College of Science
Department of Physics
Fourth Class
Lecture 19

Quantum Mechanics

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Lecture 19: Angular momentum

Preparation

Assist. prof. Alaa Abdul Hakeim

Unit 9

Angular momentum

9.1 Angular Momentum Operators in Cartesian and Spherical Polar form.

Angular momentum is very useful for studying the dynamics of systems that move under the influence of spherically symmetric, or central, potentials, V(r), for as in classical mechanics, the orbital angular momenta of these systems are conserved quantum mechanically too. Angular momentum plays a critical role in the description of

1- molecular rotations
2- motion of electrons in atoms
3- the motion of nucleons in nuclei

The quantum theory of angular momentum is thus a prerequisite for studying molecular, atomic, and nuclear systems.

From Schrӧedinger eq. in cartesian coordinate

$$-\frac{\hbar^2}{2m}\nabla^2\Psi\ (x,y,z)+V\Psi\ \ (x,y,z)=E\ \Psi\ (x,y,z)$$

Where $V=-\frac{1}{4\pi\varepsilon o}\frac{e^2}{r}$ is the potential of atomic system. also, the Schrӧedinger eq. in polar coordinate equal

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\left(rR_{nl}(r)\right)+\left[\frac{l(l+1)\hbar^2}{2mr^2}+V(r)\right]R_{nl}(r)=ER_{nl}(r)$$

The solution of this eq. is Ψ (r, θ,Φ)= R(r)Θ(θ)Φ(∅)

So, R(r) is radial part and Θ(θ)Φ (∅)=Y(θ, ∅) angular part.

The angular solution consists of $\theta_{lm}(\theta)\Phi_{ml}(\emptyset)=Y_{lm}(\theta,\emptyset)=sphyrical\ harmonic$.

A spherical harmonic $Y_{lm}(\theta,\emptyset)$ is a single valued, continuous, bounded complex function of two real arguments θ,Φ with $0\leq\theta\leq\pi\ and\ 0\leq\emptyset\leq 2\pi$. It is characterized by two parameters $l\ and\ m$, which take values $l=0,1,2,---and\ m=l,l-1,l-2,---\ -l+2,-l+1,-l$.

Therefore, for a given l there exists a $(2l+1)$ functions corresponding to different m. All derivatives of $Y_{lm}(\theta, \emptyset)$ are single- valued, continuous and finite functions.

Spherical harmonics play an important role in quantum mechanics. They are eigen functions of the operator of orbital angular momentum and describe the angular distribution of particles which move in a spherically symmetric field with the orbital angular momentum l and projection m. Strictly speaking, l specifics the absolute value of orbital angular momentum because $l(l+1)$ is the eigen value of the square of the orbital angular momentum operator $\hat{L}^2$, m is the eigen value of l_x which is the projection of the orbital angular momentum operator on the quantization axis.

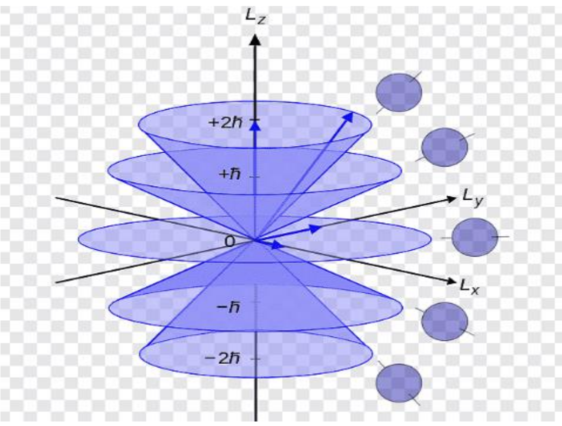
The radial solution R(r) depends on principal quantum number n and orbital quantum number l , $R_{nl}(r)$.

