f(a+h) = f(a) + f'(a)h/1! + f''(a)h^2/2! + \dots$. Changing a to x and letting $h=1$, we get
 $f(x+1) = f(x) + f'(x)/1! + f''(x)/2! + \dots$, which shows that $e^{\hat{D}} f = \hat{T}_1 f$.

3.23 (a) $(d^2/dx^2)e^x = e^x$ and the eigenvalue is 1.

(b) $(d^2/dx^2)x^2 = 2$ and x^2 is not an eigenfunction of d^2/dx^2 .

(c) $(d^2/dx^2)\sin x = (d/dx)\cos x = -\sin x$ and the eigenvalue is -1 .

(d) $(d^2/dx^2)3\cos x = -3\cos x$ and the eigenvalue is -1 .

(e) $(d^2/dx^2)(\sin x + \cos x) = -(\sin x + \cos x)$ so the eigenvalue is -1 .

3.24 (a) $(\partial^2/\partial x^2 + \partial^2/\partial y^2)(e^{2x}e^{3y}) = 4e^{2x}e^{3y} + 9e^{2x}e^{3y} = 13e^{2x}e^{3y}$. The eigenvalue is 13.

(b) $(\partial^2/\partial x^2 + \partial^2/\partial y^2)(x^3y^3) = 6xy^3 + 6x^3y$. Not an eigenfunction.

(c)

$(\partial^2/\partial x^2 + \partial^2/\partial y^2)(\sin 2x \cos 4y) = -4\sin 2x \cos 4y - 16\sin 2x \cos 4y = -20\sin 2x \cos 4y$.

The eigenvalue is -20 .

(d) $(\partial^2/\partial x^2 + \partial^2/\partial y^2)(\sin 2x + \cos 3y) = -4\sin 2x - 9\cos 3y$. Not an eigenfunction,

3.25 $-(\hbar^2/2m)(d^2/dx^2)g(x) = kg(x)$ and $g''(x) + (2m/\hbar^2)kg(x) = 0$. This is a linear homogenous differential equation with constant coefficients. The auxiliary equation is $s^2 + (2m/\hbar^2)k = 0$ and $s = \pm i(2mk)^{1/2}/\hbar$. The general solution is $g = c_1 e^{i(2mk)^{1/2}x/\hbar} + c_2 e^{-i(2mk)^{1/2}x/\hbar}$. If the eigenvalue k were a negative number, then $k^{1/2}$ would be a pure imaginary number; that is, $k^{1/2} = ib$, where b is real and positive. This would make $ik^{1/2}$ a real negative number and the first exponential in g would go to ∞ as $x \rightarrow -\infty$ and the second exponential would go to ∞ as $x \rightarrow \infty$. Likewise, if k were an imaginary number ($k = a + bi = re^{i\theta}$, where a and b are real and b is nonzero), then $k^{1/2}$ would have the form $c + id$, and $ik^{1/2}$ would have the form $-d + ic$, where c and d are real. This would make the exponentials go to infinity as x goes to plus or minus infinity. Hence to keep g finite as $x \rightarrow \pm\infty$, the eigenvalue k must be real and nonnegative, and the allowed eigenvalues are all nonnegative numbers.

