

B.Sc. (Semester - 6)
Course: US06CPHY21
Quantum Mechanics

UNIT- IV Exactly Soluble Eigen value Problem

The Angular Momentum Operators:

The angular momentum of the particle about origin O is expressed as

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

Where, $\vec{r}(x, y, z)$ and $\vec{p}(p_x, p_y, p_z)$.

Now,

$$\begin{aligned} L^2 &= \vec{L} \cdot \vec{L} \\ &= (\vec{r} \times \vec{p}) \cdot \vec{L} \\ &= \vec{r} \cdot (\vec{p} \times \vec{L}) \\ &= \vec{r} \cdot [\vec{p} \times (\vec{r} \times \vec{p})] \\ &= \vec{r} \cdot [\vec{r}(\vec{p} \cdot \vec{p}) - \vec{p}(\vec{p} \cdot \vec{r})] \\ &= \vec{r} \cdot \vec{r}(\vec{p} \cdot \vec{p}) - \vec{r} \cdot \vec{p}(\vec{p} \cdot \vec{r}) \\ \therefore L^2 &= r^2 p^2 - (\vec{r} \cdot \vec{p})(\vec{p} \cdot \vec{r}) \end{aligned} \quad \dots (4.1)$$

But,

$$\begin{aligned} [\vec{r}, \vec{p}] &= i\hbar \\ \therefore \vec{r} \cdot \vec{p} - \vec{p} \cdot \vec{r} &= i\hbar \\ \therefore \vec{p} \cdot \vec{r} &= \vec{r} \cdot \vec{p} - i\hbar \end{aligned}$$

Therefore, equation (4.1) becomes,

$$\begin{aligned} L^2 &= r^2 p^2 - (\vec{r} \cdot \vec{p})(\vec{r} \cdot \vec{p} - i\hbar) \\ \therefore L^2 &= r^2 p^2 - (\vec{r} \cdot \vec{p})^2 + i\hbar(\vec{r} \cdot \vec{p}) \end{aligned} \quad \dots (4.2)$$

The components of angular momentum in Cartesian coordinates are

$$\begin{aligned} \vec{L} &= \vec{r} \times \vec{p} \\ \therefore \begin{bmatrix} L_x \\ L_y \\ L_z \end{bmatrix} &= \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{bmatrix} \\ \left. \begin{aligned} L_x &= yp_z - zp_y \\ L_y &= zp_x - xp_z \\ L_z &= xp_y - yp_x \end{aligned} \right\} \end{aligned} \quad \dots (4.3)$$

But,

$$\begin{aligned} p_x &\rightarrow -i\hbar \frac{\partial}{\partial x}, p_y \rightarrow -i\hbar \frac{\partial}{\partial y}, p_z \rightarrow -i\hbar \frac{\partial}{\partial z} \\ \therefore L_x &= -y i\hbar \frac{\partial}{\partial z} + z i\hbar \frac{\partial}{\partial y} \\ \therefore L_x &= i\hbar \left[z \frac{\partial}{\partial y} - y \frac{\partial}{\partial z} \right] \end{aligned} \quad \dots (4.4)$$

And,

$$L_y = -z i\hbar \frac{\partial}{\partial x} + x i\hbar \frac{\partial}{\partial z}$$

$$\therefore L_y = i\hbar \left[x \frac{\partial}{\partial z} - z \frac{\partial}{\partial x} \right] \quad \dots (4.5)$$

Similarly,

$$L_z = -x i\hbar \frac{\partial}{\partial y} + y i\hbar \frac{\partial}{\partial x}$$

$$\therefore L_z = i\hbar \left[y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right] \quad \dots (4.6)$$

The transformation equations are

$$\begin{cases} x = r \sin \Theta \cos \Phi \\ y = r \sin \Theta \sin \Phi \\ z = r \cos \Theta \end{cases} \quad \dots (4.7)$$

We have,

$$\frac{y}{x} = \frac{r \sin \Theta \sin \Phi}{r \sin \Theta \cos \Phi} = \frac{\sin \Phi}{\cos \Phi} = \tan \Phi$$

$$\therefore \Phi = \tan^{-1} \left(\frac{y}{x} \right) \quad \dots (4.8)$$

And

$$z = r \cos \Theta \rightarrow \cos \Theta = \frac{z}{r}$$

$$\therefore \Theta = \cos^{-1} \left(\frac{z}{r} \right) \quad \dots (4.9)$$

Also,

$$r^2 = x^2 + y^2 + z^2$$

$$\therefore r = (x^2 + y^2 + z^2)^{1/2}$$

Putting this value of r in equation (4.9), we get

$$\therefore \Theta = \cos^{-1} \frac{z}{(x^2 + y^2 + z^2)^{1/2}} \quad \dots (4.10)$$

Now,

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \Theta}{\partial x} \frac{\partial}{\partial \Theta} + \frac{\partial \Phi}{\partial x} \frac{\partial}{\partial \Phi} \quad \dots (4.11)$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y} \frac{\partial}{\partial r} + \frac{\partial \Theta}{\partial y} \frac{\partial}{\partial \Theta} + \frac{\partial \Phi}{\partial y} \frac{\partial}{\partial \Phi} \quad \dots (4.12)$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z} \frac{\partial}{\partial r} + \frac{\partial \Theta}{\partial z} \frac{\partial}{\partial \Theta} + \frac{\partial \Phi}{\partial z} \frac{\partial}{\partial \Phi} \quad \dots (4.13)$$

We have,

$$r^2 = x^2 + y^2 + z^2$$

$$\therefore 2r \frac{\partial r}{\partial x} = 2x$$

$$\therefore \frac{\partial r}{\partial x} = \frac{x}{r} = \frac{r \sin \Theta \cos \Phi}{r}$$

$$\therefore \frac{\partial r}{\partial x} = \sin \Theta \cos \Phi \quad \dots (4.14)$$

Similarly,

$$\therefore \frac{\partial r}{\partial y} = \frac{y}{r} = \sin \theta \sin \phi \quad \dots (4.15)$$

and $\therefore \frac{\partial r}{\partial z} = \frac{z}{r} = \cos \theta \quad \dots (4.16)$

Now,

$$\begin{aligned} \theta &= \cos^{-1} \frac{z}{(x^2 + y^2 + z^2)^{1/2}} \\ \therefore \frac{\partial \theta}{\partial x} &= - \frac{1}{\sqrt{1 - \frac{z^2}{x^2 + y^2 + z^2}}} \frac{z \left(-\frac{1}{2}\right)}{(x^2 + y^2 + z^2)^{3/2}} 2x \\ \therefore \frac{\partial \theta}{\partial x} &= \frac{zx(x^2 + y^2 + z^2)^{1/2}}{\sqrt{x^2 + y^2}} \frac{1}{(x^2 + y^2 + z^2)^{3/2}} \\ \therefore \frac{\partial \theta}{\partial x} &= \frac{zx}{\sqrt{x^2 + y^2} (x^2 + y^2 + z^2)} \\ \therefore \frac{\partial \theta}{\partial x} &= \frac{r \cos \theta \cdot r \sin \theta \cos \phi}{r \sin \theta} \frac{1}{r^2} = \frac{\cos \theta \cos \phi}{r} \\ \therefore \frac{\partial \theta}{\partial x} &= \frac{\cos \theta \cos \phi}{r} \quad \dots (4.17) \end{aligned}$$

Similarly,

$$\therefore \frac{\partial \theta}{\partial y} = \frac{\cos \theta \sin \phi}{r} \quad \dots (4.18)$$

and, $\frac{\partial \theta}{\partial z} = \frac{\sin \theta}{r} \quad \dots (4.19)$

Also we have,

$$\begin{aligned} \phi &= \tan^{-1} \left(\frac{y}{x} \right) \\ \therefore \frac{\partial \phi}{\partial x} &= \frac{1}{1 + \frac{y^2}{x^2}} y \left(-\frac{1}{x^2} \right) = -\frac{y}{x^2 + y^2} \\ \therefore \frac{\partial \phi}{\partial x} &= -\frac{r \sin \theta \cos \phi}{r^2 \sin^2 \theta} = -\frac{\sin \theta}{r \sin \theta} \\ \therefore \frac{\partial \phi}{\partial x} &= -\frac{\sin \theta}{r \sin \theta} \quad \dots (4.20) \end{aligned}$$

