CHEM*3860 Fall 2022 Final Exam Equation Sheet

Professor L. D. Chen

The Schrödinger Equation

$$E_{\mathrm{k}} = h\nu - \phi$$

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

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

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

$$\int_{-\infty}^{\infty}|\psi|^2\mathrm{d}x = 1$$

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

The Particle in a Box

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

$$y = c_1e^{a_1x} + c_2e^{a_2x}$$

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

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

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

Operators

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\int\int\int F(x)G(y)H(z)\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int F(x)\mathrm{d}x\int G(y)\mathrm{d}y\int H(z)\mathrm{d}z$$

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

The Harmonic Oscillator

$$y(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + \cdots = \sum_{n=0}^{\infty}a_nx^n$$

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 + \cdots = \sum_{n=0}^{\infty}x^n$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{n=0}^{\infty}\frac{x^n}{n!}$$

$$\cos cx = 1 - \frac{c^2x^2}{2!} + \frac{c^4x^4}{4!} - \frac{c^6x^6}{6!} + \cdots = \sum_{n=0}^{\infty}(-1)^n\frac{c^{2n}x^{2n}}{(2n)!}$$

$$\sin cx = x - \frac{c^3x^3}{3!} + \frac{c^5x^5}{5!} - \frac{c^7x^7}{7!} + \cdots = \sum_{n=0}^{\infty}(-1)^n\frac{c^{2n+1}x^{2n+1}}{(2n+1)!}$$

$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \cdots = \sum_{n=1}^{\infty}(-1)^{n+1}\frac{x^n}{n}$$

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

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

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

$$E = T + V = 2\pi^2v^2mA^2$$

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

$$\int_{-a}^{+a}f(x)\mathrm{d}x = 2\int_0^a f(x)\mathrm{d}x \quad \text{for } f(x) \text{ even}$$

$$\int_{-a}^{+a}g(x)\mathrm{d}x = 0 \quad \text{for } g(x) \text{ odd}$$

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

$$\psi_1 = \left(\frac{4\alpha^3}{\pi}\right)^{1/4}xe^{-\alpha x^2/2}$$

$$\psi_2 = \left(\frac{\alpha}{4\pi}\right)^{1/4}\left(2\alpha x^2 - 1\right)e^{-\alpha x^2/2}$$

Angular Momentum

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

$$\left[\hat{A}, \hat{A}^n\right] = 0, \quad n = 1, 2, 3, \ldots$$

$$\left[k\hat{A}, \hat{B}\right] = \left[\hat{A}, k\hat{B}\right] = k\left[\hat{A}, \hat{B}\right]$$

$$\left[\hat{A}, \hat{B} + \hat{C}\right] = \left[\hat{A}, \hat{B}\right] + \left[\hat{A}, \hat{C}\right]$$

$$\left[\hat{A} + \hat{B}, \hat{C}\right] = \left[\hat{A}, \hat{C}\right] + \left[\hat{B}, \hat{C}\right]$$

$$\left[\hat{A}, \hat{B}\hat{C}\right] = \left[\hat{A}, \hat{B}\right]\hat{C} + \hat{B}\left[\hat{A}, \hat{C}\right]$$

$$\left[\hat{A}\hat{B}, \hat{C}\right] = \left[\hat{A}, \hat{C}\right]\hat{B} + \hat{A}\left[\hat{B}, \hat{C}\right]$$

$$\sigma(x)\sigma(p_x) \equiv \Delta x\Delta p_x \geq \frac{1}{2}\hbar$$

$$\mathbf{A} = A_x\mathbf{i} + A_y\mathbf{j} + A_z\mathbf{k}$$

$$\mathbf{A} + \mathbf{B} = \left(A_x + B_x\right)\mathbf{i} + \left(A_y + B_y\right)\mathbf{j} + \left(A_z + B_z\right)\mathbf{k}$$