- 3.26** $(\int dx)f = \int f dx = kf$. Differentiation of both sides of this equation gives $(d/dx)\int f dx = f = kf'$. So $df/dx = k^{-1}f$ and $(1/f)df = k^{-1}dx$. Integration gives $\ln f = k^{-1}x + c$ and $f = e^c e^{x/k} = Ae^{x/k}$, where A is a constant and k is the eigenvalue. To prevent the eigenfunctions from becoming infinite as $x \rightarrow \pm\infty$, k must be a pure imaginary number. (Strictly speaking, $Ae^{x/k}$ is an eigenfunction of $\int dx$ only if we omit the arbitrary constant of integration.)
- 3.27** $d^2 f/dx^2 + 2df/dx = kf$ and $f'' + 2f' - kf = 0$. The auxiliary equation is $s^2 + 2s - k = 0$ and $s = -1 \pm (1+k)^{1/2}$. So $f = Ae^{[-1+(1+k)^{1/2}]x} + Be^{[-1-(1+k)^{1/2}]x}$, where A and B are arbitrary constants. To prevent the eigenfunctions from becoming infinite as $x \rightarrow \pm\infty$, the factors multiplying x must be pure imaginary numbers: $-1 \pm (1+k)^{1/2} = ci$, where c is an arbitrary real number. So $\pm(1+k)^{1/2} = 1 + ci$ and $1+k = (1+ci)^2 = 1+2ic - c^2$ and $k = 2ic - c^2$.
- 3.28** (a) $\hat{p}_y^3 = (\hbar/i)^3 (\partial/\partial y)^3 = i\hbar^3 \partial^3/\partial y^3$;
 (b) $\hat{x}\hat{p}_y - \hat{y}\hat{p}_x = x(\hbar/i)\partial/\partial y - y(\hbar/i)\partial/\partial x$;
 (c) $[x(\hbar/i)\partial/\partial y]^2 f(x, y) = -\hbar^2 (x\partial/\partial y)(x\partial f/\partial y) = -\hbar^2 (x^2 \partial^2 f/\partial y^2)$.
 Hence $(\hat{x}\hat{p}_y)^2 = -\hbar^2 (x^2 \partial^2/\partial y^2)$.
- 3.29** $(\hbar/i)(dg/dx) = kg$ and $dg/g = (ik/\hbar) dx$. Integration gives $\ln g = (ik/\hbar)x + C$ and $g = e^{ikx/\hbar} e^C = Ae^{ikx/\hbar}$, where C and A are constants. If k were imaginary ($k = a + bi$, where a and b are real and b is nonzero), then $ik = ia - b$, and the $e^{-bx/\hbar}$ factor in g makes g go to infinity as x goes to minus infinity if b is positive or as x goes to infinity if b is negative. Hence b must be zero and $k = a$, where a is a real number.
- 3.30** (a) $[\hat{x}, \hat{p}_x]f = (\hbar/i)[x\partial/\partial x - (\partial/\partial x)x]f = (\hbar/i)[x\partial f/\partial x - (\partial/\partial x)(xf)] = (\hbar/i)[x\partial f/\partial x - f - x\partial f/\partial x] = -(\hbar/i)f$, so $[\hat{x}, \hat{p}_x] = -(\hbar/i)$.
 (b) $[\hat{x}, \hat{p}_x^2]f = (\hbar/i)^2 [x\partial^2/\partial x^2 - (\partial^2/\partial x^2)x]f = -\hbar^2 [x\partial^2 f/\partial x^2 - (\partial^2/\partial x^2)(xf)] = -\hbar^2 [x\partial^2 f/\partial x^2 - x\partial^2 f/\partial x^2 - 2\partial f/\partial x] = 2\hbar^2 \partial f/\partial x$. Hence $[\hat{x}, \hat{p}_x^2] = 2\hbar^2 \partial/\partial x$.
 (c) $[\hat{x}, \hat{p}_y]f = (\hbar/i)[x\partial/\partial y - (\partial/\partial y)x]f = (\hbar/i)[x\partial f/\partial y - x(\partial f/\partial y)] = 0$, so $[\hat{x}, \hat{p}_y] = 0$.
 (d) $[\hat{x}, \hat{V}(x, y, z)]f = (xV - Vx)f = 0$.
 (e) Let $A \equiv -\hbar^2/2m$. Then $[\hat{x}, \hat{H}]f = \{x[A(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) + V] - [A(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) + V]x\}f =$

$A[x\partial^2 f/\partial x^2 + x\partial^2 f/\partial y^2 + x\partial^2 f/\partial z^2 - x\partial^2 f/\partial x^2 - 2\partial f/\partial x - x\partial^2 f/\partial y^2 - x\partial^2 f/\partial z^2] + xAVf - AVxf = -2A\partial f/\partial x = (\hbar^2/m)\partial f/\partial x$, so $[\hat{x}, \hat{H}] = (\hbar^2/m)\partial/\partial x$.