Similarly, $\frac{\partial \phi}{\partial y} = -\frac{\cos \phi}{r \sin \theta} \quad \dots (4.21)$

and, $\frac{\partial \phi}{\partial z} = 0 \quad \dots (4.22)$

put all these values in equations (4.11), (4.12) & (4.13), we get

$$\frac{\partial}{\partial x} = \sin \theta \cos \phi \frac{\partial}{\partial r} + \cos \theta \cos \phi \frac{\partial}{\partial \theta} - \frac{\sin \theta}{r \sin \theta} \frac{\partial}{\partial \phi} \quad \dots (4.23)$$

$$\frac{\partial}{\partial y} = \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \quad \dots (4.24)$$

$$\frac{\partial}{\partial z} = \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \quad \dots (4.24)$$

Now,

$$L_x = -i\hbar \left[y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right]$$

$$\begin{aligned} \therefore L_x &= -i\hbar \left[(r \sin \theta \sin \phi) \left(\cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right) \right. \\ &\quad \left. - (r \cos \theta) \left(\sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \right) \right] \\ \therefore L_x &= -i\hbar \left[r \sin \theta \sin \phi \cos \theta \frac{\partial}{\partial r} - \sin^2 \theta \sin \phi \frac{\partial}{\partial \theta} - r \sin \theta \cos \theta \sin \phi \frac{\partial}{\partial r} \right. \\ &\quad \left. - \cos^2 \theta \sin \phi \frac{\partial}{\partial \theta} - \frac{\cos \theta \cos \phi}{\sin \theta} \frac{\partial}{\partial \phi} \right] \\ &= -i\hbar \left[-\sin \phi \frac{\partial}{\partial \theta} - \cos \phi \cot \theta \frac{\partial}{\partial \phi} \right] \\ \therefore L_x &= i\hbar \left[\sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right] \quad \dots (4.25) \end{aligned}$$

Similarly,

$$L_y = i\hbar \left[-\cos \phi \frac{\partial}{\partial \theta} + \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right] \quad \dots (4.26)$$

$$L_z = -i\hbar \frac{\partial}{\partial \phi} \quad \dots (4.27)$$

This gives operator for L_z

We have,

$$L^2 = r^2 p^2 - (\vec{r} \cdot \vec{p})^2 + i\hbar(\vec{r} \cdot \vec{p})$$

Now,

$$r^2 p^2 = -r^2 \hbar^2 \nabla^2$$

And,

$$\vec{r} \cdot \vec{p} = \vec{r} \cdot (-i\hbar \vec{\nabla}) = -i\hbar(\vec{r} \cdot \vec{\nabla}) \quad \dots (4.28)$$

We know that,

$$\begin{aligned} r^2 &= x^2 + y^2 + z^2 \\ \therefore 2r \frac{\partial}{\partial r} &= 2x \frac{\partial}{\partial x} + 2y \frac{\partial}{\partial y} + 2z \frac{\partial}{\partial z} \\ \therefore r \frac{\partial}{\partial r} &= x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} + z \frac{\partial}{\partial z} = (\hat{i}x + \hat{j}y + \hat{k}z) \cdot \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) \\ \therefore r \frac{\partial}{\partial r} &= \vec{r} \cdot \vec{\nabla} \\ \therefore \vec{r} \cdot \vec{\nabla} &= r \frac{\partial}{\partial r} \quad \dots (4.29) \end{aligned}$$

Using equation (4.29) in (4.28), we get

$$\begin{aligned}
\vec{r} \cdot \vec{p} &= -i\hbar r \frac{\partial}{\partial r} \\
\therefore (\vec{r} \cdot \vec{p})^2 &= (\vec{r} \cdot \vec{p}) \cdot (\vec{r} \cdot \vec{p}) \\
&= \left(-i\hbar r \frac{\partial}{\partial r}\right) \left(-i\hbar r \frac{\partial}{\partial r}\right) \\
&= -\hbar^2 r \left[\frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) \right] \\
\therefore (\vec{r} \cdot \vec{p})^2 &= -\hbar^2 r^2 \frac{\partial^2}{\partial r^2} - \hbar^2 r \frac{\partial}{\partial r}
\end{aligned}$$

Hence operator L^2 can be written as,

$$\begin{aligned}
L^2 &= -r^2 \hbar^2 \nabla^2 + \hbar^2 r^2 \frac{\partial^2}{\partial r^2} + \hbar^2 r \frac{\partial}{\partial r} + \hbar^2 r \frac{\partial}{\partial r} \\
&= -r^2 \hbar^2 \nabla^2 + \hbar^2 r^2 \frac{\partial^2}{\partial r^2} + 2 \hbar^2 r \frac{\partial}{\partial r} \\
&= -r^2 \hbar^2 \nabla^2 + \hbar^2 \frac{\partial}{\partial r} \left[r^2 \frac{\partial}{\partial r} \right] \\
\therefore L^2 &= -\hbar^2 \left[r^2 \nabla^2 - \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right] \quad \dots (4.30)
\end{aligned}$$

Substituting the value of operator ∇^2 in spherical polar coordinates we get,

$$\begin{aligned}
L^2 &= -\hbar^2 \left\{ r^2 \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] - \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right\} \\
\therefore L^2 &= -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad \dots (4.31)
\end{aligned}$$

This is expression for L^2 operator in spherical polar coordinates.

The Eigen Value Equation for L^2 ; Separation of Variables:

The eigen value equation is given by

$$A\phi_a = a\phi_a \quad \dots (4.32)$$

Where,

$A \rightarrow$ operator

$\phi_a \rightarrow$ eigen function and

$a \rightarrow$ eigen value

Here,

$$L^2 v(\theta, \phi) = \lambda \hbar^2 v(\theta, \phi) \quad \dots (4.33)$$

This is the eigen value equation for L^2 operator.

$v(\theta, \phi) \rightarrow$ eigen function of L^2

$\lambda \hbar^2 \rightarrow$ eigen value of L^2

Here, we have used the $\lambda \hbar^2$ for the eigen value parameter of L^2 operator.

$$-\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] v(\theta, \phi) = \lambda \hbar^2 v(\theta, \phi) \quad \dots (4.34)$$

To solve eigen value equation L^2 , we use the method of separation of variable.

Let,

$$v(\theta, \phi) = \theta(\theta) \Phi(\phi) \quad \dots (4.35)$$

Hence, equation (4.34) becomes

$$-\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] [\theta(\theta) \Phi(\phi)] = \lambda \hbar^2 [\theta(\theta) \Phi(\phi)]$$

$$- \left[\frac{\Phi(\phi)}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \theta(\theta) \right) \right] - \frac{\theta(\theta)}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) = \lambda \theta(\theta) \Phi(\phi)$$

Multiplying both sides by $\frac{\sin^2 \theta}{\theta(\theta) \Phi(\phi)}$ we get,

$$- \left[\frac{\sin \theta}{\theta(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \theta(\theta) \right) \right] - \frac{1}{\Phi(\phi)} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) = \lambda \sin^2 \theta$$

$$\therefore - \frac{1}{\Phi(\phi)} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) = \lambda \sin^2 \theta + \frac{\sin \theta}{\theta(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \theta(\theta) \right) \quad \dots (4.36)$$

The L.H.S of this equation is independent of θ and R.H.S is independent of ϕ . There equality implies that both sides must be independent of θ & ϕ , and hence both sides must be equal to some constant m^2 .

$$\therefore \frac{\sin \theta}{\theta(\theta)} \frac{d}{d\theta} \left(\sin \theta \frac{d}{d\theta} \theta(\theta) \right) + \lambda \sin^2 \theta = m^2 \quad \dots (4.37)$$

$$\text{and,} \quad - \frac{1}{\Phi(\phi)} \frac{d^2 \Phi(\phi)}{d\phi^2} = m^2 \quad \dots (4.38)$$

Multiplying equation (4.37) by $\frac{\theta(\theta)}{\sin^2 \theta}$, we get

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d}{d\theta} \theta(\theta) \right) + \left(\lambda - \frac{m^2}{\sin^2 \theta} \right) \theta(\theta) = 0 \quad \dots (4.39)$$

Admissibility Conditions on Solutions; Eigen Values:

We know that,

$$- \frac{1}{\Phi(\phi)} \frac{d^2 \Phi(\phi)}{d\phi^2} = m^2$$

$$\therefore \frac{d^2 \Phi(\phi)}{d\phi^2} = -m^2 \Phi(\phi) \quad \dots (4.40)$$

There are two solution of equation (4.40)

$$\Phi(\phi) = e^{im\phi} \quad \text{and} \quad \Phi(\phi) = e^{-im\phi}$$

The wave function should be finite and single valued. This is known as admissibility conditions. Since values of ϕ differing by integer multiplies of 2π refer to the same physical point, these solutions will satisfy the condition of single-valued ness only if

$$e^{im\phi} = e^{im(\phi+2\pi)}$$

$$\therefore e^{im2\pi} = 1 \quad \dots (4.41)$$

$$\therefore \cos(2m\pi) + i \sin(2m\pi) = 1 \quad \dots (4.42)$$

When $2m\pi = 0, 2\pi, 4\pi, \dots$ above equation will be satisfied.

$$\therefore m = 0, \pm 1, \pm 2, \dots$$

These are the possible values of m .

