Potentially Useful Equations

$E=h\nu$ $c=\lambda\nu$ $\lambda=h/p$ $\hbar = h/2\pi$

$$\hat{x} = x \qquad \hat{p}_x = \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x} \qquad \hat{l}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi} \qquad \Delta x\,\Delta p \geq \frac{\hbar}{2} \qquad \hat{H} = \hat{E}_K + \hat{V}$$

$$\hat{H}\psi = E\psi \qquad -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x)\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \qquad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Lambda^2$$

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} \qquad \Lambda^2 Y_{l,m_l}(\theta,\phi) = -l(l+1)Y_{l,m_l}(\theta,\phi) \qquad \hat{l}_z Y_{l,m_l}(\theta,\phi) = m_l\hbar Y_{l,m_l}(\theta,\phi)$$

$$\langle A\rangle = \int_{\text{all x}} \psi^*(x)\hat{A}\psi(x)\,\mathrm{d}x \qquad \langle A\rangle = \int_{\text{all space}} \psi^*\hat{A}\psi\,\mathrm{d}\tau \qquad \mathrm{d}\tau = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi$$

Particle in a 1-D Box: $\psi_n(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}}\sin\frac{n\pi x}{L}$ $\qquad E_n = \frac{h^2 n^2}{8mL^2}$

Particle in a 2-D Box: $\psi_{n_1,n_2}(x,y) = \left(\frac{2}{L_1}\right)^{\frac{1}{2}}\left(\frac{2}{L_2}\right)^{\frac{1}{2}}\sin\frac{n_1\pi x}{L_1}\sin\frac{n_2\pi y}{L_2}$ $\qquad E_{n_1,n_2} = \frac{h^2}{8m}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2}\right)$

Free particle: $\psi(x) = \exp\{ikx\}$ $\qquad E_k = \frac{k^2\hbar^2}{2m}$

Particle in a barrier: $\psi(x) = \exp\{\kappa x\}$ $\qquad \kappa\hbar = [2m(V-E)]^{1/2}$

Harmonic oscillator: $V(x) = \frac{1}{2}kx^2$ $\qquad k = \frac{\mathrm{d}^2V(x)}{\mathrm{d}x^2} = m\omega^2$ $\qquad E_v = (v+\frac{1}{2})\hbar\omega$ $\qquad v = 0,1,2,\cdots$

$$\psi_v(x) = N_v H_v(y)e^{-y^2/2} \qquad y = \frac{x}{\alpha} \qquad \alpha = \left(\frac{\hbar^2}{mk}\right)^{1/4}$$

Particle on a ring: $\psi_{m_l}(\phi) = \frac{1}{(2\pi)^{1/2}}e^{im_l\phi}$ $\qquad m_l = 0,\pm1,\pm2,\cdots$ $\qquad E_{m_l} = \frac{m_l^2\hbar^2}{2I}$

Particle on a sphere: $\psi_{l,m_l}(\theta,\phi) = Y_{l,m_l}(\theta,\phi)$ $\qquad l = 0,1,2,\cdots$ $\qquad m_l = l, l-1,\cdots,-l$

$$E_l = l(l+1)\frac{\hbar^2}{2I} \qquad L = \sqrt{l(l+1)}\hbar$$

Transition dipole integral: $\underset{\rightarrow}{\mu}_{fi} = \int \Psi_f^*\,\underset{\rightarrow}{\hat{\mu}}\,\Psi_i\,\mathrm{d}\tau$ $\qquad \underset{\rightarrow}{\mu} = -e\sum_i \underset{\rightarrow}{r_i} + e\sum_I Z_I\,\underset{\rightarrow}{R_I}$

Moment of inertia: $I = \sum_i m_i (r_i^{\perp})^2$ (diatomic molecule: $I = \mu R_e^2$, $\mu = \frac{m_1 m_2}{m_1 + m_2}$)