(f) $[\hat{x}\hat{y}\hat{z}, \hat{p}_x^2]f = -\hbar^2[xyz\partial^2 f/\partial x^2 - (\partial^2/\partial x^2)(xyzf)] = -\hbar^2[xyz\partial^2 f/\partial x^2 - xyz\partial^2 f/\partial x^2 - 2yz\partial f/\partial x] = 2\hbar^2 yz\partial f/\partial x$, so $[\hat{x}\hat{y}\hat{z}, \hat{p}_x^2] = 2\hbar^2 yz\partial/\partial x$.

$$3.31 \quad \hat{T} = -\frac{\hbar^2}{2m_1}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2}\right) - \frac{\hbar^2}{2m_2}\left(\frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2}\right)$$

$$3.32 \quad \hat{H} = -(\hbar^2/2m)\nabla^2 + c(x^2 + y^2 + z^2), \text{ where } \nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2.$$

$$3.33 \quad \text{(a) } \int_0^2 |\Psi(x, t)|^2 dx;$$

$$\text{(b) } \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^2 |\Psi(x, y, z, t)|^2 dx dy dz;$$

$$\text{(c) } \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^2 |\Psi(x_1, y_1, z_1, x_2, y_2, z_2, t)|^2 dx_1 dy_1 dz_1 dx_2 dy_2 dz_2.$$

3.34 (a) $|\psi|^2 dx$ is a probability and probabilities have no units. Since dx has SI units of m, the SI units of ψ are $m^{-1/2}$.

(b) To make $|\psi|^2 dx dy dz$ dimensionless, the SI units of ψ are $m^{-3/2}$.

(c) To make $|\psi|^2 dx_1 dy_1 dz_1 \cdots dx_n dy_n dz_n$ dimensionless, the SI units of ψ are $m^{-3n/2}$.

3.35 Let the x , y , and z directions correspond to the order used in the problem to state the edge lengths. The ground state has $n_x n_y n_z$ quantum numbers of 111. The first excited state has one quantum number equal to 2. The quantum-mechanical energy decreases as the length of a side of the box increases. Hence in the first excited state, the quantum-number value 2 is for the direction of the longest edge, the z direction. Then

$$h\nu = \frac{\hbar^2}{8m}\left(\frac{1^2}{a^2} + \frac{1^2}{b^2} + \frac{2^2}{c^2}\right) - \frac{\hbar^2}{8m}\left(\frac{1^2}{a^2} + \frac{1^2}{b^2} + \frac{1^2}{c^2}\right)$$

$$\nu = \frac{3\hbar}{8mc^2} = \frac{3(6.626 \times 10^{-34} \text{ J s})}{8(9.109 \times 10^{-31} \text{ kg})(6.00 \times 10^{-10} \text{ m})^2} = 7.58 \times 10^{14} \text{ s}^{-1}$$

$$3.36 \quad \text{(a) Use of Eqs. (3.74) and (A.2) gives } \int_{2.00 \text{ nm}}^{3.00 \text{ nm}} \int_{1.50 \text{ nm}}^{2.00 \text{ nm}} \int_0^{0.40 \text{ nm}} |\psi|^2 dx dy dz = \int_0^{0.40 \text{ nm}} (2/a)\sin^2(\pi x/a) dx \int_{1.50 \text{ nm}}^{2.00 \text{ nm}} (2/b)\sin^2(\pi y/b) dy \int_{2.00 \text{ nm}}^{3.00 \text{ nm}} (2/c)\sin^2(\pi z/c) dz =$$

$$\left[\frac{x}{a} - \frac{\sin(2\pi x/a)}{2\pi} \right] \Big|_0^{0.40 \text{ nm}} \left[\frac{y}{b} - \frac{\sin(2\pi y/b)}{2\pi} \right] \Big|_{1.50 \text{ nm}}^{2.00 \text{ nm}} \left[\frac{z}{c} - \frac{\sin(2\pi z/c)}{2\pi} \right] \Big|_{2.00 \text{ nm}}^{3.00 \text{ nm}} =$$

$$\left[\frac{0.40}{1.00} - \frac{\sin(2\pi \cdot 0.40/1.00)}{2\pi} \right] \left[\frac{2.00 - 1.50}{2.00} - \frac{\sin(2\pi \cdot 2.00/2.00) - \sin(2\pi \cdot 1.50/2.00)}{2\pi} \right] \times$$

$$\left[\frac{3.00 - 2.00}{5.00} - \frac{\sin(2\pi \cdot 3.00/5.00) - \sin(2\pi \cdot 2.00/5.00)}{2\pi} \right] =$$

$$(0.3065)(0.09085)(0.3871) = 0.0108.$$

(b) The y and z ranges of the region include the full range of y and z , and the y and z factors in ψ are normalized. Hence the y and z integrals each equal 1. The x integral is the same as in part (a), so the probability is 0.3065.

(c) The same as (b), namely, 0.3065.

