

Ch # 5 Angular Momentum:

Angular momentum is an important quantity, especially when we study the dynamics of the systems that moves under the influence of spherically symmetric or central potentials. i.e.  $V(\vec{r}) = V(r)$  - depends on position not direction.

For example, in hydrogen atom, where  $e^-$  moves in the proton's Coulomb potential or central potential. and, ~~It~~ is based on the quantization of angular momentum. Angular momentum also play a critical role in the description of molecular rotations, the motion of an  $e^-$  in atom, and the motion of nucleons in nuclei.

Therefore, the quantum theory of angular momentum is thus a vital for studying molecular, atomic and nuclear systems.

# Spherically Symmetric or Central Potentials:

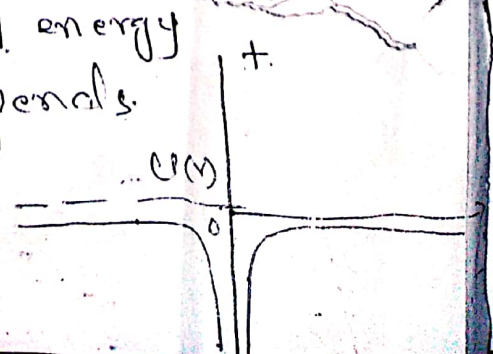
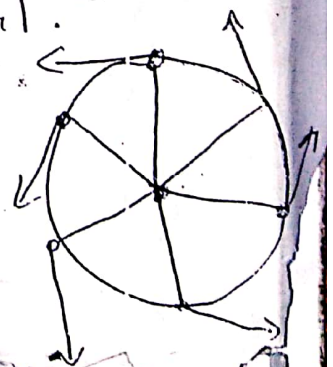
In 3D, we often encounter spherically symmetric potential energy functions. For example, the potential energy of the electron in the hydrogen atom is the electrostatic potential energy of the proton-electron system: It depends only on the distance " $r$ " of the electron from the proton, not on the direction of the position vector  $\underline{r}$ . Hence,

"A potential that depends only on the distance between the particle and a well defined center point; not the direction, called spherically symmetric or central potential."

For the proton- $e^-$  system, the potential energy is

$$U(r) = -\frac{q^2}{4\pi\epsilon_0 r}$$

It means the potential energy  $U(r)$  of the particle depends only on the particle's distance from its origin.



In classical mechanics, the <sup>orbital</sup> angular momentum  $\vec{L}$  of a particle can be written as

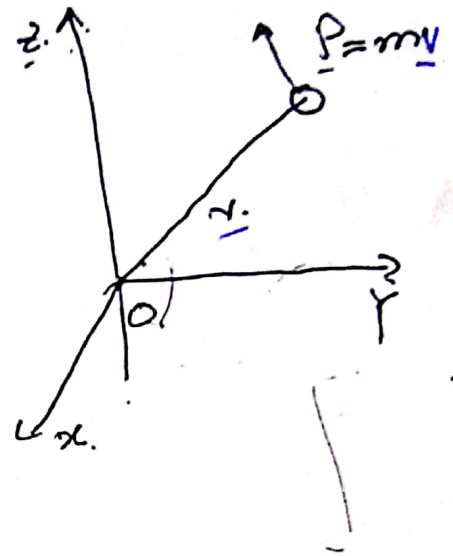
$$\vec{L} = \vec{r} \times \vec{p}$$

Here,

$\vec{r}$  = position vector

$\vec{p}$  = linear momentum

$\vec{L}$  = orbital angular momentum



But in quantum mechanics, the orbital angular momentum is associated with operators  $\hat{L}$ ,  $\hat{r}$  of position and momentum, i.e.  $\hat{p}$  and  $\hat{r}$

Hence As.  $\hat{p} = -i\hbar \vec{\nabla}$ ,  $\vec{\nabla} = \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k}$

Hence,  $\hat{r} = x\hat{i} + y\hat{j} + z\hat{k}$

$$\hat{L} = \hat{L}_x \hat{i} + \hat{L}_y \hat{j} + \hat{L}_z \hat{k}$$

Also.

