E-Learning materials by Dr. Ashok Kr. Acharya, Asst. Professor, University Department of Chemistry, DSPMU, Ranchi. M.Sc. Angular momentum Chapter - 5

There are a number of examples of Angular momentum in quantum mechanics. Angular momentum is possessed by a rotating molecular, an electron revolving around an atom spinning electrons and spinning nuclei.

Let a particle of mass m is revolving around a point at a distance, r, the angular momentum L is given by

Where u is the linear velocity,  $\omega$  is the angular velocity and l (=mr<sup>2</sup>) is the moment of inertia of the particle, The kinetic energy  $E_k$  of the particle is given by

From equation (1) and (2) we get

 $E_k = \frac{L^2}{2I}$ .....(3)

In three dimensions, the angular momentum is represented by a vector  $\vec{L}$ . suppose a mass m is rotating about a fixed point P with a linear velocity.  $\vec{u}$ , it's angular momentum is given by

$$\vec{L}\vec{r}$$
. $m\vec{v} = \vec{r}$ . $\vec{p}$ 

Where  $\vec{r}$  is the vector from the fixed point P to the mass point and  $\vec{p}$  is linear momentum vector. The vector  $\vec{r}$ and  $\vec{p}$  can be written in terms of their components as

$$\vec{r} = i\jmath + j\jmath + k$$

And  $\vec{p} = ii + jj + k$ 

Where Lj and k ar unit vectors along x, y and z axes. Thus, the angular momentum. L in terms of the component  $\vec{r}$ and  $\vec{p}$  is given by

L = i(ypz-zpy)+j(zpx)+k(xpy-ypx).....(4)

Replacing px, py and pz by the corresponding mechanical operators, the operators for the components of angular momentum are given by

$$\hat{L}_x = \frac{h}{2\pi} \left( y \frac{\partial}{\partial} - \frac{\partial}{\partial} \right)$$
$$\hat{L}_x = \frac{h}{2\pi} \left( z \frac{\partial}{\partial} - x \frac{\partial}{\partial} \right)$$

$$\hat{L}_x = \frac{h}{2\pi} \left( x \frac{\partial}{\partial} - y \frac{\partial}{\partial} \right)$$

Thus, the total angular momentum is given by

In quantum mechanics, the scalar pr9duct orf L is more important. i.e.

$$L = iL_x + jL_y + kL_z$$

In quantum mechanics, the scalar product of l is more important. i.e

$$L.L = L^2 = L_x^2 + L_y^2 + L_z^2$$

In terms of spherical polar co –ordinates, the angular momentum operators are given by

$$\hat{L}_{x} = \frac{h}{2\pi} \begin{bmatrix} -s_{1} & \frac{\partial}{\partial} - c_{1} & \frac{\partial}{\partial} \end{bmatrix}$$
$$\hat{L}_{y} = \frac{h}{2\pi} \begin{bmatrix} -c_{1} & \frac{\partial}{\partial} - c_{1} & \frac{\partial}{\partial} \end{bmatrix}$$
$$\hat{L}_{z} = \frac{h}{2\pi} \begin{bmatrix} \frac{\partial}{\partial} \end{bmatrix}$$

$$L^{2} = \frac{h^{2}}{4\pi^{2}} \left[ \frac{1}{s} \cdot \frac{\partial}{\partial} \left( s \cdot \frac{\partial}{\partial} \right) + \frac{1}{s} \cdot \frac{\partial^{2}}{\partial^{2}} \right]$$

Suppose the component of angular momentum about Z-axis (i.e. $\hat{L}_z$ ) and thus, operator is Hermintian as given below:

$$\int_{0}^{2\pi} \Psi 2^{*} \left[ \frac{h}{2\pi} \cdot \frac{\partial}{\partial} \right] \Psi 1 d\phi =$$

$$\frac{h}{2\pi} \left\{ [\Psi 2^{*} \Psi 1]_{0}^{2\pi} - \int_{0}^{2\pi} \Psi 1 \frac{\partial \Psi 2^{*}}{\partial} \cdot d \right\} \dots \dots (6)$$

