Quadrant II – Transcript and Related Materials

Programme: Bachelor of Science (Third Year)

Subject : Physics

Course Code: PYC 108

Course Title : DSC: Atomic and Molecular Physics

Unit : Many Electron Atoms

Module Name: Electron configuration, Hund's rule, Spin orbit interaction, Vector atom model

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Notes :

Electron configuration

Electronic configuration of an atom is the distribution of electrons around the nucleus of the atom. Shells are denoted by capital letters according to the following scheme:

n = 1	2	3	4	5	. . .
K	L	M	N	O	. . .

Each subshell is identified by its principal quantum number n followed by the letter corresponding to its orbital quantum number l.

l = 0,	1,	2,	3,	4,	5,	…….
s,	p,	d,	f,	g,	h,	…….

If an electron is in a shell for which l = 0, it is called s electron; for l = 1, a p electron and so on.

A subscript after the letter indicates the number of electrons in that subshell.

For example, the electron configuration of sodium is written

$1s^2 2s^2 2p^6 3s^1$

Which means that the 1s (n = 1, l = 0) and 2s (n = 2, l = 0) subshells contain two electrons each, the 2p (n = 2, l = 1) subshell contains six electrons, and the 3s (n = 3, l = 0) subshell contains one electron.

The electron configuration of a few elements:

1) Hydrogen : $1s^1$
2) Helium :$1s^2$
3) Lithium : $1s^2 2s^1$
4) Beryllium : $1s^2 2s^2$
5) Boron : $1s^2 s^2 2p^1$

The **aufbau principle** states that in the ground state of an atom, electrons fill atomic orbitals of the lowest available energy levels before occupying higher levels. In neutral atoms, the approximate order in which subshells are filled is given by the *n + ℓ rule*,

Orbitals with a lower *n + ℓ* value are filled before those with higher n + ℓ values. In the case of equal *n + ℓ* values, the orbital with a lower *n* value is filled first.

For example, in copper (Z= 29) , the 4s orbital ($n + \ell = 4 + 0 = 4$) is occupied before the 3d orbital ($n + \ell = 3 + 2 = 5$). The rule then predicts the electron configuration $1s^2 2s^2 2p^6 3s^2\ 3p^6 3d^9 4s^2$.

Hund's rule :

The electrostatic potential energy of the system in the case of parallel spins is smaller than that in the case of antiparallel spins. As the tendency of any system is to have the least energy, the electrons in an atom tend to remain unpaired, i.e. they have parallel spins. This is known as Hund's rule. The ferromagnetism of iron, cobalt and nickel (Z = 26, 27,28) is in part a consequence of Hund's rule. The 3d subshells of their atoms are only partially occupied, and the electrons in these subshells do not pair off to permit their spin magnetic moment to cancel out. In iron, five out of the six 3d electrons have parallel spins, so that each iron atom have a large resultant magnetic moment.

The spin -orbit interaction:

Hydrogen spectrum could not be fully accounted on the basis of the Bohr atom model. H_α line of Balmer series of hydrogen is found to be doublet, the separation between the components being about 1.14 A^0. According to Bohr atom model, it should be a single line.

Fine structure of a spectral line is observed also in the case of other elements. The cause of fine structure is the spin-orbit interaction. Spin orbit interaction is an interaction between an electron's spin magnetic moment and the internal magnetic field of the atom which arises from the orbital motion of the electron.

In the reference frame of the electron the nucleus is seen orbiting the electron. As the positively charged nucleus orbits the electron it creates a positive current loop that in turn creates a magnetic field B. Each electron has an intrinsic property called electron spin that induces a spin angular momentum. The electron spin also creates a spin magnetic dipole moment $\mu_{s.}$ the spin magnetic dipole moment μ_s of electron experiences a torque due magnetic field B created by the orbit of the nucleus. This torque tends to rotate the spin magnetic dipole moment and thus change the energy of the electron.

When a magnetic dipole of magnetic moment μ is placed in a magnetic field of induction B the energy of the dipole is given by $U_m = - \mu . B = - \mu B \cos\Theta$ where Θ is the angle between the vectors μ and B. The quantity $\mu\cos\Theta$ is the component of μ parallel to B .

When we consider the magnetic moment associated with the spin of the electron, we have $\mu\cos\Theta = \pm \frac{e\hbar}{2m}$.

Thus $U_m = \pm \frac{e\hbar}{2m} B$.

$U_m = 0$ in absence of spin-orbit coupling.

