Quadrant II- Transcript and Related Materials

Programme : Bachelor of Science (Third Year)

Subject : Physics

Paper Code : PYC-108

Paper Title : DSC: Atomic and Molecular Physics

Unit I : Hydrogen Atom

Module Name : Spin, magnetic moment, J and mj, Angular momentum.

Name of the Presenter : Mandakini Kundaikar, Associate Prof. PESRSN College of Arts and Science, Farmagudi, Goa.

Notes :

Applications of Quantum numbers:

Total quantum number n=1,2,3,4,------------

Orbital quantum number l=0,1,2,3,----------(n-1)

Orbital magnetic quantum number m_l =0,±1, ±2,----±l

1) Total quantum number n:

Electron energy is constant and it should have –ve value to remain in the orbit.

$$E_n = \frac{-me^4}{32\,\pi^2 \quad \epsilon_0^2\,\hbar^2}\left(\frac{1}{n^2}\right)$$

$$E_1 = \frac{-me^4}{32\,\pi^2 \quad \epsilon_0^2\,\hbar^2}(\frac{1}{1^2})$$

$$E_2 = \frac{-me^4}{32\,\pi^2 \quad \epsilon_0^2\,\hbar^2}(\frac{1}{2^2})$$

Hence Energy of the electron is quantized. The quantization of electron energy in the hydrogen atom is therefore described by the total quantum number n.

Orbital quantum number l :

Expression for Orbital angular momentum:

Differential equation for the radial part R(r) of the wave function is

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + [\frac{2m}{\hbar^2}(\frac{e^2}{4\pi \epsilon_0\, r} + E) - \frac{l(l+1)}{r^2}]R = 0\_\_\_\_\_1$$

Kinetic energy $\mathrm{T} = \mathrm{T}_{\mathrm{radial}} + \mathrm{T}_{\mathrm{Orbital}}$

Potential energy $V = -\frac{e^2}{4\pi\epsilon_0 r}$

Hence total energy$E = T_{radial} + T_{orbital} - \frac{e^2}{4\pi \epsilon_0\, r}$

Therefore equation 1 becomes

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2m}{\hbar^2}[T_{radial} + T_{Orbital} - \frac{\hbar^2 l(l+1)}{2mr^2}]R = 0 \;\_\_\_\_\_\_2$$

If

$$T_{Orbital} = \frac{\hbar^2 l(l+1)}{2mr^2}$$

Then equation 2 will have
only R(r) which is a function of r only.

Consider

$$T_{Orbital} = \frac{\hbar^2 l(l+1)}{2mr^2}$$

Angular momentum, $\mathrm{L} = \mathrm{mv_{orb}r}$

$$\text{Therefore}\ , \mathrm{T_{Orbital}} = \frac{\mathrm{L}^2}{2\mathrm{mr}^2} = \frac{\hbar^2 l(l+1)}{2\mathrm{mr}^2}$$

$$L^2 = \hbar^2 l(l+1)$$

$$L = \hbar\sqrt{l(l+1)}$$

Since $l = 0, 1, 2, 3 - - -$

States: s, p, d, f ------

s state has no angular momentum because $l = 0$

l=1 means p state which has angular momentum
$L = \hbar\sqrt{2}$
l=2. Is a d state, which has angular momentum

$L = \hbar\sqrt{6}$

Hence angular momentum is quantized . Quantization of angular momentum is described by orbital quantum number l.

Space quantization :

Magnitude of angular momentum is quantized and is given by $L = \hbar\sqrt{l(l+1)}$ Where l= 0, 1,2,3-------

Direction of L is also quantized with respect to an external magnetic field. This is referred to as **space quantization.** The magnetic quantum number m_l specifies the direction of L by determining the component of L in the field direction . ie. $L_z = m_l\hbar$

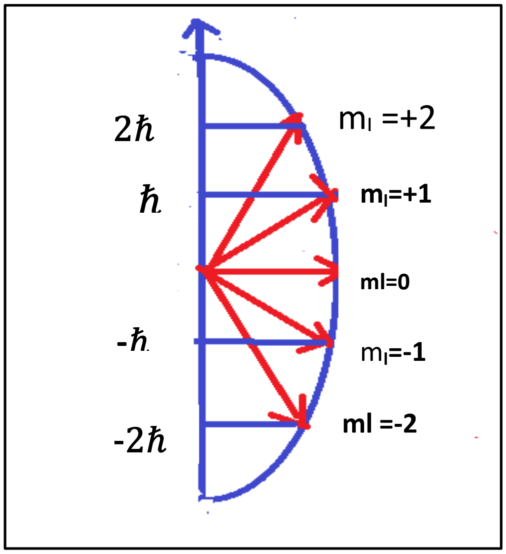
The value of **m_l** range from **+ *l*** through 0 to **–l** so that number of possible orientations of L in a magnetic are (2l+1).