As the functions  $\Psi_1(\phi)$  and  $\Psi_2(\phi)$  must be single valued i.e. for any  $\phi_1$ 

$$\Psi(\phi) = \Psi(2\pi + \phi) \tag{7}$$

The first terms on the RHS of equation (6) must disappear. Hence equation (6) may be written as follows:

$$- \frac{h}{2\pi} \int_0^{2\pi} \Psi 1 \frac{\partial}{\partial} \Psi 2^* d = -\frac{h}{2\pi} \int_0^{2\pi} \Psi 1 \frac{\partial \Psi 2^*}{\partial} d$$
$$= \int_0^{2\pi} \Psi 1 \left[ \frac{h}{2\pi} \cdot \frac{\partial}{\partial} \right] \Psi 2^* d$$
.....(8)

Since  $\hat{L}_{x,}\hat{L}_{y}a$   $\hat{L}_{z}$  are equivalent, an operator corresponding to any component of angular momentum ishermitian. Thus  $L^{2}$  Must also be hermitian. We can thus conclude that from quantum mechanical view. Not only any component of angular momentum about any axis but also the total angular momentum in system is observable.

## **Eigen values of angular momentum**

Where  $\hat{A}$  is the operator for the Physical quantity, Ψ is the eigen function and  $\lambda$  is the eigenvalues.

On the basis of equation (1), the possible values of the component of angular momentum about z-axis ( the axis of rotation) are given by,

 $\hat{L}_{\gamma}\Psi = \lambda \Psi$ 

Or  $\frac{\partial \Psi}{\partial} = \Psi \frac{2\pi}{h} \lambda \cdot \Psi$ 

Or  $\Psi = \exp\left[\frac{2\pi}{h}\lambda\right] = \cos\left[\frac{2\pi}{h}\phi\right] + i\sin\left[\frac{2\pi}{h}\phi\right]$ 

The function  $\Psi$  is single valued, thus from equation (7) we get,

$$\exp\left[\frac{2\pi}{h}\lambda\right] = \exp\left[\frac{2\pi}{h}(\phi + 2\pi)\right]$$

orexp (i k  $\phi$ ) = exp( $\phi$  + 2 $\pi$ )

where 
$$K = \frac{2\pi}{h} \cdot \lambda o \exp(2\pi) = 1$$

in other words

$$\cos(2\pi k) + I\sin(2\pi) = 1$$
 .....(2)

Equation (2) is po9ssible only if

 $K = 0, \neq 1, \neq 2, \dots, \neq n$ 

In other words  $\lambda$  must be zero or integral multiple of  $\frac{h}{2\pi}$ . This is in accordance with Bohr's postulate about angular momentum of an electron in an atom. Thus, the component of angular momentum about any axis forms discrete Eigen spectrum. We shall now discuss the various properties of orbital angular Momentum, spin angular momentum obtained from vector coupling of orbital and spin angular moment.

If  $L_x$ ,  $L_y$  and the three components of the orbital angular momentum. Then

 $L^2 = L.L = L_x^2 + L_y^2 + L_z^2$ 

L2 is called the total orbital angular momentum squared. It has been shown that wave functions Of rigid rotator were also Eigen function of L2 and  $\hat{L}_z$ . The Eigen value equation in atomic units are

 $\hat{L}^2$  Yl,m = l(l+1) yl,m

## $\hat{L}_x$ Yl, m =myl, m

Where the functions  $Y_{lm}$  are the spherical harmonics. The quantum number I can have the values 0, 1,2..... And for a given value of 1, m can have (21+1) values. i.e.l(l-1),((i-2).....o....-(l-1).

We know3 that the functions  $Y_{lm}$ describes the angular variation of atomic orbital. Thus, we indentify 1 and m respectively with quantum numbers determining the total orbital angular momentum and a compound of this momentum in an arbitrary angular momentum and a compound of this momentum in an arbitrary direction.

