Exam 2: Theory of Atomic Structure

Due Nov. 20, 2000

You may use any resource you like to complete this exam including computers, Mathematica, integral tables, and the text. If you do, make sure you cite that resource. You are, however, to complete this exam on your own. Any plots should be computer generated.

This exam is due promptly at the beginning of class Monday, Nov. 20. No exceptions will be made.

1. (a) Using your Hartree-Fock program for the singlet states of a two-electron atom, calculate the ground state of H^-. What do you find for the total energy? Is H^- bound in this approximation?
   (b) Examine the orbital you calculated in (a). How does it behave at small r? At large r? Does this behavior match your expectations?
   (c) Using Hartree-Fock single particle wave functions [from (a)], perform a CI calculation to determine which configurations are needed to yield a bound state. Use (and state) any physical insight to choose the most important configurations and thus minimize your computational effort.
   (d) To what term, ${}^{2S+1}L$, do these configurations correspond? Assuming the same configurations are important for the ground state of He, what states (configurations and terms) are accessible by an electric dipole transition?

2. Show that Eq. 8-3 holds for a properly symmetrized two-electron wave function.

3. (a) What is the ground state configuration of N?

   Assuming that L-S coupling holds,
   (b) List the possible terms ${}^{2S+1}L$ that result from the ground state configuration.
   (c) List the corresponding fine structure terms ${}^{2S+1}L_J$.
   (d) Draw these terms on an energy level diagram. Does the ground state term agree with Hund's rules?

4. Including spin-orbit effects, what is the J value of the lowest energy ${}^3P$ state of He? What are the terms of the states to which this state can decay? Hint: Write out the wave function explicitly in the independent particle approximation including especially the angular momentum part of the wave function.