$$c\mathbf{A} = cA_x\mathbf{i} + cA_y\mathbf{j} + cA_z\mathbf{k}$$

$$\mathbf{A}\cdot\mathbf{B} = |\mathbf{A}||\mathbf{B}|\cos\theta = \mathbf{B}\cdot\mathbf{A}$$

$$(\mathbf{A} + \mathbf{B})\cdot\mathbf{C} = \mathbf{A}\cdot\mathbf{C} + \mathbf{B}\cdot\mathbf{C}$$

$$\mathbf{A}\cdot\mathbf{B} = A_xB_x + A_yB_y + A_zB_z$$

$$\mathbf{A}\cdot\mathbf{A} = |\mathbf{A}|^2$$

$$|\mathbf{A}| = \left(A_x^2 + A_y^2 + A_z^2\right)^{1/2}$$

$$|\mathbf{A}\times\mathbf{B}| = |\mathbf{A}||\mathbf{B}|\sin\theta$$

$$\mathbf{A}\times\mathbf{B} = -\mathbf{B}\times\mathbf{A}$$

$$\mathbf{A}\times(\mathbf{B} + \mathbf{C}) = \mathbf{A}\times\mathbf{B} + \mathbf{A}\times\mathbf{C}$$

$$\mathbf{A}\times\mathbf{B} = \left(A_yB_z - A_zB_y\right)\mathbf{i}$$
$$+ \left(A_zB_x - A_xB_z\right)\mathbf{j} + \left(A_xB_y - A_yB_x\right)\mathbf{k}$$

$$\mathbf{grad}\ g(x,y,z) \equiv \nabla g(x,y,z) \equiv \frac{\partial g}{\partial x}\mathbf{i} + \frac{\partial g}{\partial y}\mathbf{j} + \frac{\partial g}{\partial z}\mathbf{k}$$

$$\mathbf{p} \equiv m\mathbf{v}$$

$$\mathbf{L} \equiv \mathbf{r}\times\mathbf{p}$$

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

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

$$\hat{L}_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

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

$$0 \le r \le \infty, \quad 0 \le \theta \le \pi, \quad 0 \le \phi \le 2\pi$$

$$\mathrm{d}\tau = r^2\mathrm{d}r\sin\theta\mathrm{d}\theta\mathrm{d}\phi$$

$$Y_l^m(\theta,\phi) = S_{l,m}(\theta)T(\phi) = \frac{1}{\sqrt{2\pi}}S_{l,m}(\theta)e^{im\phi}$$

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

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

The Hydrogen Atom

$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$$

$$x = x_2 - x_1, \quad y = y_2 - y_1, \quad z = z_2 - z_1$$

$$\mathbf{R} = X\mathbf{i} + Y\mathbf{j} + Z\mathbf{k}$$

$$X = \frac{m_1x_1 + m_2x_2}{m_1+m_2}, \quad Y = \frac{m_1y_1 + m_2y_2}{m_1+m_2}, \quad Z = \frac{m_1z_1 + m_2z_2}{m_1+m_2}$$

$$M \equiv m_1 + m_2, \quad \mu \equiv \frac{m_1m_2}{m_1+m_2}$$

$$H = \frac{p_M^2}{2M} + \left[\frac{p_\mu^2}{2\mu} + V(x,y,z)\right]$$

$$I = \mu d^2$$

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

$$\nu = 2(J+1)B, \quad B \equiv \frac{h}{8\pi^2 I}$$

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r}$$

$$\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi), \quad l = 0,1,2,\ldots, \quad |m| \le l$$

$$-\frac{\hbar^2}{2\mu}\left(R'' + \frac{2}{r}R'\right) + \frac{l(l+1)\hbar^2}{2\mu r^2}R - \frac{Ze^2}{4\pi\epsilon_0 r}R = ER(r)$$

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

$$n = 1,2,3,\ldots, \quad l = 0,1,2,\ldots,n-1,$$

$$m = -l,-l+1,\ldots,0,\ldots,l-1,l$$

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a}\right)^{3/2}e^{-Zr/a}, \quad a \equiv \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$$