(ii) Ladder operators for angular momentum : Instead of  $\hat{L}_x$ and  $\hat{L}_Y$ , it is more convenient to write the complex combination ( $\hat{L}_x \pm \hat{L}_y$ )

Of these operators. They are known as step up and step down operator. we represent these two operators by the symbols.

The  $\hat{L}_z \hat{L}_+ = \hat{L}_z \left( \hat{L}_x + i \hat{L}_y \right) = \hat{L}_z \hat{L}_x + i \hat{L}_z \hat{L}_y$  .....(1)

Using commutation relation, the above equation may be written as

Similarly we can write

 $\hat{L}_{z}\hat{L}_{-}Y_{lm}) = \hat{L}_{-} \qquad (\hat{L}_{z} - 1)$ 

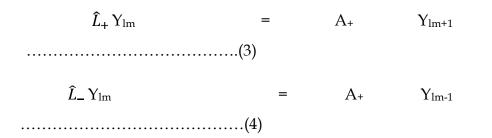
Since  $Y_{lm}$  are the eigen functions of  $L^2$  and  $\hat{L}_z$  consider th 3e operation of  $\hat{L}_z$  on  $\hat{L}_+ Y_{lm}$ . Using equation (2) we get

$$\hat{L}_{z}(\hat{L}_{+}Y_{lm}) = \hat{L}_{+}(\hat{L}_{z} + 1)Y_{lm}$$

 $= (m+1)((\hat{L}_{+} + Ylm))$ 

Similarly,  $\hat{L}_z(\hat{L}_+ Y_{lm}) = (m+1)((\hat{L}_+ + Y_{lm}))$ 

Thus,  $\hat{L}_+$  and  $\hat{L}_-$  are the step up and step down operators with respect to the eigen value of  $\hat{L}_z$ . The  $\hat{L}_+ Y_{\rm lm}$  is an eigen value (i.e m+1) one unit greater and  $\hat{L}_- Y_{\rm lm}$  and eigen vector of  $\hat{L}_z$  with wigen value (i.e m-1)one unite than the eigen value of  $Y_{\rm lm}$ . Therefore, the operators. $\hat{L}_+$  and $\hat{L}_-$  are alas known as ladder operators as the successive application of  $\hat{L}_+$  or  $\hat{L}_-$  creates a ladder of eigen states of  $\hat{L}_z$ . Thus, we may write



Where  $A_+$  and  $A_-$  are constants. This ladder can not extended infinitely because the value of m is limited (i.e+1,0,l). Thus, and attempt to raise the state $Y_{lm}$ (Where m =+1) must give zero. Hence

 $Y_{l,m}Y_{l,l}=0$ 

Similarly,  $\hat{L}_{1,-1} = 0$ 

As There is not state whose eigne value for  $\hat{L}_z$  is – (l +1) for given l. thus when m has lowest value,

 $\hat{L}_{-}$  destroys the rotating electron and when m ha sthe maximum value,  $\hat{L}_{+}$  destroys it. To determine the values of A<sub>+</sub> and A<sub>-</sub> we us the requirement that the function Y<sub>l,m</sub> are normalizes. Multiplying the LHS of equation (3) with  $\hat{L}_{+}$  Yl, m

And integrating over all space we get,

 $\langle \hat{L}_{+} \text{Ylml} \hat{L}_{+} \text{Ylm} \rangle = |A_{+}|^{2} \langle \text{Y}_{l,m+1} | \text{Y}_{l,m+1} \rangle = |A_{+}|^{2} \dots (5)$ 

By using definition of  $\hat{L}_+$  (equation A), the LHS of equation (5) may be written as:

$$\langle \left[ \left( \hat{L}_{x} + i \hat{L}_{y} \right) \mathbf{Y}_{l,m} \right] | L_{x} | \mathbf{Y}_{l,m} \rangle + i \langle \left[ \left( \hat{L}_{x} + i \hat{L}_{y} \right) \mathbf{Y}_{l,m} \right] | L_{x} | \mathbf{Y}_{l,m} \rangle \right]$$