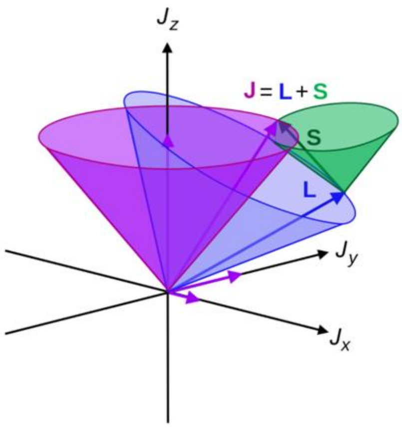
$$\therefore n\ represented\ principl\ Q.n. related\ with\ energy$$

$$l\ represented\ orbital\ Q.n. related\ with\ angular\ momentum\ \hat{L}^2$$

$$m\ represented\ magnetic\ Q.n. related\ with\ angular\ momentum$$

$$component\ about\ z\ direction\ l_z$$





9.1.1 Orbital Angular Momentum.

The orbital angular momentum of a body is associated with its rotation about certain axis. In classical mechanics the orbital angular momentum of a particle about a point is defined as the momentum of linear momentum of the body (under consideration) about the axis of particle about a point is defined as

$$\vec{L} = \vec{r} \times \vec{P} \quad - - - - - 1$$

Where $\vec{r}$ is position vector of the particle form that point and $\vec{P}$ is the linear momentum of the particle.

Orbital angular momentum is perpendicular to both $\vec{r}\ and\ \vec{P}$ and therefore perpendicular to the plane in which $\vec{r}$ rotates.

Equation1 defines the components of $\vec{L}$ about x, y, z axes respectively.

By vector analysis:

$$\vec{L} = il_x + jl_y + kl_z \qquad \vec{r} = i\,x + j\,y + k\,z$$

$$\vec{P} = iP_x + j\,P_y + kP_z$$

Substituting these values in eq1

$$\vec{L} = il_x + jl_y + kl_z = \begin{vmatrix} i & j & k \\ x & y & z \\ P_x & P_y & P_z \end{vmatrix}$$

Compare the coefficients of i , j, k, on either side

$$\vec{L} = il_x + jl_y + kl_z = i\left(yP_z - zP_y\right) + j\,(zP_x - xP_z) + k(xP_y - yP_x)$$

$$l_x = yP_z - zP_y \qquad l_y = zP_x - xP_z \qquad l_z = xP_y - yP_x$$

If we substitute operators for P_x, P_y, P_z

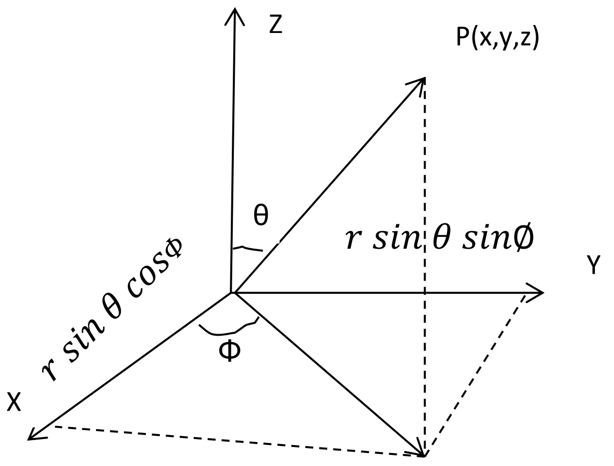
$$P_x = \frac{\hbar}{i}\frac{\partial}{\partial x}\ , \qquad P_y = \frac{\hbar}{i}\frac{\partial}{\partial y}\ , \quad P_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

The components of orbital angular momentum are defined as :

$$l_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \quad l_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \quad l_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - - - 2$$

9.1.2 Orbital Angular Momentum in Polar Coordinates

$$\left.\begin{aligned} x &= r\sin\theta\cos\emptyset \\ y &= r\sin\theta\sin\emptyset \\ z &= r\cos\theta \end{aligned}\right\} ------\mathbf{3}$$



$$\left.\begin{aligned} r^2 &= x^2+y^2+z^2 \\ \cos\theta &= \frac{z}{r} = \frac{z}{\sqrt{x^2+y^2+z^2}} \\ \tan\emptyset &= \frac{y}{x} \end{aligned}\right\} ------ 4$$

$$\left.\begin{aligned} l_x &= \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ l_y &= \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ l_z &= \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned}\right\} ------5$$

To evaluate l_x, l_y *and* l_z in polar coordinate we have to evaluate

$$\left.\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial r}{\partial x}.\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}.\frac{\partial}{\partial\theta} + \frac{\partial\emptyset}{\partial x}.\frac{\partial}{\partial\emptyset} \\ \frac{\partial}{\partial y} &= \frac{\partial r}{\partial y}.\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}.\frac{\partial}{\partial\theta} + \frac{\partial\emptyset}{\partial y}.\frac{\partial}{\partial\emptyset} \\ \frac{\partial}{\partial z} &= \frac{\partial r}{\partial z}.\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial z}.\frac{\partial}{\partial\theta} + \frac{\partial\emptyset}{\partial z}.\frac{\partial}{\partial\emptyset} \end{aligned}\right\} ------ 6$$

