Potentially Useful Equations

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

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

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

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

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

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

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

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

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: $\psi_{l,m_l}(\theta,\phi) = Y_{l,m_l}(\theta,\phi) \quad l = 0,1,2,\cdots \quad m_l = l, l-1,\cdots,-l$

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

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*):

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

Hydrogenic atom: $\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r) Y_{l,m_l}(\theta,\phi)$ $n = 1,2,\cdots$ $l = 1,2,\cdots,n-1$ $P_{n,l}(r) = r^2 R_{n,l}^2(r)$

$$E_n = -\frac{\hbar^2}{2m_e a_0^2}\frac{Z^2}{n^2} \qquad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$$

$$W = \frac{N!}{n_0! n_1! n_2! \cdots} \quad N = \sum_i n_i \quad E = \sum_i n_i \varepsilon_i \quad p_i = \frac{n_i}{N} = \frac{e^{-\beta\varepsilon_i}}{q} \quad q = \sum_i e^{-\beta\varepsilon_i} = \sum_j g_j e^{-\beta\varepsilon_j} \quad \beta = \frac{1}{kT}$$

$$E = U - U(0) = -\frac{N}{q}\left(\frac{\partial q}{\partial\beta}\right)_V = -N\left(\frac{\partial \ln q}{\partial\beta}\right)_V \qquad S = k\ln W = \frac{U - U(0)}{T} + kN\ln q$$

Canonical Ensemble: $E = -\frac{1}{Q}\left(\frac{\partial Q}{\partial\beta}\right)_V = -\left(\frac{\partial \ln Q}{\partial\beta}\right)_V$ $S = \frac{U - U(0)}{T} + k\ln Q$

$$H - H(0) = -\left(\frac{\partial \ln Q}{\partial\beta}\right)_V + kTV\left(\frac{\partial \ln Q}{\partial V}\right)_T$$

$$A - A(0) = -kT\ln Q \qquad G - G(0) = -kT\ln Q + kTV\left(\frac{\partial \ln Q}{\partial V}\right)_T$$

Identical, *distinguishable* particles: $Q = q^N$

Identical, *indistinguishable* particles: $Q = \frac{q^N}{N!}$

$$q = q^T q^R q^V q^E \qquad q^T = \frac{V}{\Lambda^3} = \left(\frac{2\pi m}{h^2\beta}\right)^{3/2} V \qquad \Lambda = \left(\frac{h^2\beta}{2\pi m}\right)^{1/2}$$

Linear rotor: $q^R = \sum_J (2J+1)e^{-\beta hcBJ(J+1)} \sim \frac{1}{\sigma}\frac{1}{\beta hcB} = \frac{1}{\sigma}\frac{kT}{hcB} \qquad \Theta_R = \frac{hcB}{k}$

Non-linear rotor: $q^R \sim \frac{1}{\sigma}\left(\frac{kT}{hc}\right)^{3/2}\left(\frac{\pi}{ABC}\right)^{1/2}$

Harmonic oscillator: $q^V = \frac{1}{(1-e^{-\beta hc\tilde{\nu}})} = \frac{1}{(1-e^{-hc\tilde{\nu}/kT})} \qquad \Theta_V = \frac{hc\tilde{\nu}}{k}$

$$K = \frac{(q^{\circ}_{C,m}/N_A)^c (q^{\circ}_{D,m}/N_A)^d}{(q^{\circ}_{A,m}/N_A)^a (q^{\circ}_{B,m}/N_A)^b} e^{-\Delta_r E_0/RT}$$

$$z = \sigma_C v_{rel} \mathcal{N}_B \qquad Z_{AB}(v_{rel}) = \sigma_C v_{rel} \mathcal{N}_A \mathcal{N}_B \qquad Z_{AB}(T) = \sigma_C \langle v_{rel}\rangle \mathcal{N}_A \mathcal{N}_B = \sigma_C \langle v_{rel}\rangle N_A^2 [A][B]$$

$$f(v_{rel})\,\mathrm{d}v_{rel} = 4\pi\left(\frac{\mu}{2\pi kT}\right)^{3/2} v_{rel}^2\, e^{-\mu v_{rel}^2/2kT}\,\mathrm{d}v_{rel} \qquad \langle v_{rel}\rangle = \left(\frac{8kT}{\pi\mu}\right)^{1/2}$$

$$Rate = k_2[A][B] \qquad k_2(v_{rel}) = \sigma_R v_{rel} N_A$$

$$k_2(T) = N_A \int_0^\infty \sigma_R(v_{rel})\, v_{rel}\, f(v_{rel})\,\mathrm{d}v_{rel} = N_A\left(\frac{8kT}{\pi\mu}\right)^{1/2} \sigma_0\, e^{-\varepsilon_{th}/kT} \quad , \quad \sigma_R = \begin{matrix} 0, & \varepsilon < \varepsilon_{th} \\ \sigma_0\left(1-\varepsilon_{th}/\varepsilon\right), & \varepsilon \ge \varepsilon_{th} \end{matrix}$$

$$Rate = \frac{k_d k_a}{k_a + k_{-d}}[A][B] \qquad k_d = 4\pi R^* D N_A \sim \frac{8}{3}\frac{kN_A T}{\eta}$$

$$k_2(T) = \frac{kT}{h}\frac{\overline{q}^{\circ}_{AB^\mp}}{q^{\circ}_A q^{\circ}_A} N_A e^{-\Delta\varepsilon_0/kT}\frac{RT}{p^\circ} = \frac{kT}{h}\overline{K}^{\mp}\frac{RT}{p^\circ} = \frac{kT}{h}\overline{K}_c^{\mp} = \frac{kT}{h}\frac{RT}{p^\circ} e^{\Delta^{\mp}S^\circ/R} e^{-\Delta^{\mp}H^\circ/RT}$$

Integrals and Other Relations

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

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

$$\int_0^\infty x^n e^{-ax} \mathrm{d}x = \frac{n!}{a^{n+1}}$$

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

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

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

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

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

Stirling's approximation: $\ln x = x \ln x - x$ for large x