UNIVERSITY of GUELPH

CHEM*3860 Fall 2024 Final Exam Equation Sheet

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The Schrödinger Equation

$$E_\mathrm{k} = h\nu - \phi, \quad h = 6.626 \times 10^{-34}\ \mathrm{J \cdot s}$$

$$\lambda = \frac{h}{p}$$

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

$$|\psi|^2 = \psi^*\psi$$

$$e^{i\theta} = \cos\theta + i\sin\theta$$

The Particle in a Box

$$y'' + py' + qy = 0, \quad a^2 + pa + q = 0$$

$$y = c_1 e^{a_1 x} + c_2 e^{a_2 x}$$

$$\psi(x) = \left(\frac{2}{l}\right)^{1/2} \sin\left(\frac{n\pi x}{l}\right), \quad n = 1, 2, 3, \ldots$$

$$E = \frac{n^2 h^2}{8ml^2}, \quad n = 1, 2, 3, \ldots$$

$$\int_{-\infty}^{\infty} \psi_i^* \psi_j \mathrm{d}x = \delta_{ij}, \quad \delta_{ij} \equiv \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}$$

Operators

$$\left(\hat{A} \pm \hat{B}\right) f(x) \equiv \hat{A}f(x) \pm \hat{B}f(x)$$

$$\hat{A}\hat{B}f(x) \equiv \hat{A}\left[\hat{B}f(x)\right]$$

$$\left[\hat{A}, \hat{B}\right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$\hat{A}\left[f(x) + g(x)\right] = \hat{A}f(x) + \hat{A}g(x)$$

$$\hat{A}\left[cf(x)\right] = c\hat{A}f(x)$$

$$\left(\hat{A} + \hat{B}\right)\hat{C} = \hat{A}\hat{C} + \hat{B}\hat{C}$$

$$\hat{A}\left(\hat{B} + \hat{C}\right) = \hat{A}\hat{B} + \hat{A}\hat{C}$$

$$\hat{A}f(x) = kf(x)$$

$$\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}, \quad \hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}, \quad \hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

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

$$\hat{H}\psi = E\psi$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\left[-\sum_{i=1}^{n}\frac{\hbar^2}{2m}\nabla_i^2 + V\left(x_1, \ldots, z_n\right)\right]\psi = E\psi$$

$$\int |\psi|^2 \mathrm{d}\tau = 1$$

$$\langle B \rangle = \int \psi^* \hat{B}\psi \mathrm{d}\tau$$

The Harmonic Oscillator

$$y(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots = \sum_{n=0}^{\infty} a_n x^n$$

$$x = A\sin(2\pi\nu t + b), \quad \nu = \frac{1}{2\pi}\left(\frac{k}{m}\right)^{1/2}$$

$$F_x = -\frac{\partial V}{\partial x}, \quad F_y = -\frac{\partial V}{\partial y}, \quad F_z = -\frac{\partial V}{\partial z}$$

$$V = \frac{1}{2}kx^2, \quad T = \frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2$$

$$E = \left(v + \frac{1}{2}\right)h\nu, \quad v = 0, 1, 2, \ldots$$

Angular Momentum

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z, \quad \left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x, \quad \left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$

$$\left[\hat{L}^2, \hat{L}_x\right] = 0, \quad \left[\hat{L}^2, \hat{L}_y\right] = 0, \quad \left[\hat{L}^2, \hat{L}_z\right] = 0$$

$$\hat{L}^2 Y_l^m(\theta, \phi) = l(l+1)\hbar^2 Y_l^m(\theta, \phi), \quad l = 0, 1, 2, \ldots$$

$$\hat{L}_z Y_l^m(\theta, \phi) = m\hbar Y_l^m(\theta, \phi), \quad m = -l, -l+1, \ldots, l-1, l$$