To evaluate $\frac{\partial}{\partial x}, \frac{\partial}{\partial y}$ *and* $\frac{\partial}{\partial z}$ we have to find $\frac{\partial r}{\partial x}, \frac{\partial r}{\partial y}, \frac{\partial r}{\partial z}, \frac{\partial\theta}{\partial x}, \frac{\partial\theta}{\partial y}, \frac{\partial\theta}{\partial z}, \frac{\partial\emptyset}{\partial x}, \frac{\partial\emptyset}{\partial y}, \frac{\partial\emptyset}{\partial z}$ using eq4.

$$\frac{\partial r}{\partial x} = \frac{x}{r} = \frac{r\sin\theta\cos\emptyset}{r} = \sin\theta\cos\emptyset --- 7$$

Similarly, $\frac{\partial r}{\partial y} = \frac{y}{r} = \sin\theta\sin\emptyset$ $-----8$

$$\frac{\partial r}{\partial z} = \frac{z}{r} = \cos\theta \ ------9$$

Using eq.4 to find $\frac{\partial \theta}{\partial x}$

$cos\theta = \frac{z}{\sqrt{x^2+y^2+z^2}}$

$$\frac{\partial y}{\partial x} = -sin\theta\ \partial\theta = -\frac{z}{2}\ (x^2+y^2+z^2)^{-\frac{3}{2}}\ (2x)\partial x$$

$$\frac{\partial \theta}{\partial x} = \frac{zx}{(x^2+y^2+z^2)^{\frac{3}{2}}\ sin\theta} = \frac{zx}{r^3 sin\theta} = \frac{r\ cos\theta\ r\ sin\theta\ cos\emptyset}{r^3 sin\theta}$$

$$\frac{\partial \theta}{\partial x} = \frac{cos\theta cos\emptyset}{r}\ ----10$$

Similarly, $\frac{\partial \theta}{\partial y} = \frac{cos\theta\ sin\emptyset}{r}\ ----11\quad and\quad \frac{\partial \theta}{\partial z} = -\frac{sin\theta}{r}\ ---12$

To find $\frac{\partial \emptyset}{\partial x}, \frac{\partial \emptyset}{\partial y}, \frac{\partial \emptyset}{\partial z}$, also from eq.4

$$tan\emptyset = \frac{y}{x}\quad ,\quad sec^2\emptyset\ \frac{\partial \emptyset}{\partial x} = -\frac{y}{x^2}$$

$$\frac{\partial \emptyset}{\partial x} = -\frac{r\ sin\theta sin\emptyset}{r^2 sin^2\theta\ cos^2\emptyset}\ .cos^2\emptyset = -\frac{sin\emptyset}{r\ sin\theta}\ ----13$$

Similarly: $\frac{\partial \emptyset}{\partial y} = \frac{cos\emptyset}{r\ sin\theta}\ ----14\quad and\quad \frac{\partial \emptyset}{\partial z} = 0 --- 15$

To evaluate l_z

$$l_z = \frac{ħ}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$l_z = -i\hbar\left[\left\{r\ sin\theta\ cos\emptyset\left(\frac{\partial r}{\partial y}.\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y}.\frac{\partial}{\partial \theta} + \frac{\partial \emptyset}{\partial y}.\frac{\partial}{\partial \emptyset}\right)\right\} - \left\{r\ sin\theta sin\emptyset\left(\frac{\partial r}{\partial x}.\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}.\frac{\partial}{\partial \theta} + \frac{\partial \emptyset}{\partial x}.\frac{\partial}{\partial \emptyset}\right)\right\}\right]$

$$l_z = -i\hbar r\, sin\theta \left[cos\emptyset \left\{sin\theta sin\emptyset \frac{\partial}{\partial r} + \frac{1}{r} cos\theta\, sin\emptyset \frac{\partial}{\partial \emptyset} + (\frac{cos\emptyset}{r\, sin\theta}) \frac{\partial}{\partial \emptyset}\right\} - sin\emptyset \left\{sin\theta cos\emptyset \frac{\partial}{\partial r} + \frac{1}{r} cos\theta cos\emptyset \frac{\partial}{\partial \theta} + (-\frac{sin\emptyset}{r\, sin\theta} \frac{\partial}{\partial \emptyset})\right\}\right]$$

$$l_z = -i\hbar \left(cos^2\emptyset \frac{\partial}{\partial \emptyset} + sin^2\emptyset \frac{\partial}{\partial \emptyset}\right)$$