For ex. 1) when l =0 , **m_l =0** so $L_z = 0$

2) When l=1 , $m_l = -1, 0, +1$ so that $L_z = -\hbar, 0, +\hbar$

3) When l=2, $m_l = -2, -1, 0, +1,$ so that $L_z = -2\hbar, -\hbar, 0, +\hbar, +2\hbar$

space quantization of orbital angular momentum Diagram :



L can never be aligned exactly parallel or anti parallel to B, since $\mathbf{L_z}$ is always smaller than the magnitude $L = \hbar\sqrt{l(l+1)}$ of the orbital angular momentum.

Electron Spin: According to Smith and back an electron as a charged sphere, spinning about its own axis . The rotation involves angular momentum. Because the electron is negatively charged, has a magnetic moment opposite in direction to its angular momentum vector $\vec{\mathbf{S}}$ is expressed in terms of spin quantum number **s.** Where $s = \frac{1}{2}$

Therefore Spin angular momentum $S = \hbar\sqrt{s(s+1)}$

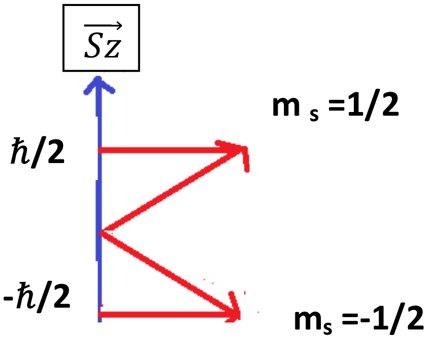
Since $s = \frac{1}{2}$

$$S = \frac{\sqrt{3}}{2}\hbar$$

Spin magnetic quantum number m_s :

Space quantization of electron spin is described by the spin magnetic quantum number m_s . Spin angular momentum vector can have

(2s+1) =2 orientations specified by $\mathbf{m_s} = \pm\frac{\mathbf{1}}{\mathbf{2}}$ The component $\mathbf{S_z}$ of



spin angular momentum of an electron along a magnetic field in the z direction is determined by spin magnetic quantum number, **m_s** so that

$$\mathbf{S}_z = \mathbf{m_s}\hbar, \quad Sz = \pm\frac{1}{2}\hbar$$

Total Angular momentum J and Total magnetic quantum number :

Orbital angular momentum **L** and Spin angular momentum **S** contribute to the total angular momentum **J** of an atom. Since magnitude of **L** and **S** is quantized, magnitude of **J** is also quantized .

ie. $J = \hbar\sqrt{j(j+1)}$ Where j is total angular momentum quantum number.

And the component in the z-direction is given by $J_z = m_j\hbar$

Let us consider an atom whose total angular momentum is provided by a single electron . For example: Hydrogen, lithium and sodium. They have single electron in the outermost orbit.

Since, $L_z = m_l\hbar$, $Sz = m_s\,\hbar$ and $J_z = m_j\hbar$

$$\vec{\mathbf{J}} = \vec{\mathbf{L}} + \vec{\mathbf{S}},$$

$$\therefore \quad \mathbf{J_z} = \mathbf{L_z} \pm \mathbf{S_z}$$

$$\mathbf{m_j}\hbar = \mathbf{m}_l\hbar \pm \mathbf{m_s}\hbar$$

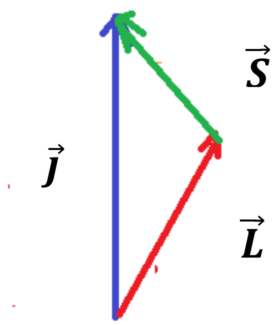
$$\therefore \mathbf{m_j} = \mathbf{m}_l \pm \mathbf{m_s}$$

The possible values of m_j range from +j through 0 to –j

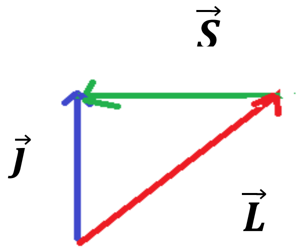
So for any value of l , $j = l \pm s$

In the case of one electron atom only two possible orientations are possible.

i) **J=l+s so that J > L**



ii) For j=l-s, so that J< L



Evidently the orbital and spin angular momentum vector can never be exactly parallel or anti- parallel to each other or to the total angular momentum vector.