$$\hat{L} = -i\hbar \hat{r} \times \vec{\nabla}$$

Cross product can be written as



$$\hat{L}_z = -i\hbar \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix}$$

$$\hat{L} = -i\hbar \left[ \hat{i} \begin{vmatrix} y & z \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix} - \hat{j} \begin{vmatrix} x & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial z} \end{vmatrix} + \hat{k} \begin{vmatrix} x & y \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{vmatrix} \right]$$

$$\hat{L} = -i\hbar \left[ \hat{i} \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) - \hat{j} \left( x \frac{\partial}{\partial z} - z \frac{\partial}{\partial x} \right) + \hat{k} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right]$$

as  $\hat{L} = \hat{L}_x \hat{i} + \hat{L}_y \hat{j} + \hat{L}_z \hat{k}$

Therefore, components of the orbital angular momentum are

$$\hat{L}_x = -i\hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \quad \text{--- (1)}$$

$$\hat{L}_y = -i\hbar \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \quad \text{--- (2)}$$

$$\hat{L}_z = -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \quad \text{--- (3)}$$

# Commutation Relations!

we need to check, <sup>whether</sup> ~~whether~~ the orbital angular momentum components  $\hat{L}_x$ ,  $\hat{L}_y$  and  $\hat{L}_z$  commute with each others or not.

$$[\hat{L}_x, \hat{L}_y] = ? = [L_x L_y - L_y L_x]$$

As we know,  $\hat{L}_x = -i\hbar [y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y}]$

and  $\hat{L}_y = -i\hbar [z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z}]$

So, first calculate  $\hat{L}_x \hat{L}_y$

$$\hat{L}_x \hat{L}_y = [-i\hbar (y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y})] [-i\hbar (z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z})]$$

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

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

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

$$\left. \left. x \frac{\partial^2}{\partial y \partial z} \right) \right]$$

we know.

$$1 = \frac{\partial y}{\partial y} = \frac{\partial x}{\partial x} = \frac{\partial z}{\partial z}$$

$$0 = \frac{\partial y}{\partial z} = \frac{\partial x}{\partial z} = \frac{\partial y}{\partial x} = \frac{\partial x}{\partial y} = \frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} = 0$$

Hence

$$\hat{L}_x \hat{L}_y = -\hbar^2 \left[ y \frac{\partial}{\partial x} + yz \frac{\partial^2}{\partial x \partial z} - yx \frac{\partial^2}{\partial z^2} - z^2 \frac{\partial^2}{\partial y \partial x} + zx \frac{\partial^2}{\partial y \partial z} \right]$$

Similarly, we can calculate  $\hat{L}_y \hat{L}_x$ , which is

$$\hat{L}_y \hat{L}_x = -\hbar^2 \left[ zy \frac{\partial^2}{\partial x \partial z} + z^2 \frac{\partial^2}{\partial x \partial y} - xy \frac{\partial^2}{\partial z^2} + x \frac{\partial}{\partial y} + xz \frac{\partial^2}{\partial z \partial y} \right]$$

So, the commutation relation will become as

$$[\hat{L}_x, \hat{L}_y] = [\hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x]$$



$$[\hat{L}_x, \hat{L}_y] = -\hbar^2 \left[ y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right]$$

$$= i\hbar \left[ i\hbar \left( y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right) \right]$$

$$= i\hbar \left[ i\hbar \left( y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right) \right]$$

$$= i\hbar \left[ y \left( -i\hbar \frac{\partial}{\partial x} \right) - x \left( i\hbar \frac{\partial}{\partial y} \right) \right]$$

$$= i\hbar \left[ -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right]$$

$$= i\hbar \left[ x \left( -i\hbar \frac{\partial}{\partial y} \right) - y \left( -i\hbar \frac{\partial}{\partial x} \right) \right]$$

So.

As  $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

and  $\hat{p}_y = -i\hbar \frac{\partial}{\partial y}$

$$[\hat{L}_x, \hat{L}_y] = i\hbar [x \hat{p}_y - y \hat{p}_x]$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$\therefore \hat{L}_z = \dots$$

$$\hat{L}_z = -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

Similarly,

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$

Hence,  $\hat{L}_x$ ,  $\hat{L}_y$ , and  $\hat{L}_z$  do not commute and, therefore, one can not measure them simultaneously. Since, cannot be diagonalized and do not possess common eigenstate.