3.37 $\hat{p}_x = -i\hbar \partial/\partial x$. (a) $\partial(\sin kx)/\partial x = k \cos kx$, so ψ is not an eigenfunction of \hat{p}_x .

(b) $\hat{p}_x^2 \psi_{(3.73)} = -\hbar^2 (\partial^2/\partial x^2) \psi_{(3.73)} = -\hbar^2 (-1)(n_x \pi/a)^2 \psi_{(3.73)}$, where $\psi_{(3.73)}$ is given by Eq. (3.73). The eigenvalue is $\hbar^2 n_x^2/4a^2$, which is the value observed if p_x^2 is measured.

(c) $\hat{p}_z^2 \psi_{(3.73)} = -\hbar^2 (\partial^2/\partial z^2) \psi_{(3.73)} = -\hbar^2 (-1)(n_z \pi/c)^2 \psi_{(3.73)}$ and the observed value is $\hbar^2 n_z^2/4c^2$.

(d) $\hat{x} \psi_{(3.73)} = x \psi_{(3.73)} \neq (\text{const.}) \psi_{(3.73)}$, so ψ is not an eigenfunction of \hat{x} .

3.38 Since $n_y = 2$, the plane $y = b/2$ is a nodal plane within the box; this plane is parallel to the xz plane and bisects the box. With $n_z = 3$, the function $\sin(3\pi z/c)$ is zero on the nodal planes $z = c/3$ and $z = 2c/3$; these planes are parallel to the xy plane.

3.39 (a) $|\psi|^2$ is a maximum where $|\psi|$ is a maximum. We have $|\psi| = |f(x)||g(y)||h(z)|$. For $n_x = 1$, $|f(x)| = (2/a)^{1/2} |\sin(\pi x/a)|$ is a maximum at $x = a/2$. Also, $|g(y)|$ is a maximum at $y = b/2$ and $|h(z)|$ is a maximum at $z = c/2$. Therefore $|\psi|$ is a maximum at the point $(a/2, b/2, c/2)$, which is the center of the box.

(b) $|f(x)| = (2/a)^{1/2} |\sin(2\pi x/a)|$ is a maximum at $x = a/4$ and at $x = 3a/4$. $|g(y)|$ is a maximum at $y = b/2$ and $|h(z)|$ is a maximum at $z = c/2$. Therefore $|\psi|$ is a maximum at the points $(a/4, b/2, c/2)$ and $(3a/4, b/2, c/2)$,

3.40 When integrating over one variable, we treat the other two variables as constant; hence $\iiint F(x)G(y)H(z) dx dy dz = \iint \left[\int F(x)G(y)H(z) dx \right] dy dz = \iint G(y)H(z) \left[\int F(x) dx \right] dy dz$

$$= \left[\int F(x) dx \right] \int \left[\int G(y) H(z) dy \right] dz = \int F(x) dx \int H(z) \left[\int G(y) dy \right] dz = \int F(x) dx \int G(y) dy \int H(z) dz .$$

- 3.41** If the ratio of two edge lengths is exactly an integer, we have degeneracy. For example, if $b = ka$, where k is an integer, then $n_x^2/a^2 + n_y^2/b^2 = (n_x^2 + n_y^2/k^2)/a^2$. The (n_x, n_y, n_z) states $(1, 2k, n_z)$ and $(2, k, n_z)$ have the same energy.

- 3.42** With $V = 0$, we have $-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) = E\psi$. Assume

$\psi(x, y, z) = F(x)G(y)H(z)$. Substitution into the Schrödinger equation followed by

division by FGH , gives $-\frac{\hbar^2}{2m} \left(\frac{1}{F} \frac{d^2 F}{dx^2} + \frac{1}{G} \frac{d^2 G}{dy^2} + \frac{1}{H} \frac{d^2 H}{dz^2} \right) = E$ and

$$-\frac{\hbar^2}{2m} \left(\frac{1}{F} \frac{d^2 F}{dx^2} \right) = E + \frac{\hbar^2}{2m} \left(\frac{1}{G} \frac{d^2 G}{dy^2} + \frac{1}{H} \frac{d^2 H}{dz^2} \right) \quad (\text{Eq. 1}). \quad \text{Let } E_x \equiv -\frac{\hbar^2}{2m} \left(\frac{1}{F} \frac{d^2 F}{dx^2} \right).$$

Then, since F is a function of x only, E_x is independent of y and z . But Eq. 1 shows E_x is equal to the right side of Eq. 1, which is independent of x , so E_x is independent of x .

