CHEM∗3860 Fall 2022 Midterm Exam Equation Sheet

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The Schrödinger Equation

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

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

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

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

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

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

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

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

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

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

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

The 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

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

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

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

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

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

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

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

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

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

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

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

The Harmonic Oscillator

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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