The above condition will satisfy if it is a real integer.

The norm is given by

$$\int \Phi^*(\phi) \Phi(\phi) d\tau = 1$$

Here,

$$\begin{aligned} \Phi(\phi) &= A e^{im\phi} \\ \text{and, } \Phi^*(\phi) &= A^* e^{-im\phi} \end{aligned}$$

Substituting these values in above equation, we get

$$\begin{aligned} \int_0^{2\pi} A^* e^{-im\phi} A e^{im\phi} d\phi &= 1 \\ \therefore |A|^2 \int_0^{2\pi} d\phi &= 1 \\ \therefore |A|^2 2\pi &= 1 \\ \therefore A &= \frac{1}{\sqrt{2\pi}} \end{aligned} \quad \dots (4.43)$$

\therefore The normalized function Φ is given by

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad \dots (4.44)$$

$\theta(\theta)$ equation is given by

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d}{d\theta} \theta(\theta) \right) + \left(\lambda - \frac{m^2}{\sin^2 \theta} \right) \theta(\theta) = 0 \quad \dots (4.45)$$

To solve $\theta(\theta)$ equation, suppose $\cos \theta = \omega$

$$\therefore -\sin \theta = \frac{d\omega}{d\theta}$$

$$\begin{aligned} \text{we can write, } \frac{d}{d\theta} &= \frac{d}{d\omega} \frac{d\omega}{d\theta} \\ \therefore \frac{d}{d\theta} &= -\sin \theta \frac{d}{d\omega} \\ \therefore \frac{1}{\sin \theta} \frac{d}{d\theta} &= -\frac{d}{d\omega} \end{aligned}$$

Now,

$$\begin{aligned} \cos \theta &= \omega \\ \therefore \sin^2 \theta &= 1 - \cos^2 \theta \\ \therefore \sin^2 \theta &= 1 - \omega^2 \end{aligned}$$

Substituting these values in equation (4.45), we get

$$\begin{aligned} -\frac{d}{d\omega} \left[\sqrt{1 - \omega^2} \left(-\sin \theta \frac{d\theta}{d\omega} \right) \right] + \left[\lambda - \frac{m^2}{1 - \omega^2} \right] \theta(\theta) &= 0 \\ \therefore \frac{d}{d\omega} \left[\sqrt{1 - \omega^2} \times \sqrt{1 - \omega^2} \frac{d\theta}{d\omega} \right] + \left[\lambda - \frac{m^2}{1 - \omega^2} \right] \theta(\theta) &= 0 \\ \therefore \frac{d}{d\omega} \left[(1 - \omega^2) \frac{d\theta}{d\omega} \right] + \left[\lambda - \frac{m^2}{1 - \omega^2} \right] \theta(\theta) &= 0 \end{aligned}$$

Take the solution $\theta(\theta) = P(\omega)$

$$\begin{aligned}\therefore \frac{d}{d\omega} \left[(1 - \omega^2) \frac{dP(\omega)}{d\omega} \right] + \left[\lambda - \frac{m^2}{1 - \omega^2} \right] P(\omega) &= 0 \\ \therefore (1 - \omega^2) \frac{d^2P}{d\omega^2} - 2\omega \frac{dP}{d\omega} + \left[\lambda - \frac{m^2}{1 - \omega^2} \right] P(\omega) &= 0 \quad \dots (4.46)\end{aligned}$$

The solution of this polynomial equation is

$$P(\omega) = (1 - \omega^2)^a K(\omega) \quad , a > 0 \quad \dots (4.47)$$

Differentiate with respect to ω

$$\begin{aligned}\frac{dP}{d\omega} &= (1 - \omega^2)^a \frac{dK}{d\omega} + K(\omega) a (1 - \omega^2)^{a-1} (-2\omega) \\ \therefore \frac{dP}{d\omega} &= (1 - \omega^2)^a \frac{dK}{d\omega} - 2a\omega K(\omega) a (1 - \omega^2)^{a-1} \quad \dots (4.48) \\ \frac{d^2P}{d\omega^2} &= (1 - \omega^2)^a \frac{d^2K}{d\omega^2} + \frac{dK}{d\omega} a (1 - \omega^2)^{a-1} (-2\omega) \\ &\quad - 2a\omega K(\omega) (a-1) (1 - \omega^2)^{a-2} (-2\omega) - 2aK(\omega) (1 - \omega^2)^{a-1} \\ &\quad - 2a\omega \frac{dK}{d\omega} (1 - \omega^2)^{a-1} \\ \therefore \frac{d^2P}{d\omega^2} &= (1 - \omega^2)^a \frac{d^2K}{d\omega^2} - 2a\omega \frac{dK}{d\omega} (1 - \omega^2)^{a-1} + 4a(a-1)\omega^2 K(\omega) (1 - \omega^2)^{a-2} \\ &\quad - 2aK(\omega) (1 - \omega^2)^{a-1} - 2a\omega \frac{dK}{d\omega} (1 - \omega^2)^{a-1} \\ \therefore \frac{d^2P}{d\omega^2} &= (1 - \omega^2)^a \frac{d^2K}{d\omega^2} - 4a\omega \frac{dK}{d\omega} (1 - \omega^2)^{a-1} + 4a(a-1)\omega^2 K(\omega) (1 - \omega^2)^{a-2} \\ &\quad - 2aK(\omega) (1 - \omega^2)^{a-1} \quad \dots (4.49)\end{aligned}$$

Substituting equations (4.47), (4.48) & (4.49) in equation (4.46), we get

$$\begin{aligned}(1 - \omega^2) \frac{d^2P}{d\omega^2} - 2\omega \frac{dP}{d\omega} + \left[\lambda - \frac{m^2}{1 - \omega^2} \right] P(\omega) &= 0 \\ (1 - \omega^2) \left[(1 - \omega^2)^a \frac{d^2K}{d\omega^2} - 4a\omega \frac{dK}{d\omega} (1 - \omega^2)^{a-1} + 4a(a-1)\omega^2 K(\omega) (1 - \omega^2)^{a-2} \right. \\ &\quad \left. - 2aK(\omega) (1 - \omega^2)^{a-1} \right] \\ &\quad - 2\omega \left[(1 - \omega^2)^a \frac{dK}{d\omega} - 2a\omega K(\omega) a (1 - \omega^2)^{a-1} \right] \\ &\quad + \left[\lambda - \frac{m^2}{1 - \omega^2} \right] (1 - \omega^2)^a K(\omega) = 0 \\ \therefore (1 - \omega^2)^{a+1} \frac{d^2K}{d\omega^2} - 4a\omega (1 - \omega^2)^a \frac{dK}{d\omega} + 4a(a-1)\omega^2 K(\omega) (1 - \omega^2)^{a-1} \\ &\quad - 2aK(\omega) (1 - \omega^2)^a - 2\omega (1 - \omega^2)^a \frac{dK}{d\omega} - 4a\omega^2 K(\omega) (1 - \omega^2)^{a-1} \\ &\quad + \lambda (1 - \omega^2)^a K(\omega) - \frac{m^2}{1 - \omega^2} (1 - \omega^2)^a K(\omega) = 0\end{aligned}$$

Dividing throughout by $(1 - \omega^2)^a$, we get

$$\begin{aligned}
& \therefore (1 - \omega^2) \frac{d^2 K}{d\omega^2} - 4a\omega \frac{dK}{d\omega} + \frac{4a(a-1)\omega^2 K(\omega)}{1 - \omega} - 2aK(\omega) - 2\omega \frac{dK}{d\omega} - \frac{4a\omega^2 K(\omega)}{1 - \omega} \\
& \quad + \lambda K(\omega) - \frac{m^2}{1 - \omega^2} K(\omega) = 0 \\
& \therefore (1 - \omega^2) \frac{d^2 K}{d\omega^2} - 2\omega(2a+1) \frac{dK}{d\omega} + \left[-2a + \frac{4a^2(\omega^2 - 1)}{1 - \omega^2} + \frac{4a^2}{1 - \omega^2} - \frac{m^2}{1 - \omega^2} + \lambda \right] K(\omega) \\
& \quad = 0 \\
& \therefore (1 - \omega^2) \frac{d^2 K}{d\omega^2} - 2\omega(2a+1) \frac{dK}{d\omega} + \left[-2a - 4a^2 + \frac{4a^2}{1 - \omega^2} - \frac{m^2}{1 - \omega^2} + \lambda \right] K(\omega) = 0 \\
& \therefore (1 - \omega^2) \frac{d^2 K}{d\omega^2} - 2\omega(2a+1) \frac{dK}{d\omega} + \left[-2a - 4a^2 + \frac{4a^2 - m^2}{1 - \omega^2} + \lambda \right] K(\omega) = 0
\end{aligned}$$

