PHY801: Survey of Atomic and Condensed Matter Physics
Michigan State University

Homework 3

3.1. Consider an open-shell atom with 4 electrons in the p-shell (p^4), such as the oxygen atom.

(i) What is the total number of configurations? Just give the number.

(ii) What are the different multiplets $^{2S+1}L_J$ for this open-shell atom? Give their degeneracies.

(iii) What is the lowest-energy multiplet according to the Hund's 1st rule (ignore the spin-orbit interaction)?

(iv) What is the lowest energy multiplet after the spin-orbit interaction is considered ($H_{so} = \lambda_{so}\vec{L}\cdot\vec{S}$)?

(v) What is the spin-orbit splitting?

3.2. Using Hund's three rules, work out the lowest energy multiplets of d^1, d^3, d^4, d^7 and f^1, f^3, f^7. Compare your results given in Table 1 and 2 of the Chapter on Diamagnetism and Paramagnetism in Kittel (Ch. 14 in 7th edition, Ch. 11 in 8th edition). Next, calculate the Landé g-factors associated with these lowest-energy multiplets. (Once you know how to do it for a few cases, it should be straight-forward to do the rest.)

3.3. The wave function of the hydrogen atom in its $1s$ ground state is $\psi = (\pi a_B^3)^{-1/2} exp(-r/a_B)$, where a_B is the Bohr radius. Show that for this state $< r^2 >= 3a_B^2$ and calculate the diamagnetic susceptibility for 1 mole of atomic hydrogen enclosed in unit volume. The correct answer is 2.32×10^{-6} cm^3/mole.

3.4. Consider the multiplet (L, S, J). Show that the average magnetization $< M >$ for N atoms the presence of an external uniform magnetic field B along the z direction is given by

$$< M >= N\mu_B g_J J B_J(x) \, ,$$

where

$$x = g_J \mu_B J B / k_B T$$

and

$$B_J(x) = \frac{2J+1}{2J} \coth\left(\frac{(2J+1)x}{2J}\right) - \frac{1}{2J} \coth\left(\frac{x}{2J}\right)$$

is the Brillouin function.
