USEFUL CONSTANTS and FORMULAS

1mW = 10^{-3}W = 10^{-3} J s^{-1} 1nm = 10^{-9}m 1eV = 1.602 x 10^{-19} J

h = 6.63 x 10^{-34} J s $\hbar$ = 1.05 x 10^{-34} J s c = 3.0 x 10^{8} m s^{-1}

hc = 2.0 x 10^{-25} J m m_e = 9.11 x 10^{-31} kg e = 1.602 x 10^{-19} C

$\lambda\nu = c$ $\varepsilon_0 = 8.854\times10^{-12}\,Cs^2kg^{-1}m^{-3}$ $E = h\nu$ $\lambda = h/p$

$l_n = mrv = n\hbar$ $r_n = n^2 a_0$ a_0 = 5.29 x 10^{-11} m

Particle in a box

$$E_n = \frac{n^2h^2}{8ma^2} = \frac{n^2\hbar^2\pi^2}{2ma^2} \quad E_n = \frac{n^2h^2}{8ma^2} = \frac{n^2\hbar^2\pi^2}{2ma^2} \qquad \psi_n(0\le x\le a) = \left(\frac{2}{a}\right)^{1/2}\sin\left(\frac{n\pi x}{a}\right)$$

Harmonic Oscillator

$$E_n = \left(n+\frac{1}{2}\right)h\nu = \left(n+\frac{1}{2}\right)\hbar\omega \qquad \alpha = \frac{\sqrt{km}}{\hbar} = \frac{m\omega}{\hbar}, \qquad \tilde{\nu} = \frac{1}{2\pi c}\left(\frac{k}{\mu}\right)^{1/2}, \; V = \tfrac{1}{2}m\omega^2x^2$$

$$\int_{-\infty}^{\infty} e^{-\alpha x^2}dx = \sqrt{\frac{\pi}{\alpha}} \qquad \int_{-\infty}^{\infty} x^2e^{-\alpha x^2}dx = \sqrt{\frac{\pi}{\alpha}}\frac{1}{2\alpha} \qquad \int_{-\infty}^{\infty} x^{2n}e^{-\alpha x^2}dx = 2\frac{1\cdot3\cdot5\cdots(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{\alpha}}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\alpha x^2/2} \qquad \psi_1(x) = \frac{1}{\sqrt{2}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(2\alpha^{1/2}x\right)e^{-\alpha x^2/2}$$

$$\psi_2(x) = \frac{1}{\sqrt{8}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(4\alpha x^2-2\right)e^{-\alpha x^2/2} \qquad \psi_3(x) = \frac{1}{\sqrt{48}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(8\alpha^{3/2}x^3-12\alpha^{1/2}x\right)e^{-\alpha x^2/2}$$

Raising and lowering operators

$$a_\pm = \left(\frac{1}{2\hbar\mu\omega}\right)^{\frac{1}{2}}(\mp ip+\mu\omega x) \qquad \hat{x} = \left(\frac{\hbar}{2\mu\omega}\right)^{1/2}\left(\hat{a}^+ + \hat{a}^-\right) \qquad \hat{p} = i\left(\frac{\hbar\mu\omega}{2}\right)\left(\hat{a}^+ - \hat{a}^-\right)$$

Normalization constants

$$\hat{a}^+|\psi_n\rangle = \hat{a}^+|n\rangle = \sqrt{n+1}\,|\psi_{n+1}\rangle == \sqrt{n+1}\,|n+1\rangle$$

$$\hat{a}^-|\psi_n\rangle = \hat{a}^-|n\rangle = \sqrt{n}\,|\psi_{n-1}\rangle = \sqrt{n}\,|n-1\rangle$$

Rigid Rotor

$$Y_0^0 = \frac{1}{(4\pi)^{1/2}} \qquad Y_1^0 = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\cos\theta \qquad Y_1^{\pm1} = \left(\frac{3}{8\pi}\right)^{\frac{1}{2}}\sin\theta e^{\pm i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{\frac{1}{2}}\left(3\cos^2\theta-1\right) \quad Y_2^{\pm1} = \left(\frac{15}{8\pi}\right)^{\frac{1}{2}}\sin\theta\cos\theta e^{\pm i\phi} \quad Y_2^{\pm2} = \left(\frac{15}{32\pi}\right)^{\frac{1}{2}}\sin^2\theta e^{\pm2i\phi}$$

$$E_J = \frac{\hbar^2}{2I} J(J+1) \qquad B \equiv \frac{h}{8\pi^2 I} \quad \text{(Hz)} \qquad \bar{B} \equiv \frac{h}{8\pi^2 cI} \quad (\text{cm}^{-1})$$

Hydrogen atom

Three-dimensional operators in spherical coordinates

$$\hat{H}(r,\theta,\phi) = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + V(r,\theta,\phi)$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \qquad \hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$U = \frac{-Ze^2}{4\pi\varepsilon_0 r}, \qquad E_n = \frac{-Z^2e^2}{8\pi\varepsilon_0 a_0 n^2} = \frac{-Z^2}{2n^2} \text{ (atomic units)} \quad n = 1,2,3,\ldots, \qquad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2}$$

$$\int_0^\infty x^n e^{x/a} dx = n! a^{n+1}$$

H atom spatial wavefunctions (where $\sigma = Zr/a_0$. In atomic units a_0=1 and $\sigma = Zr$.)

$$n=1 \quad l=0 \quad m=0 \quad \psi_{100} = \psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$$

$$n=2 \quad l=0 \quad m=0 \quad \psi_{200} = \psi_{2s} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (2-\sigma) e^{-\sigma/2}$$

$$l=1 \quad m=0 \quad \psi_{210} = \psi_{2p_z} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\cos\theta$$

$$l=1 \quad m=\pm1 \quad \psi_{21\pm1} = \frac{1}{\sqrt{64\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\sin\theta\, e^{\pm i\phi}$$

$$n=3 \quad l=0 \quad m=0 \quad \psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3} = \psi_{3s}$$

Independent Electron Model

$$\Psi(1,2,3,4..) = \begin{pmatrix} \psi_{k1}(1) & \psi_{k2}(1) & \ldots & \psi_{kn}(1) \\ \psi_{k1}(2) & \psi_{k2}(2) & & \ldots \\ \ldots & & \ldots & \\ \psi_{k1}(n) & \ldots & & \psi_{kn}(n) \end{pmatrix}$$

$$E = \sum_i \varepsilon_i + \sum_i \sum_{j<i} \tilde{J}_{ij} - \tilde{K}_{ij} \quad \text{where } \tilde{J}_{ij} = J_{ij} \text{ and } \tilde{K}_{ij} = \begin{cases} K_{ij} & \text{if } S_i = S_j \\ 0 & \text{if } S_i \neq S_j \end{cases}$$