Problem Set 11
To be returned before class on Wednesday, December 2, 2015 (give to me in person or slide under office door).

1. Atomic Term Symbols:
   a.) Consider the ground state electron configuration of oxygen O(1s)²(2s)²(2p)⁴. You could of course couple the four \( p \) electrons in a rather lengthy microstate table. Instead, think of what’s missing to get a full \( 2p \) subshell: two holes. You can view holes in an electron configuration as particles with spin \( \frac{1}{2} \) and the same \( \ell \) as the missing electrons). With that in mind, construct the possible term symbols of the ground state configuration of oxygen. (4 credits)
   b.) Consider the N(1s)²(2s)²(2p)³ ground state configuration in nitrogen. Construct all possible term symbols corresponding to this configuration. (4 credits)
   c.) Consider an excited state configuration for Ne: (1s)²(2s)²(2p)⁵(3s). Construct all possible term symbols. Give the energetic order of the excited states according to Hund’s rules (note, however, that Hund’s rules apply strictly only for the ground state). (4 credits)

2. Spin-Orbit Interaction
   a.) Prove the relation we used implicitly in class that
   \[
   \vec{S} \cdot \vec{L} = \frac{1}{2} (\vec{J}^2 - \vec{L}^2 - \vec{S}^2)
   \]
   Sketch the vectors first, so you get some geometric insight how to proceed. (3 credits)
   b.) How large is the magnetic field at the proton generated by the electron, if you assume that the electron orbits classically as given by the Bohr model? (3 credits)
   c.) Assume that the expectation value of the inverse cubed radius in the H-atom is given by
   \[
   \left\langle \frac{1}{r^3} \right\rangle = \frac{Z^3}{n^3 a_0^3 \ell (\ell + \frac{1}{2}) (\ell + 1)}
   \]
   Calculate the spin-orbit splitting in all possible states of the H-atom for \( n = 2 \) and \( n = 3 \). (3 credits)
3. Electron-electron repulsion in the He atom:
The Hartree-Fock method treats each electron as moving in an effective potential generated by the averaged electron density of all other electrons. Let’s get an explicit expression for the effective potential of one electron in the averaged field of the other for the ground state of He, using H-functions. The wave function of a $1s$ orbital in a H-like ion with nuclear charge $Z$ is given by

$$\psi_{1s} = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0},$$

and the distance between the two electrons, $r_{12}$ can be expanded in spherical harmonics as

$$\frac{1}{r_{12}} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell + 1} \frac{r_\ell}{r_>^{\ell+1}} Y_\ell^m(\theta_1, \varphi_1) (Y_\ell^m(\theta_2, \varphi_2))^*,$$

where $r_>$ is the larger of $r_1$ and $r_2$, and $r<$ is the lesser. Use this to calculate the effective potential of electron 1 in the average field of electron 2 as a function of $r_1$. No other variables (only natural constants) may appear in the result. Hint: Interpret the effective potential as the average value of the electron-electron repulsion.  

(6 credits)