Chem. 562
Fall 2009

Name Please put your name on all pages.

Exam 1

1. This exam contains 6 pages of questions and instructions, two pages of equations and integrals, a page of tables, a periodic table, and a set of constants and conversion factors.

2. Show your work and make your reasoning clear.

3. You have 1.5 hours to work on the exam.

1.__________/25

2.__________/25

3.__________/25

4.__________/25

Total_______/100

Chem. 562 Name ___________________________

Fall 2009

1a. (13 pts.) Evaluate the commutator $[\hat{A}, \hat{B}]\psi$ for the two operators

$$\hat{A} = \frac{d}{dx} + x \text{ and } \hat{B} = \frac{d}{dx} - x.$$

1b. (12 pts) Use your result from above to determine the uncertainty principle for these two operators using $\Delta\hat{A}\Delta\hat{B} \geq \frac{1}{2}\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle\right|$.

Chem. 562 Name _________________________
Fall 2009

2a. (5 pts.) Using the two eigenfuctions ψ_m and ψ_n, mathematically define orthonormal.

2b. (10 pts.) Prove that the wavefunctions of a Hermetian operator $\hat{A}$ are orthogonal. The definition of a Hermitian operator is

$$\int \psi_m^* \hat{A} \psi_n dx = \int \psi_n \hat{A}^* \psi_m^* dx .$$

Start by using the equations

$$\hat{A}\psi_n = a_n \psi_n \quad \text{and} \quad \hat{A}\psi_m = a_m \psi_m .$$

2c. (10 pts.) Use the boundary conditions for the particle-on-a-ring wavefunction $\psi(\varphi)$ to derive the allowed quantum numbers $m_l = 0, \pm 1, \pm 2, ...$

Chem. 562 Name __________________________

Fall 2009

3. (25 pts.) Consider the particle-in-a-box for a box from x = 0 to x = L that has the eigenfunctions.

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right).$$

3a. (5 pts) Normalize the wavefunction $\Psi(x) = c\psi_1(x) + c\psi_2(x)$, which is a particle with equal probability of being in n=1 and n=2.

3b. (10 pts) Calculate $\langle p^2 \rangle$ for $\psi_1(x)$.

Name ________________________

3c. (5 pts) Consider a box that instead has walls at x = –L and x = +L. Draw the two lowest eigenstates $\psi_1(x)$ and $\psi_2(x)$.

3d. (5 pts) Derive or write the eigenfunction $\psi_1(x)$ that you drew in question 3c above.

4. (25 pts) A particle exists in a rectangular box with infinitely high potentials on all sides. Along the x-dimension the box has straight walls separated by a distance L. Along the y-dimension, the box has curved walls with a potential $V(y)=ky^2/2$.

4a. (5 pts) Write down the 2D Hamiltonian for this system.

4b. (10 pts) Write down the 2D eigenfunctions, eigenenergies, and quantum numbers for this particle.

4c. (10 pts) Draw the wavefunction as a contour plot for the particle that has been excited by <u>one</u> quantum along x but is in its <u>ground</u> state along y. Also draw the projections of the wavefunction along the x and y axes.