CHM 3411, Dr. Chatfield, Spring 2018
Problem Set 7
Due Monday, March 5

Suggested "warmups" (not to turn in): Discussion questions 9B.1-3, 9C1-3; Exercises [(b) unless otherwise specified]] 9B.1,2; 9C.1,2,4,5,8,9,10

These problems explore multi-electron atoms.

1. Multiply out the Slater determinant for the ground state of Lithium. Demonstrate that it is antisymmetric with respect to the exchange of at least one pair of the three electrons (it needs to be antisymmetric with the respect to the exchange of any pair).

2. In this problem, Spartan is used to calculate Z_{eff} (effective nuclear charge) and σ (shielding constant) for Ne.

   BACKGROUND: When only one electron is present in an atom, the energies are given by:

$$E_n = \frac{-m_e e^4}{32\pi^2 \epsilon_o^2 \hbar^2} \cdot \frac{Z^2}{n^2}\ Joules = \frac{-Z^2}{2n^2} Hartrees$$

   [This problem will be much easier if you use the expression in Hartrees (atomic energy units).] In a multi-electron atom, electrons shield each other from the nucleus, resulting in an effective nuclear charge of $Z_{eff}e$ where $Z_{eff} = Z - \sigma$ and σ is the shielding constant. The equation for E_n above *does not hold* for multi-electron atoms, but E_n can be determined approximately as the orbital energies calculated for an atom with Spartan. Z_{eff} can then be determined from atomic orbital energies using $E_n = \frac{-Z_{eff}^2}{2n^2}$ where E_n is the orbital energy and the units are Hartrees.

   PROBLEM: With Spartan, do an Energy calculation for a single Neon atom. Use the Hartree-Fock method with the 6-31G* basis set. Check the Print option for Orbitals & Energies. In the output, identify the energies of the five lowest-energy orbitals (given in units of Hartrees in the line "Eigenvalue," which you have used before).

   (a) Make images of the five lowest-energy orbitals, save them as screen shots, and copy them to your homework. Labelling the orbitals (1s, 2s etc), identifying any that are degenerate.
   (b) Determine Z_{eff} and σ from the orbital energies, and discuss the values. Are they what you would expect?

   NOTE: The Hartree-Fock method gives meaningful results for this problem, but it is not exact.

3. Suppose you have a friend who is a sophomore majoring in physics. Explain the concept of spin correlation to her.

4. Exercise 9C.3(b)

5. Exercise 9C.5(b)

6. Exercise 9C.11(b)

7. Exercise 9C.12(b)

8. Problem P9C.2

9. Problem P9C.4