The Rigid Rotor

$$\psi = Y_J^m\left(\theta, \phi\right)$$

$$\mu \equiv \frac{m_1 m_2}{m_1 + m_2}$$

$$E = \frac{J(J+1)\hbar^2}{2\mu d^2}, \quad J = 0, 1, 2, \ldots$$

The Hydrogen Atom

$$\psi = R(r)Y_l^m\left(\theta, \phi\right)$$

$$\mathbf{F} = -\frac{Ze^2}{4\pi\epsilon_0 r^2}\frac{\mathbf{r}}{r}$$

$$E = -\frac{Z^2\mu e^4}{8\epsilon_0^2 n^2 h^2}, \quad a \equiv \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$$

$$\psi_{nlm} = R_{nl}(r)Y_l^m\left(\theta, \phi\right), \quad n = 1, 2, 3, \ldots,$$

$$l = 0, 1, 2, \ldots, n-1, \quad m = -l, -l+1, \ldots, 0, \ldots, l-1, l$$

Theorems of Quantum Mechanics

$$\int f_m^* \hat{A} f_n \mathrm{d}\tau \equiv \langle f_m|\hat{A}|f_n\rangle \equiv \langle m|\hat{A}|n\rangle$$

$$\int f_m^* f_n \mathrm{d}\tau \equiv \langle f_m|f_n\rangle \equiv \langle m|n\rangle$$

$$\langle f|\hat{B}|g\rangle = \langle f|\hat{B}g\rangle$$

$$\langle cf|\hat{B}|g\rangle = c^*\langle f|\hat{B}g\rangle$$

$$\langle f|\hat{B}|cg\rangle = c\langle f|\hat{B}g\rangle$$

$$\langle m|n\rangle^* = \langle n|m\rangle$$

$$\int f_m^* \hat{A} f_n \mathrm{d}\tau = \int f_n \left(\hat{A} f_m\right)^* \mathrm{d}\tau$$

$$\langle f_m|\hat{A}|f_n\rangle = \langle f_n|\hat{A}|f_m\rangle^*$$

Electron Spin

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$$

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z, \quad \left[\hat{S}_y, \hat{S}_z\right] = i\hbar\hat{S}_x, \quad \left[\hat{S}_z, \hat{S}_x\right] = i\hbar\hat{S}_y$$

$$\left[\hat{S}^2, \hat{S}_x\right] = 0, \quad \left[\hat{S}^2, \hat{S}_y\right] = 0, \quad \left[\hat{S}^2, \hat{S}_z\right] = 0$$

$$\hat{S}^2 f = s(s+1)\hbar^2 f, \quad s = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$$

$$\hat{S}_z f = m_s\hbar f, \quad m_s = -s, -s+1, \ldots, s-1, s$$

$$\hat{S}^2\alpha = \frac{3}{4}\hbar^2\alpha, \quad \hat{S}^2\beta = \frac{3}{4}\hbar^2\beta$$

$$\hat{S}_z\alpha = +\frac{1}{2}\hbar\alpha, \quad \hat{S}_z\beta = -\frac{1}{2}\hbar\beta$$

Coordinate Systems

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta$$

$$r^2 = x^2 + y^2 + z^2$$

$$\cos\theta = \frac{z}{\left(x^2 + y^2 + z^2\right)^{1/2}}, \quad \tan\phi = \frac{y}{x}$$

If $f\left[r(x,y,z), \theta(x,y,z), \phi(x,y,z)\right] = g(x,y,z)$, then

$$\left(\frac{\partial g}{\partial x}\right)_{y,z} = \left(\frac{\partial f}{\partial r}\right)_{\theta,\phi}\left(\frac{\partial r}{\partial x}\right)_{y,z} + \left(\frac{\partial f}{\partial \theta}\right)_{r,\phi}\left(\frac{\partial \theta}{\partial x}\right)_{y,z} + \left(\frac{\partial f}{\partial \phi}\right)_{r,\theta}\left(\frac{\partial \phi}{\partial x}\right)_{y,z}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} r^2\mathrm{d}r\,\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$$