

CHEM*3860 Fall 2024 Midterm Exam Equation Sheet

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The Schrödinger Equation

$$E_k = h\nu - \phi, \quad h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s}$$

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

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

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

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

The Particle in a Box

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

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

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

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

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

Operators

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\int |\psi|^2 d\tau = 1$$

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

The Harmonic Oscillator

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

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

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

$$V = \frac{1}{2} kx^2, \quad T = \frac{1}{2} m \left(\frac{dx}{dt} \right)^2$$

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

Angular Momentum

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

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

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

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

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

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

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

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

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

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

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

Mathematical Relations

Logarithms and Exponentials

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

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

$$e^x e^y e^z \dots = e^{x+y+z+\dots}$$

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

Derivatives

$$d(f+g) = df + dg$$

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

$$\frac{df}{dt} = \left(\frac{df}{dg}\right) \left(\frac{dg}{dt}\right) \quad \text{for } f = f(g(t))$$

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

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

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

Integrals

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

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

$$\int e^{-kx} dx = -\frac{1}{k} e^{-kx} + C$$

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

$$\int \sin(kx) \cos(kx) dx = \frac{1}{2k} \sin^2(kx) + C$$

$$\int_{-\infty}^{\infty} \cos(kx) \sin(kx) dx = 0$$

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

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