$l_z = -i\hbar \frac{\partial}{\partial \emptyset}$ ------16

Similarly

$$l_x = i\hbar \left(sin\emptyset \frac{\partial}{\partial \theta} + cos\emptyset\, cot\theta \frac{\partial}{\partial \emptyset}\right) \quad ----17$$

$$l_y = i\hbar \left(sin\emptyset cot\theta \frac{\partial}{\partial \emptyset} - cos\emptyset \frac{\partial}{\partial \theta}\right) ------ 18$$

9.1.3 $\hat{L}^2$ Operator in Polar Coordinates:

$$\hat{L}^2 = \hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2 \quad ------ \quad 19$$

Sub. Eq. (16,17,and 18) in to eq.19

$$L^2 = -\hbar^2 \left\{\frac{\partial^2}{\partial \emptyset^2} + \left(sin\emptyset \frac{\partial}{\partial \theta} + cot\theta cos\emptyset \frac{\partial}{\partial \emptyset}\right)^2 + \left(sin\emptyset cot\theta \frac{\partial}{\partial \emptyset} - cos\emptyset \frac{\partial}{\partial \theta}\right)^2\right\}$$

$$L^2 = -\hbar^2 \left\{\frac{1}{sin^2\theta} \frac{\partial^2}{\partial \emptyset^2} + \frac{1}{sin\theta} \frac{\partial}{\partial \theta}\left(sin\theta \frac{\partial}{\partial \theta}\right)\right\} ------ 20$$

Eq.20 has especial importance:

Since $\hat{\nabla}^2$ (Laplacian Operator) in spherical coordinates has the form

$$\hat{\nabla}^2 = \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{sin\theta} \frac{\partial}{\partial \theta}\left(sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{sin^2\theta} \frac{\partial^2}{\partial \emptyset^2}\right] ----21$$

$$\hat{\nabla}^2 = \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2} \quad -------- 22$$

From eq.22 it may be shown that $[\hat{\mathcal{H}}, \hat{L}^2] = 0$, $[\hat{\nabla}^2, L^2] = 0$

$V \equiv V(r)$ function of (r) only, then the angular part in $\hat{\nabla}^2$ can be represented by $\hat{L}^2$, while the reminded part depends on r.

This fact enable to represent schr$\ddot{o}$Edinger's eq. in one dimension rather than 3- dimension, as V (r) is function of r only.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\big(rR_{nl}(r)\big)+\left[\frac{l(l+1)\hbar^2}{2mr^2}+V(r)\right]R_{nl}(r)=ER_{nl}(r)$$

9.2 Eigen Values of l_z Operator:

Let $\hat{l}_z\Psi(r,\theta,\emptyset)=m\,\Psi(r,\theta,\emptyset)$

$$-i\hbar\frac{\partial}{\partial\emptyset}\Psi(r,\theta,\emptyset)=m\,\Psi(r,\theta,\emptyset)$$

Then eq.23 becomes

$$-i\hbar\Psi(r,\theta)\frac{\partial}{\partial\emptyset}\Phi(\emptyset)=m\,\Psi(r,\theta)\Phi(\emptyset)$$

$$\frac{\partial\Phi(\emptyset)}{\Phi(\emptyset)}=\frac{i}{\hbar}m\partial\emptyset \qquad \therefore \qquad \ln\Phi(\emptyset)=\frac{i}{\hbar}m\emptyset$$

$\Phi(\emptyset)=\exp\,(\frac{i}{\hbar}m\emptyset)$ $\quad\therefore\quad$ $\Psi(r,\theta,\emptyset)=\varphi(r,\theta)e^{\frac{i}{\hbar}m\emptyset}$

$\exp(im\emptyset)=exp[im(\emptyset+2\pi)]$ $\qquad$ $\exp(im2\pi)=1$

Then $m=0,\pm1,\pm2,\pm3,-----etc$

$$\Psi(r,\theta,\emptyset)=\varphi(r,\theta)e^{\frac{i}{\hbar}m(\emptyset+2\pi)}$$

This means that $\hat{l}_z$ has definite eigen values discrete by $\hbar$.