Mathematical Relations

Logarithms and Exponentials

$$\ln x + \ln y + \cdots = \ln xy\cdots, \quad \ln x - \ln y = \ln\frac{x}{y}$$

$$a\ln x = \ln x^a$$

$$e^xe^ye^z\cdots = e^{x+y+z+\cdots}$$

$$\frac{e^x}{e^y} = e^{x-y}, \quad (e^x)^a = e^{ax}$$

Derivatives

$$\mathrm{d}(f+g) = \mathrm{d}f + \mathrm{d}g$$

$$\mathrm{d}(fg) = f\mathrm{d}g + g\mathrm{d}f, \quad \mathrm{d}\left(\frac{f}{g}\right) = \frac{1}{g}\mathrm{d}f - \frac{f}{g^2}\mathrm{d}g$$

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \left(\frac{\mathrm{d}f}{\mathrm{d}g}\right)\left(\frac{\mathrm{d}g}{\mathrm{d}t}\right) \quad \text{for} \quad f = f(g(t))$$

$$\left(\frac{\partial y}{\partial x}\right)_z = \left(\frac{1}{(\partial x/\partial y)}\right)_z$$

$$\left(\frac{\partial y}{\partial x}\right)_z\left(\frac{\partial x}{\partial z}\right)_y\left(\frac{\partial z}{\partial y}\right)_x = -1$$

$$\frac{\mathrm{d}x^n}{\mathrm{d}x} = nx^{n-1}, \quad \frac{\mathrm{d}e^{ax}}{\mathrm{d}x} = ae^{ax}, \quad \frac{\mathrm{d}\ln(ax)}{\mathrm{d}x} = \frac{1}{x}$$

$$\mathrm{d}f = g(x,y)\,\mathrm{d}x + h(x,y)\,\mathrm{d}y \text{ is exact if } \left(\frac{\partial g}{\partial y}\right)_x = \left(\frac{\partial h}{\partial x}\right)_y$$

Integrals

$$\int x^n\mathrm{d}x = \frac{1}{n+1}x^{n+1} + C, \quad n \ne -1$$

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

$$\int \frac{1}{ax+b}\mathrm{d}x = \frac{1}{a}\ln(ax+b) + C$$

$$\int e^{-kx}\mathrm{d}x = -\frac{1}{k}e^{-kx} + C$$

$$\int xe^{-kx}\mathrm{d}x = -\frac{1}{k^2}e^{-kx} - \frac{x}{k}e^{-kx} + C$$

$$\int xe^{-kx^2}\mathrm{d}x = -\frac{1}{2k}e^{-kx^2} + C$$

$$\int x^3e^{-kx^2}\mathrm{d}x = -\frac{1}{2k^2}e^{-kx^2} - \frac{x^2}{2k}e^{-kx^2} + C$$

$$\int \sin(kx)\,\mathrm{d}x = -\frac{1}{k}\cos(kx) + C$$

$$\int \sin^2(kx)\,\mathrm{d}x = \frac{1}{2}x - \frac{1}{4k}\sin(2kx) + C$$

$$\int \sin(kx)\cos(kx)\,\mathrm{d}x = \frac{1}{2k}\sin^2(kx) + C$$

$$\int_{-\infty}^{\infty}\cos(kx)\sin(kx)\,\mathrm{d}x = 0$$

$$\int_{-\infty}^{\infty}e^{-a(x+b)^2}\mathrm{d}x = \left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_{-\infty}^{\infty}x^{2n}e^{-\alpha x^2}\mathrm{d}x = \left(\frac{\pi}{\alpha}\right)^{1/2}\frac{(2n-1)!!}{(2\alpha)^n}$$

$$\int_0^{\infty}x^ne^{-kx}\mathrm{d}x = \frac{n!}{k^{n+1}}, \quad n \ge 0, k > 0$$