

Potentially Useful Equations

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

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

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

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

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

$$\langle A \rangle = \int_{\text{all } x} \psi^*(x) \hat{A} \psi(x) dx \quad \langle A \rangle = \int_{\text{all space}} \psi^* \hat{A} \psi d\tau \quad d\tau = dx dy dz = r^2 \sin \theta dr d\theta d\phi$$

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

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

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

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

$$\text{Harmonic oscillator: } V(x) = \frac{1}{2} kx^2 \quad k = \frac{d^2 V(x)}{dx^2} = m\omega^2 \quad E_v = (v + \frac{1}{2}) \hbar \omega \quad v = 0, 1, 2, \dots$$

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

$$\text{Particle on a ring: } \psi_{m_l}(\phi) = \frac{1}{(2\pi)^{1/2}} e^{im_l \phi} \quad m_l = 0, \pm 1, \pm 2, \dots \quad E_{m_l} = \frac{m_l^2 \hbar^2}{2I}$$

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

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

$$\text{Transition dipole integral: } \underline{\mu}_{fi} = \int \Psi_f^* \hat{\underline{\mu}} \Psi_i d\tau \quad \underline{\mu} = -e \sum_i r_i + e \sum_l Z_l R_l$$

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

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

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

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

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

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

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

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

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

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

$E_n = -\frac{\hbar^2 Z^2}{2m_e a_0^2 n^2} \quad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2}$

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

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

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

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

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

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

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

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

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

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

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

$$z = \sigma_C v_{rel} N_B \quad Z_{AB}(v_{rel}) = \sigma_C v_{rel} N_A N_B \quad Z_{AB}(T) = \sigma_C \langle v_{rel} \rangle N_A N_B = \sigma_C \langle v_{rel} \rangle N_A^2 [A][B]$$

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

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

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

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

Integrals and Other Relations

$$\int x^n dx = \frac{x^{n+1}}{n+1} + \text{constant} \quad \int \frac{1}{x} dx = \ln x + \text{constant}$$

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

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

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

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

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