We assume that, $4a^2 = |m|^2$

$$\therefore 2a = |m|$$

By putting the above assumption, we get

$$\therefore (1 - \omega^2) \frac{d^2 K}{d\omega^2} - 2\omega(|m| + 1) \frac{dK}{d\omega} + [\lambda - |m| - |m|^2] K(\omega) = 0 \quad \dots (4.50)$$

The above equation can be solved by series method. The series solution of the above equation is given by

$$\begin{aligned}
K(\omega) &= \sum a_n \omega^{n+s} \\
\therefore \frac{dK}{d\omega} &= \sum a_n (n+s) \omega^{n+s-1} \\
\text{and, } \frac{d^2 K}{d\omega^2} &= \sum a_n (n+s)(n+s-1) \omega^{n+s-2}
\end{aligned}$$

put $s = 0$, we have

$$\begin{aligned}
K(\omega) &= \sum a_n \omega^n \\
\therefore \frac{dK}{d\omega} &= \sum a_n (n) \omega^{n-1} \\
\text{and, } \frac{d^2 K}{d\omega^2} &= \sum a_n (n)(n-1) \omega^{n-2}
\end{aligned}$$

Substituting these values in equation (4.50), we get

$$\begin{aligned}
& (1 - \omega^2) \sum a_n n(n-1) \omega^{n-2} - 2\omega(|m| + 1) \sum a_n (n) \omega^{n-1} \\
& \quad + [\lambda - |m| - |m|^2] \sum a_n \omega^n = 0 \\
& \therefore \sum a_n n(n-1) \omega^{n-2} - \sum a_n n(n-1) \omega^n - 2(|m| + 1) \sum a_n n \omega^{n-1} \\
& \quad + [\lambda - |m| - |m|^2] \sum a_n \omega^n = 0 \\
& \therefore \sum a_n n(n-1) \omega^{n-2} - \sum a_n [n(n-1) + 2(|m| + 1)n - (\lambda - |m| - |m|^2)] \omega^n \\
& \quad = 0 \quad \dots (4.51)
\end{aligned}$$

Now, equate the coefficients of ω^r to zero.

We substitute $n = r + 2$ in first term and $n = r$ in the second term, we have

$$\begin{aligned}\therefore a_{r+2}(r+2)(r+1)\omega^r - a_r[r(r-1) + 2(|m|+1)r - \lambda + |m| + |m|^2]\omega^r &= 0 \\ \therefore a_{r+2}(r+2)(r+1) &= a_r[r(r-1) + 2(|m|+1)r - \lambda + |m| + |m|^2] \\ \therefore \frac{a_{r+2}}{a_r} &= \frac{r^2 - r + 2|m|r + 2r - \lambda + |m| + |m|^2}{(r+2)(r+1)} \\ \therefore \frac{a_{r+2}}{a_r} &= -\frac{\lambda - (r+|m|)(1+r+|m|)}{(r+1)(r+2)} \quad \dots (4.52)\end{aligned}$$

This is the recurrence relation for the series $K(\omega)$

$$\begin{aligned}K(\omega) &= \sum a_n \omega^n \\ \therefore K(\omega) &= a_0 + a_2 \omega^2 + a_4 \omega^4 + \dots \\ \text{Here, } a_1 &= a_3 = a_5 = \dots = 0\end{aligned}$$

If the ratio of successive coefficients $\frac{a_{r+2}}{a_r} \rightarrow 0$, then series is called convergent.

$$\therefore \lim_{r \rightarrow \infty} \frac{a_{r+2}}{a_r} \rightarrow 0$$

Here, r is very large, then we can neglect λ .

$$\begin{aligned}\therefore \frac{a_{r+2}}{a_r} &= -\frac{(r+|m|)(r+|m|+1)}{(r+1)(r+2)} \\ &= \frac{r^2 \left(1 + \frac{|m|}{r}\right) \left(1 + \frac{|m|+1}{r}\right)}{r^2 \left(1 + \frac{1}{r}\right) \left(1 + \frac{2}{r}\right)} \\ \therefore \frac{a_{r+2}}{a_r} &= \left(1 + \frac{|m|}{r}\right) \left(1 + \frac{|m|+1}{r}\right) \left(1 + \frac{1}{r}\right)^{-1} \left(1 + \frac{2}{r}\right)^{-1}\end{aligned}$$

Neglect the higher order terms

$$\begin{aligned}\therefore \frac{a_{r+2}}{a_r} &= \left(1 + \frac{|m|}{r}\right) \left(1 + \frac{|m|+1}{r}\right) \left(1 - \frac{1}{r}\right) \left(1 - \frac{2}{r}\right) \\ \therefore \frac{a_{r+2}}{a_r} &= 1 + \frac{2|m| - 2}{r}\end{aligned}$$

Putting $2a = |m|$, we get

$$\therefore \frac{a_{r+2}}{a_r} = 1 + \frac{4a - 2}{r} + \dots \dots \dots \quad \dots (4.53)$$

Since the coefficients tend to equality as $r \rightarrow \infty$, the series $K(\omega)$ diverges for $\omega = 1$. In fact, the asymptotic behavior of the ratio in the series $K(\omega)$ is exactly the same as that of the ratio of successive coefficient in the expansion of series $(1 - \omega^2)^{-2a}$.

$$\begin{aligned}P(\omega) &= (1 - \omega^2)^a K(\omega) \\ \therefore P(\omega) &= (1 - \omega^2)^a (1 - \omega^2)^{-2a} \\ \therefore P(\omega) &= (1 - \omega^2)^{-a}\end{aligned}$$

But, $\omega = \cos \theta$, $\therefore \omega^2 \rightarrow 1$, $\therefore P(\omega) \rightarrow \infty$

Therefore, in the neighborhood of $\omega^2 = 1$, not only $K(\omega)$ diverges like $(1 - \omega^2)^{-2a}$, but also $P(\omega)$ would diverges like $(1 - \omega^2)^{-a}$. The only way to escape this unacceptable singularity of $P(\omega)$ at $\omega = \pm 1$ is by terminating the series $K(\omega)$ after a certain number of terms.

This can be done by choosing numerator in the recursion relation

$$\lambda - (r + |m|)(r + |m| + 1) = 0$$

$$\therefore \lambda = (r + |m|)(r + |m| + 1)$$

Take $r = t$, $t = 0, 1, 2, \dots$, where t may have any values $0, 1, 2, \dots$

$$\therefore \lambda = (t + |m|)(t + |m| + 1)$$

Assume, $t + |m| = l$

$$\therefore \lambda = l(l + 1) \quad \dots (4.54)$$

$t + |m| = l$ is non-negative integer.

\therefore The eigen values of L^2 operator is given by

$$\therefore \lambda \hbar^2 = l(l + 1) \hbar^2 \quad \dots (4.55)$$

The Eigen Functions of L^2 – Operator: [Spherical Harmonics]

The θ equation can be written as

$$(1 - \omega^2)K''(\omega) - 2\omega(|m| + 1)K'(\omega) + [\lambda - |m| - |m|^2]K(\omega) = 0$$

But, $\lambda = l(l + 1)$

$$\therefore (1 - \omega^2)K''(\omega) - 2\omega(|m| + 1)K'(\omega) + [l(l + 1) - |m| - |m|^2]K(\omega) = 0 \quad \dots (4.56)$$

This equation is closely related to Legendre's differential equation.

