Atomic & Molecular Physics Problem Sheet 2224.2
Issued Thursday 7 February 2008, due Thursday 14 February 2008

1. If the electron spin wavefunctions that are simultaneous eigenstates of $\hat{s}^2$ (spin) and $\hat{s}_z$ (z-component of spin) are denoted as α and β, for spin 'up' and spin 'down' respectively, write out the results of operating with $\hat{s}^2$ and $\hat{s}_z$ on each of α and β.

   Make two-electron wavefunctions by writing down the possible combinations of $\alpha(i)$ and $\beta(i)$ for electron number $i = 1, 2$. Find the $z-$components of *total* spin, $\hat{S}_z = \hat{s}_{z_1} + \hat{s}_{z_2}$ for each of these two-electron wavefunctions, and hence group them into a spin singlet and a spin triplet.

   Explain qualitatively how the exchange interaction leads to a difference in the energies of spin singlet and spin triplet states in helium. **[10]**

2. Explain the central field approximation and why it is a useful description for atoms that have a single optically active electron. How is the quantum defect used in this model? What trends are observed for the value of the quantum defect with quantum numbers n and l?

   The element magnesium (Mg) has atomic number $Z = 12$. Write out the electronic configuration for the ground state of singly ionised magnesium, Mg^+. Why might you expect the central field model to produce a good approximation to the energy levels of Mg^+?

   The table below gives the energies of a number of transitions nd $\rightarrow$ 3s in Mg^+. By plotting a suitable graph determine how much energy is needed to completely remove an electron from Mg^+. **[10]**

n	$E_{n\mathrm{d}\rightarrow 3\mathrm{s}}/\mathrm{cm}^{-1}$
3	71 491
4	93 311
5	103 420
6	108 900
7	112 197
8	114 332
9	115 794
10	116 838

3. State Hund's Rules for the ordering of the energies of terms according to the values of spin, S, orbital, L, and total, J, angular momentum in a given electronic configuration.

   The element aluminium has atomic number $Z = 13$. Write out the electronic configuration for the ground state of aluminium.

   Now deduce the possible term symbols for this configuration, and use Hund's Rules to arrange them in order of energy from lowest to highest.

   Now write out the configuration for singly ionised aluminium, Al^+ in the ground state. What are the possible terms? (*Hint: You may find it useful to consider the allowed terms for helium known from the lectures*) **[10]**