Since the operators  $L_x$  and  $L_y$  are herminitian, we may write the above integral as

$$\begin{aligned} \langle \mathbf{Y}_{\mathbf{l},\mathbf{m}} | L_{x} | \langle \left[ \left( \hat{L}_{x} \pm i \hat{L}_{y} \right) \mathbf{Y}_{\mathbf{l},\mathbf{m}} \right] \rangle \\ &+ \langle \mathbf{Y}_{\mathbf{l},\mathbf{m}} | L_{y} | \left[ \left( \hat{L}_{x} + i \hat{L}_{y} \right) \mathbf{Y}_{\mathbf{l},\mathbf{m}} \right] | L_{y} | \mathbf{Y}_{\mathbf{l},\mathbf{m}} \end{aligned}$$

We know that

$$\left(\widehat{L}_{x} \pm i\widehat{L}_{y}\right) = \widehat{L}_{x}$$

In integral notation, we get

We can write the integral in equation (6) in bracket notation as

$$Y_{l,m}|(L^2 - L_z^2 - L_z)|Y_{l,m}| = Y_{l,m}|L^2|Y_{l,m} - Y_{l,m}|L_z^2|Y_{l,m}| = Y_{l,m}|L_z|Y_{l,m}| = Y_{l,m}|L_z|Y_{l,m}| = Y_{l,m}|Z_{l,m}| = Y_{l,m}|Z_{l,m}|Z_{l,m}| = Y_{l,m}|Z_{l,m}|Z_{l,m}| = Y_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}| = Y_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}| = Y_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}| = Y_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,m}|Z_{l,$$

 $\mathsf{Y}_{\mathbf{l},m}|\mathit{L}^2|\mathsf{Y}_{\mathbf{l},m}$ 

Since the4 functions  $Y_{l,m}$  are normalized and the operator hermitain, we have

$$[A_+]^2 = l(l+1) - m^2 - m$$

$$= l(l+1)-m(m+1)$$

Similarly 
$$[A_{-}]^{2}=l(l+1)-m(m-1)$$
  
Therefore,  $\hat{L}_{+}Y_{l,m} = \sqrt{l(l+1) - m(m+1)Y_{l,m-1}}$   
.....(7)  
And  $\hat{L}_{-}Y_{l,m} = \sqrt{l(l+1) - m(m+1)Y_{l,m-1}}$   
......(8)

• • •

The relations given in equation (7) and (8) are very useful because if we know one eigenfunction of  $\hat{L^2}$  and  $\hat{L}_z$ with eigen values 1 and m, we can construct the corresponding eigenfunctionhaving same l and m+ 1or m-1. We may then find the relation between  $\hat{L}_+,\hat{L}_-$  and  $\hat{L}^2$  . we have

$$\hat{L}_{+,}\hat{L}_{-} = (\hat{L}_x + i\hat{L}_Y)(\hat{L}_x - i\hat{L}_Y)$$
$$= \hat{L}_x^2 + \hat{L}_y^2 + i\hat{L}_y\hat{L}_x - i\hat{L}_x\hat{L}_Y$$

$$= \hat{L}_x^2 + \hat{L}_y^2 + i(-i\hat{L}_z)$$

$$= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_y^2$$
Hence  $\hat{L}^2 = \hat{L}_+, \hat{L}_- - \hat{L}_x + \hat{L}_z^2$ 
Similarly we can shown that
$$\hat{L}^2 = \hat{L}_+, \hat{L}_- + \hat{L}_z, + \hat{L}_z^2$$

. . . . .

A number of properties of angular momentum operators can be derived from their commutation relation. The commutation of  $\hat{L}_{x_i}$  and  $\hat{L}_{y_i}$  is obtained as follows. Using definition of Using definition of  $\hat{L}_{x_i}$  and  $\hat{L}_{y_i}$  we get,

$$\hat{L}_{x}\hat{L}_{y_{i}} = \frac{1}{!} \left[ y \frac{\partial}{\partial} - z \frac{\partial}{\partial} \right] \frac{1}{!} \left[ z \frac{\partial}{\partial} - x \frac{\partial}{\partial} \right]$$