Due to spin-orbit coupling, energy of the electron changes by $\pm \frac{e\hbar}{2m}$ B depending upon the orientation of the spin angular momentum. Each energy level is split into two levels. If a quantum state has energy E in the absence of spin-orbit coupling, Now it can have two values E + $\frac{e\hbar}{2m}$ B or E - $\frac{e\hbar}{2m}$ B.

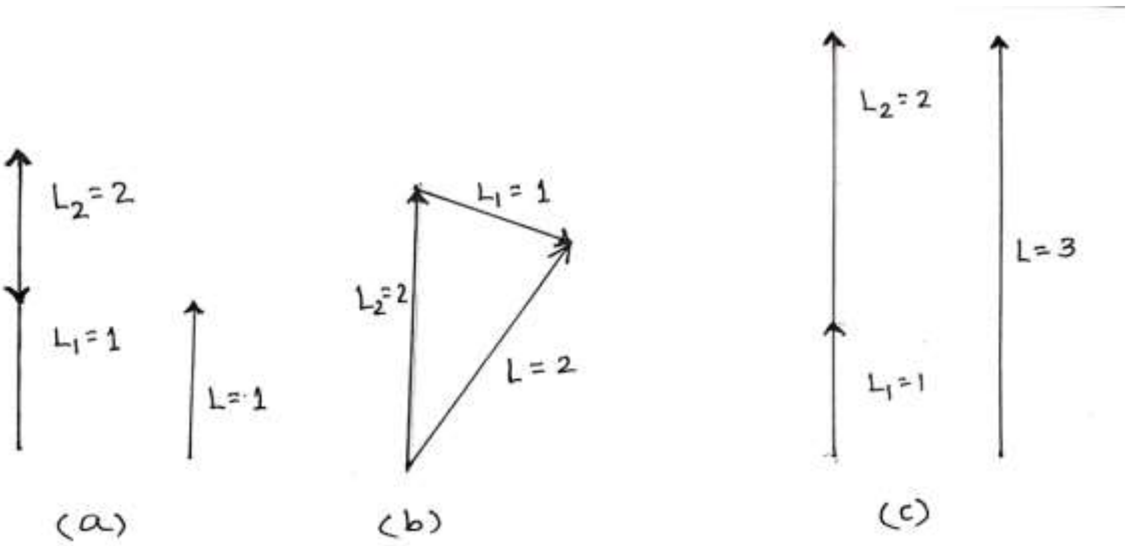
Vector Atom Model :

An electron in an atom has orbital as well as spin motion. According to quantum theory, the orbital and spin motions are both quantized in magnitude and direction. Hence they are considered as quantized vectors. Hence the atom model based on those quantized vectors is called the vector atom model to which vector laws apply.

In case of one electron systems like hydrogen atom or any other atom in which only one electron contributes to the angular momentum and hence to the magnetic moment of the atom, we have orbital angular momentum $l\sqrt{l(l+1)}\,\hbar$ and spin angular momentum of magnitude $s\sqrt{s(s+1)}\,\hbar$.

In the case of two electron systems, there will be two orbital angular momenta $l_1\sqrt{l_1(l_1+1)}\,\hbar$ and $l_2\sqrt{l_2(l_2+1)}\,\hbar$ and two spin angular momenta $s_1\sqrt{s_1(s_1+1)}\,\hbar$ and $s_2\sqrt{s_2(s_2+1)}\,\hbar$ of the two electrons. Vector atom model helps to find the resultant angular momentum of the atom.

For many electron atoms, the total angular momentum ($\vec{L}$) of an atom is given by the vector sum of the orbital angular momenta of all the electrons in the atom. i.e. $\vec{L} = \vec{L}_1 + \vec{L}_2 + \vec{L}_3 + \ldots\ldots\ldots$ with the condition that L can have only integral values. For example, For $L_1 = 1$ and $L_2 = 2$, the allowed values of L are 1,2 and 3. The spin quantum number is always $\pm\frac{1}{2}$, so that there are two possibilities for the sum S_1+S_2 , S =0 or S =1. J can have all the values from L+S to L-S. Thus J can have values 0,1,2,3,4 .



(a) $\overrightarrow{L_1}$ and $\overrightarrow{L_2}$ in opposite directions

(b) $\overrightarrow{L_1}$ and $\overrightarrow{L_2}$ inclined to each other

(c) $\overrightarrow{L_1}$ and $\overrightarrow{L_2}$ in the same direction