If $m = 0$, then it reduces to Legendre's equation.

$$\therefore (1 - \omega^2)K''(\omega) - 2\omega K'(\omega) + l(l + 1)K(\omega) = 0 \quad \dots (4.57)$$

$$\therefore (1 - \omega^2)P_l''(\omega) - 2\omega P_l'(\omega) + l(l + 1)P_l(\omega) = 0 \quad \dots (4.58)$$

Here, $P_l(\omega)$ is Legendre polynomials. Actually equation (4.56) is m^{th} derivatives of equation (4.57)

According to Leibnitz theorem

$$\frac{d^m}{dx^m}(f_1 f_2) = f_1 \frac{d^m}{dx^m} f_2 + mC_1 \frac{df_1}{dx} \frac{d^{m-1}}{dx^{m-1}} f_2 + mC_2 \frac{d^2 f_1}{dx^2} \frac{d^{m-2}}{dx^{m-2}} f_2 + \dots \dots \dots \quad \dots (4.59)$$

Using Leibnitz theorem, taking m^{th} derivatives of 1st term of equation (4.58), we get

➤ **1st term:**

$$\begin{aligned} \frac{d^m}{dx^m} [(1 - \omega^2)P_l''(\omega)] &= (1 - \omega^2) \frac{d^{m+2}P_l}{d\omega^{m+2}} + mC_1(-2\omega) \frac{d^{m+1}P_l}{d\omega^{m+1}} + mC_2(-2) \frac{d^m P_l}{d\omega^m} \\ &= (1 - \omega^2) \frac{d^{m+2}P_l}{d\omega^{m+2}} + \frac{m!}{1!(m-1)!} (-2\omega) \frac{d^{m+1}P_l}{d\omega^{m+1}} + \frac{m!}{2!(m-2)!} (-2) \frac{d^m P_l}{d\omega^m} \\ \therefore \frac{d^m}{dx^m} [(1 - \omega^2)P_l''(\omega)] &= (1 - \omega^2) \frac{d^{m+2}P_l}{d\omega^{m+2}} - 2m\omega \frac{d^{m+1}P_l}{d\omega^{m+1}} - m(m-1) \frac{d^m P_l}{d\omega^m} \dots (4.60) \end{aligned}$$

Similarly, m^{th} derivatives of 2nd term of equation (4.58) is given by

➤ **2nd term:**

$$\begin{aligned} \frac{d^m}{dx^m} [2\omega P_l'(\omega)] &= 2\omega \frac{d^{m+1}P_l}{d\omega^{m+1}} + mC_1 2 \frac{d^m P_l}{d\omega^m} \\ \therefore \frac{d^m}{dx^m} [2\omega P_l'(\omega)] &= 2\omega \frac{d^{m+1}P_l}{d\omega^{m+1}} + 2m \frac{d^m P_l}{d\omega^m} \quad \dots (4.61) \end{aligned}$$

➤ **3rd term:**

$$\frac{d^m}{dx^m} [l(l+1)P_l(\omega)] = l(l+1) \frac{d^m P_l}{d\omega^m} \quad \dots (4.62)$$

The m^{th} derivative of Legendre's differential equation is

$$(1-\omega^2) \frac{d^{m+2} P_l(\omega)}{d\omega^{m+2}} - 2\omega(|m|+1) \frac{d^{m+1} P_l(\omega)}{d\omega^{m+1}} + [l(l+1) - |m| - |m|^2] \frac{d^m P_l(\omega)}{d\omega^m} = 0 \quad \dots (4.63)$$

Now comparing equations (4.56) & (4.63)

$K(\omega)$ is the m^{th} derivative of $P_l(\omega)$.

$$K(\omega) = \frac{d^m P_l(\omega)}{d\omega^m} = P_l^m(\omega) \quad \dots (4.64)$$

The polynomial solution of θ equation is

$$\begin{aligned} \theta(\theta) &= (1-\omega^2)^a K(\omega) \\ \therefore \theta(\theta) &= (1-\omega^2)^a P_l^m(\omega) \end{aligned}$$

Now, $\omega = \cos \theta$

$$\therefore 1 - \omega^2 = \sin^2 \theta$$

and, $2a = |m|$

$$\begin{aligned} \therefore a &= \frac{|m|}{2} \\ \therefore \theta(\theta) &= (\sin^2 \theta)^{\frac{|m|}{2}} \frac{d^m}{d\omega^m} P_l(\omega) \\ \therefore \theta(\theta) &= \sin^{|m|} \theta \frac{d^m}{d\omega^m} P_l(\omega) \\ \therefore P_l^m(\omega) &= \sin^{|m|} \theta \frac{d^m}{d\omega^m} P_l(\omega) \quad \dots (4.65) \end{aligned}$$

The above equation is now seen to be identical with associated Legendre function. For fixed value of m , associate Legendre function $P_l^m(\omega)$ & $P_{l'}^m(\omega)$ are mutually orthogonal.

The orthogonality property is defined as

$$\begin{aligned} \int P_l^m(\omega) P_{l'}^m(\omega) d\omega &= \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{ll'} \quad \dots (4.66) \\ \delta_{ll'} &= 1 \quad \text{for } l = l' \\ \delta_{ll'} &= 0 \quad \text{for } l \neq l' \end{aligned}$$

If we take $l = l'$, then

$$\begin{aligned} \int P_l^m(\omega) P_l^m(\omega) d\omega &= \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \\ \int |P_l^m(\omega)|^2 d\omega &= \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \quad \dots (4.67) \end{aligned}$$

The function $\theta(\theta)$ can now be written as

$$\theta(\theta) = N \cdot P_l^m(\omega) \quad \dots (4.68)$$

N is a normalization constant. The orthogonality property for $\theta(\theta)$ function defined as

$$\int \theta_{lm}(\theta) \theta_{lm}(\theta) \sin \theta d\theta = 1 \quad \dots (4.69)$$

Using equation (4.68) in (4.69), we get

$$- \int N P_l^m(\omega) \times N P_l^m(\omega) d\omega = 1$$

$$\therefore N^2 \int |P_l^m(\omega)|^2 d\omega = 1$$

Because, $\omega = \cos \theta$, $\therefore d\omega = -\sin \theta d\theta$

The limit of θ is from $0 \rightarrow \pi$, $\omega = \cos \theta$ is from -1 to $+1$.

Substituting the value of integral from equation (4.67), we get

$$N^2 \left[\frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \right] = 1$$

$$\therefore N = \left[\frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \right]^{1/2} \quad \dots (4.70)$$

The normalized $\theta(\theta)$ function is given by

$$\theta_{lm}(\theta) = \left[\frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \right]^{1/2} P_l^m(\omega) \quad \dots (4.71)$$

The complete eigen function of L^2 operator is

$$v(\theta, \phi) = \theta(\theta) \Phi(\phi)$$

$$\therefore v(\theta, \phi) = \left[\frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \right]^{1/2} P_l^m(\omega) \times \frac{1}{\sqrt{\pi}} e^{im\phi}$$

Putting $v(\theta, \phi) = Y_{lm}(\theta, \phi)$, we get

$$Y_{lm}(\theta, \phi) = \left[\frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \right]^{1/2} P_l^m(\omega) (-1)^m e^{im\phi} \quad \dots (4.72)$$

This is the eigen function for L^2 operator.

➤ SPHERICAL HARMONICS:

(i) $l = m = 0$

$$Y_{0,0} = \left[\frac{1}{4\pi} \right]^{1/2} (-1)^0 P_0^0(\cos \theta) e^0$$

$$\therefore Y_{0,0} = \left[\frac{1}{4\pi} \right]^{1/2}$$

(ii) $l = 0, m = 0$

$$Y_{1,0} = \left[\frac{3}{4\pi} \right]^{1/2} (-1)^0 P_1^0(\cos \theta) e^0$$

$$\therefore Y_{1,0} = \left[\frac{3}{4\pi} \right]^{1/2} \cos \theta$$

(iii) $l = m = 1$

$$Y_{1,1} = \left[\frac{3}{4\pi} \frac{1}{2} \right]^{1/2} (-1)^1 P_1^1(\cos \theta) e^{i\phi}$$

$$= - \left[\frac{3}{8\pi} \right]^{1/2} P_1^1(\cos \theta) e^{i\phi}$$

$$\begin{aligned} \therefore Y_{1,1} &= -\left[\frac{3}{8\pi}\right]^{1/2} \sin \theta e^{i\phi} \\ \text{(iv)} \quad l &= 1, m = -1 \\ Y_{1,-1} &= \left[\frac{3}{8\pi}\right]^{1/2} \sin \theta e^{-i\phi} \\ \text{(v)} \quad l &= 2, m = 0 \\ Y_{2,0} &= \left[\frac{10}{8\pi}\right]^{1/2} \frac{1}{2} [3\cos^2 \theta - 1] \\ \therefore Y_{2,0} &= \left[\frac{5}{16\pi}\right]^{1/2} (3\cos^2 \theta - 1) \\ \text{(vi)} \quad l &= 2, m = 1 \\ Y_{2,1} &= \left[\frac{5}{4\pi} \frac{1}{6}\right]^{1/2} (-1)^1 P_2^1(\cos \theta) e^{i\phi} \\ \therefore Y_{2,1} &= -\left[\frac{5}{24\pi}\right]^{1/2} \sin \theta \cos \theta e^{i\phi} \end{aligned}$$