Hence E_x is a constant and $-(\hbar^2/2m)(d^2 F/dx^2) = E_x F$. This is the same as the one-dimensional free-particle Schrödinger equation (2.29), so $F(x)$ and E_x are given by (2.30) and (2.31). By symmetry, G and H are given by (2.30) with x replaced by y and by z , respectively.

- 3.43** For a linear combination of eigenfunctions of \hat{H} to be an eigenfunction of \hat{H} , the eigenfunctions must have the same eigenvalue. In this case, they must have the same value of $n_x^2 + n_y^2 + n_z^2$. The functions (a) and (c) are eigenfunctions of \hat{H} and (b) is not.

- 3.44** In addition to the 11 states shown in the table after Eq. (3.75), the following 6 states have $E(8ma^2/h^2) < 15$:

$n_x n_y n_z$	123	132	213	231	312	321
$E(8ma^2/h^2)$	14	14	14	14	14	14

These 6 states and the 11 listed in the textbook give a total of 17 states. These 17 states have 6 different values of $E(8ma^2/h^2)$, and there are 6 energy levels.

- 3.45** (a) From the table after Eq. (3.75), there is only one state with this value, so the degree of degeneracy is 1, meaning this level is nondegenerate.
 (b) From the table in the Prob. 3.44 solution, the degree of degeneracy is 6.

(c) The following $n_x n_y n_z$ values have $E(8ma^2/h^2) = 27; 115, 151, 511, 333$. The degree of degeneracy is 4.

3.46 (a) These are linearly independent since none of them can be written as a linear combination of the others.

(b) Since $3x^2 - 1 = 3(x^2) - \frac{1}{8}(8)$, these are not linearly independent.

(c) Linearly independent.

(d) Linearly independent.

(e) Since $e^{ix} = \cos x + i \sin x$, these are linearly dependent.

(f) Since $1 = \sin^2 x + \cos^2 x$, these are linearly dependent.

(g) Linearly independent.

3.47 See the beginning of Sec. 3.6 for the proof.

3.48 (a) $\langle x \rangle = \int_0^c \int_0^b \int_0^a x |f(x)|^2 |g(y)|^2 |h(z)|^2 dx dy dz = \int_0^a x |f(x)|^2 dx \int_0^b |g(y)|^2 dy \int_0^c |h(z)|^2 dz$, where f, g , and h are given preceding Eq.

(3.72). Since g and h are normalized, $\langle x \rangle = \int_0^a x |f(x)|^2 dx = (2/a) \int_0^a x \sin^2(n_x \pi x/a) dx =$

$$\frac{2}{a} \left[\frac{x^2}{4} - \frac{ax}{4n_x \pi} \sin(2n_x \pi x/a) - \frac{a^2}{8n_x^2 \pi^2} \cos(2n_x \pi x/a) \right] \Bigg|_0^a = \frac{a}{2}, \text{ where Eq. (A.3) was used.}$$

(b) By symmetry, $\langle y \rangle = b/2$ and $\langle z \rangle = c/2$.

(c) The derivation of Eq. (3.92) for the ground state applies to any state, and $\langle p_x \rangle = 0$.

(d) Since g and h are normalized,

$$\langle x^2 \rangle = \int_0^a x^2 |f(x)|^2 dx = (2/a) \int_0^a x^2 \sin^2(n_x \pi x/a) dx =$$

$$\frac{2}{a} \left[\frac{x^3}{6} - \left(\frac{ax^2}{4n_x \pi} - \frac{a^3}{8n_x^3 \pi^3} \right) \sin(2n_x \pi x/a) - \frac{a^2 x}{4n_x^2 \pi^2} \cos(2n_x \pi x/a) \right] \Bigg|_0^a = \frac{a^2}{3} - \frac{a^2}{2n_x^2 \pi^2},$$

where Eq. (A.4) was used. We have $\langle x \rangle^2 = a^2/4 \neq \langle x^2 \rangle$. Also,

$$\langle xy \rangle = \int_0^c \int_0^b \int_0^a xy |f(x)|^2 |g(y)|^2 |h(z)|^2 dx dy dz =$$

$$\int_0^a x |f(x)|^2 dx \int_0^b y |g(y)|^2 dy \int_0^c |h(z)|^2 dz = \langle x \rangle \langle y \rangle.$$

