Chemistry 30321 Fall 2012
Professor J. Daniel Gezelter Due Mon. 11/12/2012

Problem Set 8
(Hydrogen and The Variational Method)

1. This problem deals with the non-classical behavior of the hydrogen atom which has an electron in the 1s orbital.

   a) Find the classical turning point (i.e. the turning radius, r_t) for an electron in the 1s state. To do this, you'll need to use both the total energy of this state as well as the potential energy between the electron and proton. Leave your answer in terms of the Bohr radius, a_0.

   b) The radial function for an electron in the 1s orbital of Hydrogen is given by

   $$R_{1s}(r) = \frac{2}{a_0^{3/2}} e^{-r/a_0}$$

   Using this function, determine the probability of finding the electron at a radius which is *outside* the classical turning point.

2. For the harmonic oscillator, the Hamiltonian is

   $$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

   and the ground state energy is given by $E_0 = \hbar\omega/2$. Approximate the energy of the ground state of the harmonic oscillator by using the **variational principle**. Use a trial function of the form $\phi(x;\alpha) = exp(-\alpha x^2)$ where α is the parameter to be varied.

3. Repeat problem 2 with a trial function of the form

   $$\phi(x;\beta) = \frac{1}{x^2 + \beta^2}$$

   where β is the variational parameter. You will need a good table of integrals (i.e. Wolfram Alpha or Mathematica) to do this problem.

4. Why is the variational estimate for the ground state energy in problem 2 so much better than the result for problem 3?

5. Extra Credit: Use a trial wavefunction for the ground state of Helium, (neglecting the spin), which is

   $$\phi(\vec{r}_1, \vec{r}_2) \propto e^{-\alpha r_1} e^{-\alpha r_2}$$

   where $\vec{r}_1$ and $\vec{r}_2$ are the coordinates of the two electrons relative to the nucleus, and α is a variational parameter, to determine an estimate for the ground state energy of helium.