HW #5 Chem 2430

1. Show that $\frac{\sin(kr)}{r}$ is a solution of the particle in the spherical box. (v = 0 inside, = ∞ outside) What are the energies if the box has radius r_0 ?

2. For an H atom in the 1s orbital, what is the probability of the electron being in the classically forbidden region?

3. What would the energy of the Helium atom be if the two electrons did not interact?

What is the wave function, ψ_{NI} , where NI DENOTES non-interacting?

Now suppose the electrons interact via a $V_0\,\delta(r_1\text{-}r_2)$ potential. Estimate how the interaction impacts the energy by evaluating $\langle \psi_{NI} | V | \psi_{NI} \rangle$.

4. Fit the $2p_z$ orbital of the H atom to Are^{-Br^2} and to $Are^{-Br^2} + Cre^{-Dr^2}$. You should be able to do this with www.mycurvefit.com. If you have trouble with this, don't spend a lot of time.

5. For the H atom suppose that for $r \le r_0$ the Coulomb potential is replaced by $-1/r_0$ (in atomic units) for $r \le r_0$. If r_0 is chosen to be,1.7x10^{-5}au, the radius of the proton, how much does the finite size of the proton change the energy of the 1s orbital of the H atom. Use first order PT as discussed in class.