In cyclic permutation, three angular momentum components can be written as in tensor form:

$$[\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k$$

where  $\epsilon_{ijk}$  is a tensor, called

Levi-Civita tensor, and can be represented,

as:

$$\epsilon_{ijk} = \begin{cases} 1 \\ -1 \\ 0 \end{cases}$$

For even permutation of (123)



For odd permutation of

(123)



For two similar indices of (143)

(143)



Proof: Square of angular Momentum. (5)

$$(i) \underline{L} \cdot \underline{L} = |\underline{L}|^2 = L^2 = L_x^2 + L_y^2 + L_z^2$$

$$(ii) \underline{L}_x \cdot \underline{L} = i\hbar \underline{L}$$

we know..

$$\underline{L} = L_x \hat{i} + L_y \hat{j} + L_z \hat{k}$$

$$\underline{L}_x \cdot \underline{L} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ L_x & L_y & L_z \\ L_x & L_y & L_z \end{vmatrix}$$

$$= \hat{i} \begin{vmatrix} L_y & L_z \\ L_y & L_z \end{vmatrix} - \hat{j} \begin{vmatrix} L_x & L_z \\ L_x & L_z \end{vmatrix} + \hat{k} \begin{vmatrix} L_x & L_y \\ L_x & L_y \end{vmatrix}$$

$$= \hat{i} (L_y L_z - L_z L_y) - \hat{j} (L_x L_z - L_z L_x) + \hat{k} (L_x L_y - L_y L_x)$$

$$= \hat{i} (L_y L_z - L_z L_y) + \hat{j} (L_z L_x - L_x L_z) + \hat{k} (L_x L_y - L_y L_x)$$

$$\hat{L}_x \hat{L}_y = \hat{i} (i\hbar \hat{L}_z) + \hat{j} (i\hbar \hat{L}_y) + \hat{k} (i\hbar \hat{L}_x)$$

$$= i\hbar [\hat{L}_z \hat{i} + \hat{L}_y \hat{j} + \hat{L}_x \hat{k}]$$

$$\boxed{\hat{L}_x \hat{L}_y = i\hbar \hat{L}_z}$$

(ii)

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

$$\boxed{\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2}$$

Commutation of  $\hat{L}^2$  with  $\hat{L}_x$ ,  $\hat{L}_y$ , and  $\hat{L}_z$

One can see that,  $\hat{L}^2$  is a scalar operator hence it should commute with  $\hat{L}_x$ ,  $\hat{L}_y$ , and  $\hat{L}_z$

$$[\hat{L}^2, \hat{L}_i] = 0, \quad i = x, y, \text{ and } z$$

Let us take:

$$[\hat{L}_x, \hat{L}^2] = \hat{L}_x \hat{L}^2 - \hat{L}^2 \hat{L}_x$$

6

$$\begin{aligned}
 [L_x, L^2] &= L_x (L_x^2 + L_y^2 + L_z^2) - (L_x^2 + L_y^2 + L_z^2) L_x \\
 &= \cancel{L_x^3} + L_x L_y^2 + L_x L_z^2 - \cancel{L_x^3} - L_y^2 L_x - L_z^2 L_x \\
 &= \boxed{L_x L_y^2} L_y + \boxed{L_x L_z^2} L_z - L_y \boxed{L_y L_x} - L_z \boxed{L_z L_x}
 \end{aligned}$$

Now.

$$[L_x, L_y] = i\hbar L_z$$

$$L_x L_y - L_y L_x = i\hbar L_z \Rightarrow L_y L_x - L_x L_y = -i\hbar L_z$$

$$L_x L_y = L_y L_x + i\hbar L_z \text{ or } L_x L_y - i\hbar L_z = L_y L_x$$

Similarly

$$L_x L_z = L_z L_x + i\hbar L_y$$

$$L_z L_x = L_x L_z - i\hbar L_y$$

or.

$$L_x L_z - L_z L_x = -i\hbar L_y$$

$$L_y L_z - L_z L_y = i\hbar L_x$$

$$L_z L_y - L_y L_z = -i\hbar L_x$$



By putting all these values, we will get

$$\langle \hat{L}_x, \hat{L}^2 \rangle = 0$$

Similarly

$$\langle \hat{L}_y, \hat{L}^2 \rangle = 0$$

$$\langle \hat{L}_z, \hat{L}^2 \rangle = 0$$

The  $\hat{L}_x$ ,  $\hat{L}_y$ ,  $\hat{L}_z$ , and  $\hat{L}^2$  are Hermitian, and their eigenvalues are real.