Legendre polynomial is defined as

$$P_l(\omega) = \frac{1}{2^l l!} \frac{d^l}{d\omega^l} (\omega^2 - 1)^l$$

For, $m = 0$

$$\begin{aligned} \text{(i)} \quad l &= 0; P_0^0(\omega) = \frac{1}{1} = 1 \\ \text{(ii)} \quad l &= 1; P_1^0(\omega) = \frac{1}{2} = \frac{d}{d\omega} (\omega^2 - 1)^1 = \frac{1}{2} 2\omega = \omega = \cos \theta \\ \text{(iii)} \quad l &= 2; P_2^0(\omega) = \frac{1}{(2)^2 (2)} \frac{d^2}{d\omega^2} (\omega^2 - 1)^2 = \frac{1}{8} \frac{d^2}{d\omega^2} (\omega^2 - 1)^2 \\ \therefore P_2^0(\omega) &= \frac{1}{8} \frac{d^2}{d\omega^2} (\omega^4 - 2\omega^2 + 1) = \frac{1}{8} \frac{d}{d\omega} (4\omega^3 - 4\omega) \\ \therefore P_2^0(\omega) &= \frac{d}{d\omega} [(4)(3)\omega^2 - 4] \\ \therefore P_2^0(\omega) &= \frac{1}{2} [3\cos^2 \theta - 1] \end{aligned}$$

$$\triangleright P_l^m(\cos \theta) = \sin^m(\theta) \frac{d^m}{d\omega^m} P_l(\cos \theta)$$

$$\text{(i)} \quad l = 1, m = 1$$

$$P_1^1(\cos \theta) = \sin \theta \frac{d^1}{d\omega^1} P_1(\cos \theta) = \sin \theta \frac{d^1}{d\omega^1} (\omega) = \sin \theta$$

$$\text{(ii)} \quad l = 2, m = 1$$

$$P_2^1(\cos \theta) = \sin \theta \frac{d}{d\omega} P_2(\cos \theta) = \sin \theta$$

➤ Polar Diagram: $[Y_{lm}(\theta, \phi) \rightarrow 0]$

Polar diagram is a diagram of spherical harmonics.

$$\text{(i)} \quad Y_{0,0} = \left[\frac{1}{4\pi}\right]^{1/2} = 0.28$$

$$(ii) \quad Y_{1,0} = \left[\frac{3}{4\pi} \right]^{1/2} \cos \theta$$

$$\text{When, } \theta = 0, Y_{1,0} = \left[\frac{3}{4\pi} \right]^{1/2} (1) = 0.488$$

$$\text{When, } \theta = 30^\circ, Y_{1,0} = \left[\frac{3}{4\pi} \right]^{1/2} (0.8660) = 0.4226$$

$$\text{When, } \theta = 45^\circ, Y_{1,0} = \left[\frac{3}{4\pi} \right]^{1/2} \frac{1}{\sqrt{2}} = 0.3450$$

$$\text{When, } \theta = 90^\circ, Y_{1,0} = 0$$

The polar diagrams for the $Y_{lm}(\theta, \phi)$ for points in the $x - z$ plane are shown in fig.(4.1)

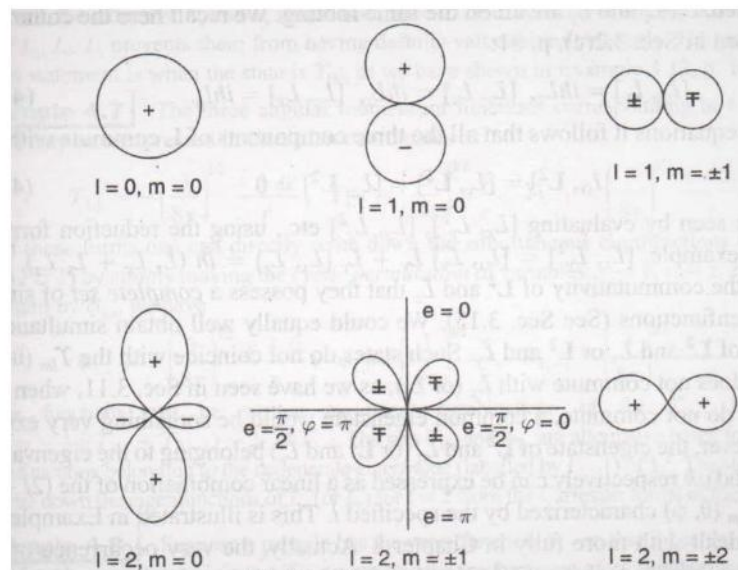


Fig: 4.1

➤ Physical Interpretation:

The z - component of angular momentum operator is

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

Eigen value equation for L^2 operator is

$$L^2 v(\theta, \phi) = \lambda \hbar^2 v(\theta, \phi)$$

Where, $\lambda = l(l+1)$

Here, $\lambda \hbar^2$ is eigen value of L^2 , $v(\theta, \phi)$ is eigen function of L^2

The spherical harmonics

$$Y_{lm}(\theta, \phi) = \Theta(\theta) \Phi(\phi)$$

$$Y_{lm}(\theta, \phi) = \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} (-1)^m P_l^m(\cos \theta) e^{im\phi}$$

$(-1)^m$ is the phase factor.

The results of our derivation may be sum in two equations.

$$L^2 v(\theta, \phi) = \lambda \hbar^2 v(\theta, \phi)$$

$$L^2 Y_{lm}(\theta, \phi) = l(l+1) \hbar^2 Y_{lm}(\theta, \phi) \quad \dots (4.73)$$

$$L_z Y_{lm}(\theta, \phi) = m \hbar Y_{lm}(\theta, \phi) \quad \dots (4.74)$$

Because,

$$\begin{aligned}
 -i\hbar \frac{\partial}{\partial \Phi} [\theta(\theta) \Phi(\phi)] &= -i\hbar \theta(\theta) \frac{\partial}{\partial \Phi} [\Phi(\phi)] \\
 &= -i\hbar \theta(\theta) \frac{\partial}{\partial \Phi} (e^{im\phi}) \\
 &= -i\hbar \theta(\theta) im (e^{im\phi}) \\
 &= -i\hbar im \theta(\theta) \Phi(\phi) \\
 \therefore -i\hbar \frac{\partial}{\partial \Phi} [\theta(\theta) \Phi(\phi)] &= m\hbar Y_{lm}(\theta, \phi)
 \end{aligned}$$

Where, $m\hbar$ is eigen value of L_z operator. L^2 and L_z have same eigen function. This happens if both the operator can commute each other.

$$\therefore [L^2, L_z] = 0$$

➤ Concept of Space Quantization:

According to it, the z – component of angular momentum L_z is quantized. It can take the values $L_z = m\hbar$, where m is integer and is called magnetic quantum number.

Equation (4.74) is the quantum mechanical statement of space quantization. It says that z – component of any momentum (L_z) can take only discrete values which are integral multiple of \hbar .

In atomic Physics, the introduction of a magnetic field whose direction is taken as the z –axis causes the energy of the atom to change by an amount proportional to the z –component of its magnetic moment, which is related to L_z . Thus, space quantization manifests it self through discrete changes in atomic levels in a magnetic field. For this reason, 'm' is called magnetic quantum number.

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

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

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

From the above equation, it follows that all the components of L commute with L^2 to produce

$$[L_x, L^2] = 0, \quad [L_y, L^2] = 0, \quad [L_z, L^2] = 0$$

Here,

$$\begin{aligned}
 [L_x, L^2] &= [L_x, L_x^2 + L_y^2 + L_z^2] \\
 &= [L_x, L_x^2] + [L_x, L_y^2] + [L_x, L_z^2] \\
 \therefore [L_x, L^2] &= [L_x, L_x L_x] + [L_x, L_y L_y] + [L_x, L_z L_z]
 \end{aligned}$$

Now,

$$\begin{aligned}
 [A, BC] &= [A, B]C + B[A, C] \\
 \therefore [L_x, L^2] &= [L_x, L_x] L_x + L_x [L_x, L_x] + [L_x, L_y] L_y + L_y [L_x, L_y] + [L_x, L_z] L_z + L_z [L_x, L_z] \\
 \therefore [L_x, L^2] &= 0 + 0 + i\hbar L_z L_y + L_y i\hbar L_z - i\hbar L_y L_z - L_z i\hbar L_y \\
 \therefore [L_x, L^2] &= 0
 \end{aligned}$$

$$\text{Similarly, } [L_y, L^2] = 0 \text{ and } [L_z, L^2] = 0$$

It is because of the commutativity of L^2 and L_z that they possess a complete set of simultaneous eigen functions, say $Y_{lm}(\theta, \phi)$.