Spherical Rotor: $E_J = hcBJ(J+1)$ $hcB = \frac{\hbar^2}{2I}$

Symmetric Rotor: $E_{JK} = hc[BJ(J+1) + (A-B)K^2]$ $hcA = \frac{\hbar^2}{2I_a}$ $hcB = \frac{\hbar^2}{2I_b}$

Linear Rotor: $E_J = hcBJ(J+1)$ $hcB = \frac{\hbar^2}{2I}$

Anharmonic Energy Levels: $E_v = hc\tilde{\nu}(v+\tfrac{1}{2}) - hc\tilde{\nu}x_e(v+\tfrac{1}{2})^2$

Morse Potential: $V(x) = hcD_e(1-e^{-ax})^2$ $a = \left(\frac{\mu\omega^2}{2hcD_e}\right)^{1/2}$ $x_e = \frac{a^2\hbar}{2\mu\omega} = \frac{\tilde{\nu}}{4D_e}$

$hc\tilde{\nu}_P(J) = hc\tilde{\nu} - 2hcBJ$ $hc\tilde{\nu}_Q(J) = hc\tilde{\nu}$ $hc\tilde{\nu}_R(J) = hc\tilde{\nu} + 2hcB(J+1)$

Some Selection Rules (*without any indication of when they are applicable*):

$\Delta J = 0, \pm 1$ $\Delta M_J = 0, \pm 1$ $\Delta v = \pm 1$ $\Delta S = 0$ $\Delta \Lambda = 0, \pm 1$

Integrals and Other Relations

$\int x^n \mathrm{d}x = \frac{x^{n+1}}{n+1} + \text{constant}$ $\int \frac{1}{x}\mathrm{d}x = \ln x + \text{constant}$

$\int_0^\infty x^n e^{-ax}\mathrm{d}x = \frac{n!}{a^{n+1}}$ $\int_0^\infty x^2 e^{-ax^2}\mathrm{d}x = \frac{1}{4a}\sqrt{\frac{\pi}{a}}$ $\int e^{ax}dx = \frac{1}{a}e^{ax}$

$\int \sin^2 ax\,\mathrm{d}x = \frac{x}{2} - \frac{1}{4a}\sin 2ax + \text{constant}$

$\int \sin ax \sin bx\,\mathrm{d}x = \frac{\sin(a-b)x}{2(a-b)} - \frac{\sin(a+b)x}{2(a+b)} + \text{constant}$ if $a^2 \neq b^2$

$e^{\pm ix} = \cos x \pm i \sin x$

$f(x) = f(0) + \left(\frac{df}{dx}\right)_0 x + \frac{1}{2}\left(\frac{d^2 f}{dx^2}\right)_0 x^2 + \ldots + \frac{1}{n!}\left(\frac{d^n f}{dx^n}\right)_0 x^n + \ldots$

Table 12.3 The spherical harmonics $Y_{l,m_l}(\theta, \phi)$

l	m_l	Y_{l,m_l}
0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
1	0	$\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$
	±1	$\mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\phi}$
2	0	$\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$
	±1	$\mp\left(\frac{15}{8\pi}\right)^{1/2}\cos\theta\sin\theta\, e^{\pm i\phi}$
	±2	$\left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{\pm 2i\phi}$
3	0	$\left(\frac{7}{16\pi}\right)^{1/2}(5\cos^3\theta - 3\cos\theta)$
	±1	$\mp\left(\frac{21}{64\pi}\right)^{1/2}(5\cos^2\theta - 1)\sin\theta\, e^{\pm i\phi}$
	±2	$\left(\frac{105}{32\pi}\right)^{1/2}\sin^2\theta\cos\theta\, e^{\pm 2i\phi}$
	±3	$\mp\left(\frac{35}{64\pi}\right)^{1/2}\sin^3\theta\, e^{\pm 3i\phi}$

Table 12.1 The Hermite polynomials $H_v(y)$

v	H_v
0	1
1	$2y$
2	$4y^2 - 2$
3	$8y^3 - 12y$
4	$16y^4 - 48y^2 + 12$
5	$32y^5 - 160y^3 + 120y$
6	$64y^6 - 480y^4 + 720y^2 - 120$