CHEM 550 Problem Set #7

Due Mon Nov 30 at 5pm –*put in Erin Riley's mailbox*

Levine Exercises:

10.18 Spin functions

11.30 Terms, levels, states of carbon

Additional Problems

Spin

1) a) Write out all of the allowed wave-functions for the first **excited** state of the He atom including electron spin as single products of a spatial term and a spin term (as we did in lecture). Which functions correspond to triplet states and which to singlet states. Explicitly apply the $S_{z\text{-total}}$ operator ($S_{z\text{-tot}} = S_{z1} + S_{z2}$) to find the z-projection of the spin angular momentum for each of these states.

b) List 5 particles that are Fermions. List 5 that are Bosons. (Google is fair game if you don't happen to know this many particles off the top of your head!). What (if any) trends do you notice as far categories the 'fundamental' particles.

Term symbol practice

1) **Derive** (do not just state) the possible term symbols for the $1s^2 2s^2 2p^3$ configuration of a nitrogen atom.

Qualitative Material

2) a) Explain (1-3 sentences) why the Hartree-Fock SCF method doesn't obtain the exact ground state energy even though it incorporates an interelectron repulsion term into the Hamiltonian.

b) Explain why the energy of an orbital depends on l for electrons in atoms other than hydrogen (1-3 sentences)? Annotate your discussion with a *plot* of the radial wave functions for 3s, 3p and 3d.

c) Rationalize why, all other things being equal, parallel (unpaired) spins *generally* (not always) produce states of lower energy that states with antiparallel (paired) (*Hund's rule*) (again 1-3 sentences)