Chemistry 562 **Spring 2012**

Problem Set 3

Due beginning of class on Friday, February 10

(Make your reasoning clear. We need to understand your reasoning, not just see the final result.)

1. Recall the normalized first excited (υ=1) wave function for the quantum harmonic oscillator from the last problem set,

$$\psi_1(x) = \sqrt{\frac{1}{2\alpha\sqrt{\pi}}}\,\frac{2x}{\alpha}\cdot e^{\frac{-x^2}{2\alpha^2}}$$

(a.) Find $\langle x \rangle$

(b.) Find $\langle p^2 \rangle$

(c.) Using (a.) and (b.) and the results from Problem Set 2, Problem 2, calculate

(i.) $(\Delta x)^2$

(ii.) $(\Delta p)^2$

(d.) Find $\Delta x \Delta p$ for $\alpha = \left(\frac{\hbar^2}{mk}\right)^{\frac{1}{4}}$. Does this result satisfy the Heisenberg Uncertainly Principle?

2. *Problem* 8.32 (Make life simple by assuming κ and L are large enough that you can treat the barrier as being "high and wide.")

3. For a normalized wave function

$$\psi(x) = c_1\psi_1(x) + \frac{1}{\sqrt{8}}\psi_2(x) + \frac{1}{\sqrt{2}}\psi_3(x)$$

where ψ_1(x), ψ_2(x), and ψ_3(x) are the normalized eigenfunctions of $\hat{H}$.

(a.) Solve for c_1.

(b.) Calculate $\langle E \rangle$ in terms of E_1, E_2, and E_3. Show all your work.

(c.) If we measure the energy of a single system, what is the probability that we will obtain E_1?

4. You can use the “living graphs” feature for Chapter 8 on the textbook website (there is a link on our course webpage) to examine the plots required to answer these questions.

   (a.) Examine the ground state and first two excited state wave functions of the particle in a 1-D box for L=10 nm. How does the number of nodes in the wave function change with increasing n? How does the magnitude of the wavefunction vary as the box size varies? Physically, why should it do that? What is the energy of the ground state? (use the mass of an electron) Why isn't it zero?

   (b.) Examine the surface plots of all the wave functions for the first and second energy levels of the 2-D particle in a box for L_x = 10 nm and L_y = 10 nm. What is the degeneracy of the second energy level? Give the quantum numbers, n_x and n_y, for the two degenerate states at that energy. Explain whether or not those same states would be degenerate if L_x = 10 nm and L_y = 15 nm?

   (c.) How does the number of nodes in the x-coordinate change as n_x increases? How does the number of nodes in the y-coordinate change as n_x increases?