## Hermitian operators.

An operator is called Hermitian operator when it can be flipped over to the other side if it appears in an inner product

$\langle f | g \rangle$  — inner product.

If  $\hat{A}$  operator is Hermitian, then

$$\langle \hat{A} f | g \rangle = \langle f | \hat{A} g \rangle$$

$\begin{cases} \hat{A}^t = \hat{A} \\ \hat{A}^* = \hat{A} \end{cases}$   
↙ dagger  
↖ conjugate

Theorem: The eigen-values of Hermitian operators are real.

Proof: Let  $\psi$  be an eigenfunction of  $\hat{A}$  with eigen value  $\lambda$ , means.

$$\hat{A} \psi = \lambda \psi$$

Then we have.

$$\int (\hat{A} \psi)^* \psi dx = \int (\lambda \psi)^* \psi dx$$

L.H.S.

$$= \int \lambda^* \psi^* \psi dx$$

$$= \int \psi^* \psi dx \quad \text{--- (1)}$$

Now R.H.S.

$$= \int \hat{A}^* \psi^* \psi dx$$

B.C. A is hermit  
 $\hat{A}^\dagger = \hat{A}$

$$= \int \psi^* \hat{A}^\dagger \psi dx$$

$$= \int \psi^* \hat{A} \psi dx = \int \psi^* \lambda \psi dx$$

or. of. one have. too. ~~an~~ inner product. ①

of wavefn.  $\psi$

then.  $\int \psi^* \hat{A} \psi dx = \int$

The operator  $(\hat{A}^\dagger)$  is called the Hermitian conjugate of  $\hat{A}$  if

$$\int (\hat{A}^\dagger \psi)^* \psi dx = \int \psi^* \hat{A} \psi dx$$

- also "Hermitian conjugate" also called "adjoint"

$$\begin{aligned} \int (\hat{A} \psi)^* \psi dx &= \int \hat{A}^\dagger \psi^* \psi dx \\ &= \int \psi^* \hat{A} \psi dx = \int \psi^* \hat{A} \psi dx \end{aligned}$$

because  $\hat{A}$  is Hermitian:  $\hat{A}^\dagger = \hat{A}$



$$= \lambda \int \psi^* \psi dx$$

Compare. L.H.S with. R.H.S.

$$\boxed{\lambda^* = \lambda}$$

Hence Hermitian operators eigenvalues are real.

## Eigenstate and Eigenvalues of the angular Momentum operators.

We confirm that  $\hat{L}^2$  commutes with each component of  $\hat{L}$  (i.e.,  $\hat{L}_x$ ,  $\hat{L}_y$ , and  $\hat{L}_z$ ), hence we can take the simultaneous eigenfns. of  $\hat{L}^2$  and  $\hat{L}_x$ ,  $\hat{L}_y$ , and  $\hat{L}_z$ :

Let  $\bar{\Psi}$  is an eigenfunction of  $\hat{L}^2$  and  $\hat{L}_z$ , Simultaneously, hence

$$\hat{L}^2 \bar{\Psi} = \lambda \bar{\Psi}$$

$$\hat{L}_z \bar{\Psi} = \mu \bar{\Psi}$$

Called the eigenvalue equations.  $\lambda$  and  $\mu$  are the eigenvalues of  $\hat{L}^2$  and  $\hat{L}_z$ , respectively, which are real. Because,

These eqs. will satisfy the following uncertainty eqn.

$$\langle L^2 \rangle \geq \langle L_z^2 \rangle$$

because, we know.

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

Raising (step up) and Lowering (step down) operators.

Let  $\hat{L}_+$  and  $\hat{L}_-$  are the step up and step down operators and can be written as

$$\hat{L}_+ = L_x + iL_y$$

$$\hat{L}_- = L_x - iL_y$$

Also,

$$\hat{L}_+ = \hat{L}_-^\dagger$$

$$\hat{L}_- = \hat{L}_+^\dagger$$

we need to prove the following commutation relations.

$$1) \quad [L^2, L_\pm] = 0$$

$$2) \quad [L_+, L_-] = 2\hbar L_z$$

$$3) \quad [L_z, L_\pm] = \pm \hbar L_\pm$$