3.49 $\langle A + B \rangle = \int \Psi^* (\hat{A} + \hat{B}) \Psi d\tau = \int \Psi^* \hat{A} \Psi d\tau + \int \Psi^* \hat{B} \Psi d\tau =$

$$\langle A \rangle + \langle B \rangle. \text{ Also } \langle cB \rangle = \int \Psi^* (c\hat{B}) \Psi d\tau = c \int \Psi^* \hat{B} \Psi d\tau = c \langle B \rangle.$$

- 3.50** (a) Not acceptable, since it is not quadratically integrable. This is obvious from a graph or from $\int_{-\infty}^{\infty} e^{-2ax} dx = -(1/2a)e^{-2ax} \Big|_{-\infty}^{\infty} = \infty$.
- (b) This is acceptable, since it is single-valued, continuous, and quadratically integrable when multiplied by a normalization constant. See Eqs. (4.49) and (A.9).
- (c) This is acceptable, since it is single-valued, continuous, and quadratically integrable when multiplied by a normalization constant. See Eqs. (4.49) and (A.10) with $n = 1$.
- (d) Acceptable for the same reasons as in (b).
- (e) Not acceptable since it is not continuous at $x = 0$.

3.51 Given: $i\hbar \partial\Psi_1/\partial t = \hat{H}\Psi_1$ and $i\hbar \partial\Psi_2/\partial t = \hat{H}\Psi_2$. Prove that $i\hbar \partial(c_1\Psi_1 + c_2\Psi_2)/\partial t = \hat{H}(c_1\Psi_1 + c_2\Psi_2)$. We have $i\hbar \partial(c_1\Psi_1 + c_2\Psi_2)/\partial t = i\hbar[\partial(c_1\Psi_1)/\partial t + \partial(c_2\Psi_2)/\partial t] = c_1 i\hbar \partial\Psi_1/\partial t + c_2 i\hbar \partial\Psi_2/\partial t = c_1 \hat{H}\Psi_1 + c_2 \hat{H}\Psi_2 = \hat{H}(c_1\Psi_1 + c_2\Psi_2)$, since \hat{H} is linear.

3.52 (a) An inefficient C++ program is

```
#include <iostream>
using namespace std;
int main() {
    int m, i, j, k, nx, ny, nz, L[400], N[400], R[400], S[400];
    i=0;
    for (nx=1; nx<8; nx=nx+1) {
        for (ny=1; ny<8; ny=ny+1) {
            for (nz=1; nz<8; nz=nz+1) {
                m=nx*nx+ny*ny+nz*nz;
                if (m>60)
                    continue;
                i=i+1;
                L[i]=m;
                N[i]=nx;
                R[i]=ny;
                S[i]=nz;
            }
        }
    }
    for (k=3; k<61; k=k+1) {
        for (j=1; j<=i; j=j+1) {
            if (L[j]==k)
                cout<<N[j]<< " "<<R[j]<< " "<<S[j]<< " "<<L[j]<<endl;
        }
    }
    return 0;
}
```

}

A free integrated development environment (IDE) to debug and run C++ programs is Code::Blocks, available at www.codeblocks.org. For a Windows computer, downloading the file with mingw-setup.exe as part of the name will include the MinGW (GCC) compiler for C++. Free user guides and manuals for Code::Blocks can be found by searching the Internet.

Alternatively, you can run the program at ideone.com.

(b) One finds 12 states.

- 3.53** (a) T. (b) F. See the paragraph preceding the example at the end of Sec. 3.3.
(c) F. This is only true if f_1 and f_2 have the same eigenvalue.
(d) F. (e) F. This is only true if the two solutions have the same energy eigenvalue.
(f) F. This is only true for stationary states.
(g) F. (h) F. $x(5x) \neq (\text{const.})(5x)$.
(i) T. $\hat{H}\Psi = \hat{H}(e^{-iEt/\hbar}\psi) = e^{-iEt/\hbar}\hat{H}\psi = Ee^{-iEt/\hbar}\psi = E\Psi$.
(j) T. (k) T. (l) F.
(m) T. $\hat{A}^2 f = \hat{A}(\hat{A}f) = \hat{A}(af) = a\hat{A}f = a^2 f$, provided \hat{A} is linear. Note that the definition of eigenfunction and eigenvalue in Sec. 3.2 specified that \hat{A} is linear.
(n) F. (o) F.