- $[L^2, L_x] = 0$. Hence, L^2 & L_x have simultaneous eigen function, say $\Phi_{lm}(\theta, \phi)$ & $Y_{lm}(\theta, \phi)$

$$[L_x, L_z] = -i\hbar L_y \neq 0$$

∴ Eigen function of $L_x \neq$ Eigen function of L_z

- $[L^2, L_y] = 0$. Hence, L^2 & L_y have simultaneous eigen function, say $f_{lm}(\theta, \phi)$ & $Y_{lm}(\theta, \phi)$

$$[L_y, L_z] = -i\hbar L_x \neq 0$$

∴ Eigen function of $L_y \neq$ Eigen function of L_z

Such functions $[\Phi_{lm}(\theta, \phi) \& f_{lm}(\theta, \phi)]$ do not coincide with $Y_{lm}(\theta, \phi)$

$$i.e. [L_z, L_x] \neq 0, [L_z, L_y] \neq 0$$

However, the eigen function of L^2 & L_x $[\Phi_{lm}(\theta, \phi)]$ can be expressed as the linear combination of $(2l + 1)$ function $Y_{lm}(\theta, \phi)$ characterized by the specific quantum number l .

$$\Phi_{lm}(\theta, \phi) = aY_{1,1} + bY_{1,0} + cY_{1,-1} \dots (4.75)$$

Angular Momentum in Stationary States of System with Spherical Symmetry: [One Dimension Square Well Potential]:

Consider a particle which is constrained to remain at a constant distance r_0 from the origin. The kinetic energy of a particle

$$\begin{aligned} T &= \frac{1}{2}mv^2 \\ \therefore T &= \frac{1}{2}I\omega^2 = \frac{I^2\omega^2}{2I} = \frac{L^2}{2I} \\ \therefore T &= \frac{L^2}{2I} \end{aligned}$$

If there are no forces effect in the motion, then potential energy will be zero.

$$\therefore \text{Total energy} = K.E + P.E = \frac{L^2}{2I} + 0 = \frac{L^2}{2I}$$

$$\therefore H = \frac{L^2}{2I}$$

The eigen value equation for this particle is

$$H v(\theta, \phi) = E v(\theta, \phi)$$

Here, H is Hamiltonian operator and $I = mr_0^2$

$$H v(\theta, \phi) = E v(\theta, \phi)$$

$$\therefore \frac{L^2}{2I} v(\theta, \phi) = E v(\theta, \phi)$$

The eigen value equation for L^2 operator is

$$L^2 Y_{lm}(\theta, \phi) = l(l + 1) \hbar^2 Y_{lm}(\theta, \phi)$$

Divide on both the sides by $2I$

$$\frac{L^2}{2I} Y_{lm}(\theta, \phi) = \frac{l(l + 1)}{2I} \hbar^2 Y_{lm}(\theta, \phi)$$

∴ The quantum mechanical energy for this particle is

$$E = \frac{l(l+1)\hbar^2}{2I} \quad \dots (4.76)$$

The Rigid Rotator:

The system of two particles held together with a constant interparticle separation r_0 and rotating about the center of mass is called rigid rotator.

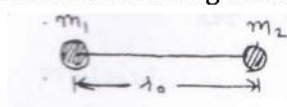


Fig: 4.2

The same result $E = \frac{l(l+1)\hbar^2}{2I}$ holds good for a system of two particles. The only difference is that, the moment of inertia is now,

$$I = \mu r_0^2$$

Where, $\mu = \frac{m_1 m_2}{m_1 + m_2}$

This system is called rigid rotator and it serves as a good approximate model for the motion of diatomic molecule.

The energy level spacing is

$$\begin{aligned} \Delta E &= E_l - E_{l-1} \\ &= \frac{l(l+1)\hbar^2}{2I} - \frac{(l-1)l\hbar^2}{2I} \\ &= \frac{\hbar^2}{2I} [l^2 + l - l^2 + l] \\ &= \frac{\hbar^2}{2I} [2l] \end{aligned}$$

$$\therefore \Delta E = \left(\frac{\hbar^2}{I} \right) l$$

$$\therefore \Delta E \propto l \quad \dots (4.77)$$

The levels are not equispaced. The spacing between two levels is not constant, it increases with increase in 'l'

A Particle in a Central Potential:

Consider a particle moving in a central potential $V(r)$ which is a function of radial co-ordinate r only,

$$H = K.E. + P.E.$$

$$H = \frac{p^2}{2m} + V(r)$$

For a system of two particles,

$$H = \frac{p^2}{2\mu} + V(r)$$

The eigen value equation is

$$Hu = Eu$$

$$\left[\frac{p^2}{2\mu} + V(r) \right] u = Eu$$

The operator for momentum p^2 is $-\hbar^2 \nabla^2$

$$\left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] u = Eu$$

Multiplying on both the sides by $-\frac{2\mu}{\hbar^2}$, we get

$$\begin{aligned} \nabla^2 u - \frac{2\mu}{\hbar^2} V(r) u &= -\frac{2\mu E}{\hbar^2} u \\ \nabla^2 u + \frac{2\mu}{\hbar^2} [E - V(r)] u &= 0 \end{aligned} \quad \dots (4.78)$$

Substituting the value of ∇^2 in spherical polar coordinates

$$\begin{aligned} &\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] u + \frac{2\mu}{\hbar^2} [E - V(r)] u = 0 \\ \therefore &\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \times \frac{\hbar^2}{\hbar^2} \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \right] u + \frac{2\mu}{\hbar^2} [E - V(r)] u = 0 \\ &\therefore \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \right] u + \frac{2\mu}{\hbar^2} [E - V(r)] u = 0 \end{aligned} \quad \dots (4.79)$$

Separating the solution in to radial and angular parts it can be written as,

$$u(r, \theta, \phi) = R(r) Y_{lm}(\theta, \phi) \quad \dots (4.80)$$

Equation (4.79) becomes,

$$\begin{aligned} &\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \right] (R(r) Y_{lm}(\theta, \phi)) + \frac{2\mu}{\hbar^2} [E - V(r)] (R(r) Y_{lm}(\theta, \phi)) = 0 \\ Y_{lm}(\theta, \phi) &\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} R(r) \right) - \frac{R(r) L^2}{\hbar^2 r^2} Y_{lm}(\theta, \phi) + \frac{2\mu}{\hbar^2} [E - V(r)] R(r) Y_{lm}(\theta, \phi) = 0 \end{aligned}$$

We take,

$$\begin{aligned} L^2 Y_{lm}(\theta, \phi) &= l(l+1) \hbar^2 Y_{lm}(\theta, \phi) \\ \therefore Y_{lm}(\theta, \phi) &\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} R(r) \right) - l(l+1) \hbar^2 Y_{lm}(\theta, \phi) \frac{R(r)}{\hbar^2 r^2} + \frac{2\mu}{\hbar^2} [E - V(r)] R(r) Y_{lm}(\theta, \phi) \\ &= 0 \end{aligned}$$

Divide throughout by $R(r) Y_{lm}(\theta, \phi)$

$$\therefore \frac{1}{R(r)} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} R(r) \right) - \frac{l(l+1) \hbar^2}{\hbar^2 r^2} + \frac{2\mu}{\hbar^2} [E - V(r)] = 0$$

Multiply by $R(r)$, we get

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) - \frac{l(l+1) \hbar^2}{\hbar^2 r^2} R(r) + \frac{2\mu}{\hbar^2} [E - V(r)] R(r) = 0$$

$$\therefore \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{2\mu}{\hbar^2} \left[E - V(r) - \frac{l(l+1) \hbar^2}{2\mu r^2} \right] R(r) = 0 \quad \dots (4.81)$$

This is known as radial equation. This equation is very useful to solve the problem of atomic physics like Hydrogen atom.

In above equation $\frac{l(l+1)\hbar^2}{2\mu r^2}$ is called centrifugal potential.

The centrifugal potential $V = \frac{l(l+1)\hbar^2}{2\mu r^2}$, and centrifugal force $\vec{F} = -\vec{\nabla}V$

Now, here $\vec{l} = l \frac{\hbar}{2\pi}$. In quantum mechanics $\vec{l} = \sqrt{l(l+1)} \hbar$.

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

The eigen value problem for a spherically symmetric potential thus reduces to determining for what values of E the radial wave equation (4.81) has admissible solution and then finding the solutions.

