HW problem week 9

A Helium atom is the second simplest atom after hydrogen: it has two electrons surrounding a nucleus of two protons and two neutrons. Unfortunately, the second simplest atom is impossible to solve exactly! Therefore we will study a model which makes some approximations, yet obtains very good agreement with experiment.

1. What is the Hamiltonian for the helium atom? You can leave it in terms of $\hat{p}_1$ and $\hat{p}_2$, i.e. dont write out the whole spherical laplacian expressions.

2. Neglecting the coulomb energy between the two electrons, what is the ground state energy of this system? How does it compare with the experimental value of -78.98 eV?

3. We can obtain a better estimate for the ground state energy by assuming that the wavefunctions for each electron are of the hydrogen type - $\psi = C_{100}e^{-rZ/a_0}$ - and calculating the expectation value of the energy now including the coulomb energy between the two electrons. Show that the potential energy due to the electron-electron interaction makes a contribution $5ke^2/4a_0$ to the energy. What is the new ground state energy?

   Hint: the following integral may be useful :

   $$\int dr_1 d\theta d\phi \, \frac{r_1^2 \sin\theta e^{-2r_1}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta}} = \frac{\pi}{r_2}\left(1 - e^{-2r_2}(1 + r_2)\right)$$

   Hint: it will be helpful for part 4 to leave your answer in terms of Z until the end.

4. In the previous part, we calculated the energy using the unperturbed hydrogenic wave functions. In reality, there are two electrons, and each electron partially ‘screens’ the nuclear charge from the other electron. We can take this into account by modifying the wavefunction to e^{-rZ_{eff}/a_0} for some $Z_{eff} < 2$. Calculate the expectation value of the energy in this state, as a function of Z_{eff}.

   Hint: by writing the Hamiltonian as

   $$p_1^2/2m + p_2^2/2m - kZ_{eff}e^2(1/r_1 + 1/r_2) - (Z - Z_{eff})ke^2(1/r_1 + 1/r_2) + V_{e-e}$$

   you can maximize your ability to use previous results and only need to do one integral.

5. Find the value of Z_{eff} which minimizes the total energy. How does your final result for the ground state energy compare with the correct value? Describe qualitatively

the effect of this modification on the electron wave function, and how the kinetic and potential energies of this new trial wavefunction compare to those with $Z = 2$.