This result is after the application of single valued condition for eigen function.

To normalize Φ (∅)

$$\int_0^{2\pi}N^2e^{-im\emptyset}e^{im\emptyset}d\emptyset=1 \qquad\qquad N=\frac{1}{\sqrt{2\pi}}$$

$\therefore\ \boxed{\Phi(\emptyset)=\frac{1}{\sqrt{2\pi}}e^{im\emptyset}}$ $\qquad$ This is the eigen function of $\hat{l}_z$

$$\hat{l}_z\Phi(\emptyset)=m\hbar\Phi(\emptyset) \qquad or\quad \hat{l}_z\Psi(r,\theta,\emptyset)=m\hbar\Psi(r,\theta,\emptyset)$$

9.3 The Commutation Relation for the Components of Orbital Angular Momentum.

$[l_x, l_y] = i\hbar l_z \quad , \qquad [l_y, l_z] = i\hbar l_x \ , \qquad [l_z, l_x] = i\hbar l_y$

The commutation relations represented above can be combined symbolically as follows $[\hat{\boldsymbol{L}}, \hat{\boldsymbol{L}}] = \boldsymbol{i}\hbar\hat{\boldsymbol{L}}$

9.4 The Commutation Relation of $\hat{\boldsymbol{L}}^2$ with $\boldsymbol{l_x}, \boldsymbol{l_y}, \boldsymbol{l_z}$.

The total orbital angular momentum is defined as follows:

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

$$[L^2, l_x] = [\hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2 \ , \ l_x]$$

$$[L^2, l_x] = (\hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2)l_x - l_x(\hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2)$$

$$[L^2, l_x] = l_x^2 l_x + l_y^2 l_x + l_z^2 l_x - (l_x l_x^2 + l_x l_y^2 + l_x l_z^2)$$

$$= (l_y^2 l_x - l_x l_y^2) + (l_z^2 l_x - l_x l_z^2)$$

$$= [l_y^2, l_x] + [l_z^2, l_x]$$

$[\hat{a}\hat{b}, \hat{c}] = \hat{a}[\hat{b}, \hat{c}] + [\hat{a}, \hat{c}]\hat{b}$

$$[l_y^2, l_x] = l_y[l_y, l_x] + [l_y, l_x]l_y$$

$$[l_z^2, l_x] = l_z[l_z, l_x] + [l_z, l_x]l_z$$

$$[l_x, l_z] = -i\hbar l_y \qquad \Rightarrow \qquad [l_z, l_x] = i\hbar l_y$$

$[l_x, l_y] = i\hbar l_z \quad \Rightarrow \quad [l_y, l_x] = -i\hbar l_z$

$$[L^2, l_x] = [l_y^2, l_x] + [l_z^2, l_x]$$

$$[L^2, l_x] = l_y(-i\hbar l_z) + (-i\hbar l_z)l_y + l_z(i\hbar l_y) + (i\hbar l_y)l_z = 0$$

$$[L^2, l_x] = 0 \quad , \quad [L^2, l_y] = 0 \quad , \quad [L^2, l_z] = 0$$

Hence $\hat{L}^2$ commutes with any of the three component of angular momentum operator.

Example:

Show that if a component of angular momentum of the electron in a hydrogen atom is known to be $2\hbar$ with 5% error, its angular orbital position in the plane perpendicular to that component can not be specified at all.

Solution:

$\Delta J \Delta\theta \sim \hbar$ where ΔJ uncertainty in angular momentum, $\Delta\theta$ uncertainty in angular position.

$\Delta J \sim \frac{\hbar}{\Delta\theta}$ from question $\Delta J \sim \frac{5}{100} \times 2\hbar = \frac{\hbar}{10}$

$$\Delta\theta \sim \frac{\hbar}{\Delta J} \sim \frac{\hbar}{\frac{\hbar}{10}} = 10\,radian$$

$$\Delta\theta > 2\pi = 2 \times 3.14 = 6.28\,radian$$

The angle in plane perpendicular to the component of angular momentum cannot be greater than ($2\pi = 6.28\,radian$. In this case uncertainty (10 rad) is greater than 2π. There fore the orbital position of the electron in the plane perpendicular to the given component of angular momentum cannot be specified at all.