QM 15-030-710-003 Spring 1999
Final: Particle Identity, Atoms
Monday, May 3

1. (15 points) The electron configuration of Cl^+ is ,

$$(1s)^2\,(2s)^2\,(2p)^6\,(3s)^2\,(3p)^4$$

Find the normal state of this ion.

Solution

For p-states

$$\begin{array}{ccc} (a)\,1,\frac{1}{2} & (b)\,0,\frac{1}{2} & (c)-1,\frac{1}{2} \\ (a')\,1,-\frac{1}{2} & (b')\,0,-\frac{1}{2} & (c')-1,-\frac{1}{2} \end{array}$$

Possible (non-negative) pairs of $M_L = \sum m$ and $M_S = \sum \sigma$ are as follows:

$$\begin{array}{cc} \left(a+a^{'}+b+b^{'}\right) & 2,0 \\ \left(a+a^{'}+b+c\right) & 1,1 \\ \left(a+a^{'}+b+c^{'}\right) & 1,0 \\ \left(a+a^{'}+b^{'}+c\right) & 1,0 \\ \left(a+b+b^{'}+c\right) & 0,1 \\ \left(a+b+b^{'}+c^{'}\right) & 0,0 \\ \left(a+a^{'}+c^{'}+c\right) & 0,0 \\ \left(b+c+a^{'}+b^{'}\right) & 0,0 \end{array}$$

so that the possible terms are ^1D: (2, 0), (1, 0), (0, 0), ^3P: (1, 1), (0, 1), (1, 0), (0, 0), and ^1S: (0, 0). By Hund's rule, the ^3P term has the lowest energy. Since the shell is more than half full, the term $^3P_2$ has the lowest energy in the multiplet ($^3P_0$, $^3P_1$, $^3P_2$).

2. (15 points) Using the Thomas-Fermi model, find the dependence on Z of

   a) Interaction energy of electrons with the nucleus;

   b) Total energy of the electron-electron interaction;

   c) Total kinetic energy of all electrons.

Hint: Find the dependence on Z of the typical electron distance from the nucleus and typical momentum.

Solution

Let ℓ be the characteristic scale for electrons in the atom. From

$$\nabla^2\phi \sim \frac{\phi}{\ell^2} \sim \phi^{3/2}$$

find

$$\phi \sim \ell^{-4}$$

On the other hand,

$$Z \sim n\ell^3 \sim \phi^{3/2}\ell^3 \sim \ell^{-3}$$

so that

$$\ell \sim Z^{-1/3}$$

Typical momentum

$$p \sim n^{1/3} \sim \phi^{1/2} \sim \ell^{-2} \sim Z^{2/3}$$

and typical kinetic energy

$$T \sim Z\frac{p^2}{2} \sim Z^{7/3}$$

Interaction energy of electrons with nucleus

$$U_{en} \sim -Z\frac{Z}{\ell} \sim -Z^{7/3}$$

Electron-electron interaction

$$U_{ee} \sim Z^2\frac{1}{\ell}$$

where Z^2 counts the number of electron-electron pairs (more precisely, $Z(Z-1)/2 \approx Z^2/2$ for $Z \gg 1$) and $1/\ell$ is the typical interaction energy between any two electrons.

3. (15 points)

   A system of two identical particles has a zero relative angular momentum, $L = 0$. What is the total spin of the system for

   a) Two $s = 0$ bosons;

   b) Two $s = 1$ bosons;

   c) Two electrons.

   Solution

   The interchange of two identical particles is identical to the coordinate inversion. The parity of a state with the angular momentum L is $(-1)^L$. On the other hand, when the particles are interchanged, the coordinate WF is multiplied by the factor of $(-1)^S$, where S is the total spin. Consequently, for a given L, the possible values of S are

$$\begin{array}{ll} L = 0, 2, 4, \ldots & S = 2s, 2s-2, \ldots, 0 \\ L = 1, 3, 5, \ldots & S = 2s-1, 2s-3, \ldots, , 1 \end{array} \quad \text{bosons}$$

$$\begin{array}{ll} L = 0, 2, 4, \ldots & S = 2s-1, 2s-3, \ldots, , 1 \\ L = 1, 3, 5, \ldots & S = 2s, 2s-2, \ldots, 0 \end{array} \quad \text{fermions}$$

   In particular, for $L = 0$ the coordinate function is symmetrical which is also the case for spinless bosons. For $s = 1$ bosons, the coordinate function is symmetrical for $S = 2$ and $S = 0$. For electrons, the coordinate function is symmetrical when the spin function is anti-symmetrical, that is for $S = 0$.