$$= - \left[ y \frac{\partial}{\partial} \cdot z \frac{\partial}{\partial} - y \frac{\partial}{\partial} x \frac{\partial}{\partial} - z \frac{\partial}{\partial} z \frac{\partial}{\partial} + z \frac{\partial}{\partial} \cdot x \frac{\partial}{\partial} \right]$$

$$= - \left[ y \frac{\partial}{\partial} + y \frac{\partial^{2}}{\partial} - y \frac{\partial^{2}}{\partial x^{2}} - z^{2} \frac{\partial^{2}}{\partial} + z \frac{\partial^{2}}{\partial} \right]$$
.....(1)

$$\hat{L}_{y,}\hat{L}_{x} = -\left[z\frac{\partial}{\partial}y\frac{\partial}{\partial} - z\frac{\partial}{\partial}z\frac{\partial}{\partial} - x\frac{\partial}{\partial}y\frac{\partial}{\partial} + x\frac{\partial}{\partial}z\frac{\partial}{\partial}\right]$$
$$= -\left[z\frac{\partial^{2}}{\partial} - z^{2}\frac{\partial^{2}}{\partial} - x\frac{\partial^{2}}{\partial z^{2}} + x\frac{\partial^{2}}{\partial} + x\frac{\partial}{\partial}\right]$$
....(2)

Subtracting e3quation (2) form equation (1), we get,

$$\begin{bmatrix} \hat{L}_{x} \hat{L}_{y,} \end{bmatrix} = \hat{L}_{x} \hat{L}_{y,} - \hat{L}_{y,} \hat{L}_{x} = -\begin{bmatrix} y \frac{\partial}{\partial} - x \frac{\partial}{\partial} \end{bmatrix}$$
$$= \begin{bmatrix} x \frac{\partial}{\partial} - y \frac{\partial}{\partial} \end{bmatrix} = i \hat{L}_{z}$$
....(3)

Thus, the operators  $\hat{L}_x$  and  $\hat{L}_{y_r}$  do not commute. Similarly

$$\begin{bmatrix} L_{y} L_{z} \end{bmatrix} = \hat{L}_{y,i} \hat{L}_{z} - \hat{L}_{z} \hat{L}_{y,i} = i \hat{L}_{x}$$

.....(4)

It is noted that the components of linear momenta commute with each other i.e.

$$\begin{bmatrix} P_{\chi} P_{y} \end{bmatrix} = \begin{bmatrix} P_{y} P_{z} \end{bmatrix} = \begin{bmatrix} P_{z} P_{\chi} \end{bmatrix}$$

In this respect angular momentum is different from the liner momentum.

Now we shall consider commutation relation between  $\hat{L}^2$  and it's components.

 $[L_{x}^{2}L_{z}] = \hat{L}_{x}^{2}L_{z} - \hat{L}_{z}\hat{L}_{x}^{2}$  $= \hat{L}_{x}\hat{L}_{x}\hat{L}_{z} - \hat{L}_{z}\hat{L}_{x}\hat{L}_{x}$  $= \hat{L}_{x}\hat{L}_{x}\hat{L}_{z} - \hat{L}_{x}\hat{L}_{z}\hat{L}_{x} + \hat{L}_{x}\hat{L}_{z}\hat{L}_{x} - \hat{L}_{z}\hat{L}_{x}\hat{L}_{x}$  $= [L_{x}^{2}L_{z}][L_{x}, L_{z}] + [L_{x}, L_{z}]\hat{L}_{x}$ 

Using equation (5), we get,

Similarly,  $[L_x^2 L_z] \quad i(\hat{L}_x \hat{L}_y + \hat{L}_y \hat{L}_x)$ .....(7)

,  $[L_{x_i}^2 L_z] = 0$  .....(8)

Adding equations (5),(7) and (8), we get

$$\left[\widehat{L}^{2}, L_{\chi}\right] = \left[\widehat{L}^{2}, L_{\gamma}\right] = 0$$

Since  $\widehat{L}^2$  commutes with any component of  $\widehat{L}$  do not commute with each other , we can conclude that the total angular momentum and only one of it's components are simultaneously will defined.