The Radial Wave Function:

The norm of the wave function μ , when expressed in spherical polar coordinates is given by

$$\begin{aligned} \text{Norm} &= \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} u(r, \theta, \phi) u^*(r, \theta, \phi) d\tau \\ &= \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} R(r) Y_{lm}(\theta, \phi) R^*(r) Y_{lm}^*(\theta, \phi) r^2 dr \sin \theta d\theta d\phi \\ \therefore \text{Norm} &= \left[\int_{r=0}^{\infty} R^*(r) R(r) r^2 dr \right] \left[\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} Y_{lm}(\theta, \phi) Y_{lm}^*(\theta, \phi) \sin \theta d\theta d\phi \right] \end{aligned}$$

Since, $Y_{lm}(\theta, \phi)$ is normalized function. It has unit norm.

$$\therefore \text{Norm} = \int R^*(r) R(r) r^2 dr = 1 \text{ for a normalized function.}$$

The expectation value of any operator A which involve r only is given by

$$\begin{aligned} \langle A \rangle &= \int \Psi^* A \Psi d\tau \\ \therefore \langle A \rangle &= \int R^*(r) A R(r) r^2 dr \end{aligned}$$

It is useful to write $R(r) = \frac{\chi(r)}{r}$

$$\begin{aligned} \therefore \langle A \rangle &= \int \frac{\chi^*(r)}{r} A \frac{\chi(r)}{r} r^2 dr \\ \therefore \langle A \rangle &= \int \chi^*(r) A \chi(r) r^2 dr \end{aligned} \quad \dots (4.82)$$

With this assumption the radial wave function now becomes

$$\begin{aligned} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \frac{\chi(r)}{r} \right) + \frac{2\mu}{\hbar^2} \left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] \frac{\chi(r)}{r} &= 0 \\ \therefore \frac{1}{r^2} \frac{d}{dr} \left[r^2 \frac{d}{dr} \left(\chi(r) \frac{1}{r} \right) \right] + \left[\frac{2\mu}{\hbar^2} (E - V(r)) - \frac{l(l+1)}{r^2} \right] \frac{\chi(r)}{r} &= 0 \\ \therefore \frac{1}{r^2} \frac{d}{dr} \left[r^2 \left(\frac{1}{r} \frac{d\chi}{dr} - \frac{\chi(r)}{r^2} \right) \right] + \left[\frac{2\mu}{\hbar^2} (E - V(r)) - \frac{l(l+1)}{r^2} \right] \frac{\chi(r)}{r} &= 0 \\ \therefore \frac{1}{r^2} \frac{d}{dr} \left[r^2 \frac{d\chi}{dr} - \chi(r) \right] + \left[\frac{2\mu}{\hbar^2} (E - V(r)) - \frac{l(l+1)}{r^2} \right] \frac{\chi(r)}{r} &= 0 \end{aligned}$$

$$\therefore \frac{1}{r^2} \left[r \frac{d^2 \chi}{dr^2} + \frac{d\chi}{dr} - \frac{d\chi}{dr} \right] + \left[\frac{2\mu}{\hbar^2} (E - V(r)) - \frac{l(l+1)}{r^2} \right] \frac{\chi(r)}{r} = 0$$

Therefore, the solution will be

$$(1) m = -l, \quad \chi(r) = \text{const.} r^{-l}$$

$$(2) m = l + 1, \quad \chi(r) = \text{const.} r^{l+1}$$

When we put $r = 0$ in above solution (1), we get

$$\chi(r) = r^{-l} = \frac{1}{r^l} = \frac{1}{0} \rightarrow \infty$$

\therefore This solution is not acceptable, since it makes $R(r)$ diverging as $r \rightarrow 0$.

\therefore we are left with the other solution $\chi(r) = r^{l+1}$, which leads to

$$R(r) = \frac{\chi(r)}{r} = \frac{r^{l+1}}{r}$$

$$\therefore R(r) = \text{const.} r^l \quad \dots (4.83)$$

Thus, any acceptable solution for angular momentum l must behave like r^l near the origin.

The Hydrogen Atom:

Consider the one- electron atom like hydrogen, singly ionized helium, doubly ionized lithium, etc. This is a two-particle system, consisting of the atomic nucleus of charge Ze , and the electron of charge $-e$. But if the nucleus is supposed to remain static, the Schrodinger equation is just that for a single particle. The electron is moving in a potential $V(r) = -Ze^2/r$. This is just the electrostatic potential energy of interaction of the two charges.

Actually, when the atom as a whole is at rest, it is not the nucleus, but the centre of mass of the two-particle system which remains static. Hence, in the kinetic energy terms in Hamiltonian taken reduced mass μ instead of the electron mass m_e . The reduced mass is given by the relation $\mu = \frac{m_e m_n}{(m_e + m_n)}$, where m_n is the mass of the nucleus.

Solution of The Radial Equation and Energy Levels:

The Hamiltonian for a conservative system is

$$H = \frac{p^2}{2\mu} + V(r)$$

The eigen value equation is

$$Hu = Eu$$

$$\left[\frac{p^2}{2\mu} + V(r) \right] u = Eu$$

The operator for momentum p^2 is $-\hbar^2 \nabla^2$

$$\left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] u = Eu$$

Multiplying on both the sides by $-\frac{2\mu}{\hbar^2}$, we get

$$\begin{aligned}\nabla^2 u - \frac{2\mu}{\hbar^2} V(r)u &= -\frac{2\mu E}{\hbar^2} u \\ \nabla^2 u + \frac{2\mu}{\hbar^2} [E - V(r)]u &= 0\end{aligned}\quad \dots (4.84)$$

Substituting the value of ∇^2 in spherical polar coordinates

$$\begin{aligned}\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] u + \frac{2\mu}{\hbar^2} [E - V(r)]u &= 0 \\ \therefore \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \times \frac{\hbar^2}{\hbar^2} \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \right] u + \frac{2\mu}{\hbar^2} [E - V(r)]u &= 0 \\ \therefore \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \right] u + \frac{2\mu}{\hbar^2} [E - V(r)]u &= 0\end{aligned}\quad \dots (4.85)$$

Separating the solution in to radial and angular parts it can be written as,

$$u(r, \theta, \phi) = R(r)Y_{lm}(\theta, \phi) \quad \dots (4.86)$$

Equation (4.85) becomes,

$$\begin{aligned}\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \right] (R(r)Y_{lm}(\theta, \phi)) + \frac{2\mu}{\hbar^2} [E - V(r)](R(r)Y_{lm}(\theta, \phi)) &= 0 \\ Y_{lm}(\theta, \phi) \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} R(r) \right) - \frac{R(r)L^2}{\hbar^2 r^2} Y_{lm}(\theta, \phi) + \frac{2\mu}{\hbar^2} [E - V(r)]R(r)Y_{lm}(\theta, \phi) &= 0\end{aligned}$$

We take,

$$\begin{aligned}L^2 Y_{lm}(\theta, \phi) &= l(l+1)\hbar^2 Y_{lm}(\theta, \phi) \\ \therefore Y_{lm}(\theta, \phi) \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} R(r) \right) - l(l+1)\hbar^2 Y_{lm}(\theta, \phi) \frac{R(r)}{\hbar^2 r^2} + \frac{2\mu}{\hbar^2} [E - V(r)]R(r)Y_{lm}(\theta, \phi) &= 0 \\ &= 0\end{aligned}$$

Divide throughout by $R(r)Y_{lm}(\theta, \phi)$

$$\therefore \frac{1}{R(r)} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} R(r) \right) - \frac{l(l+1)\hbar^2}{\hbar^2 r^2} + \frac{2\mu}{\hbar^2} [E - V(r)] = 0$$

Multiply by $R(r)$, we get

$$\begin{aligned}\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) - \frac{l(l+1)\hbar^2}{\hbar^2 r^2} R(r) + \frac{2\mu}{\hbar^2} [E - V(r)]R(r) &= 0 \\ \therefore \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{2\mu}{\hbar^2} \left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] R(r) &= 0\end{aligned}\quad \dots (4.87)$$

For H-atom, the coulomb potential as central potential given by

$$V(r) = -\frac{Ze^2}{r} \quad \dots (4.88)$$

Using equation (4.88) in (4.87), we get

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{2\mu}{\hbar^2} \left[E + \frac{Ze^2}{r} - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] R(r) = 0 \quad \dots (4.89)$$

This is radial wave equation for H-atom.

Equation (6) can be solved for:

- (i) Bound states → lower energy states, responsible for binding
- (ii) Unbound states → close to continuum states, higher energy states, come across in scattering phenomena

Let us consider bound states, for which $E < 0$, and define the positive real parameters α and λ through

$$\alpha^2 = -\frac{8\mu E}{\hbar^2} \quad \text{and} \quad \lambda = \frac{2\mu Ze^2}{\alpha \hbar^2} = \frac{Ze^2}{\hbar} \left(\frac{\mu}{-2E} \right)^{\frac{1}{2}} \quad \dots (4.90)$$

Dividing equation (4.89) throughout by α^2 , we have

$$\begin{aligned} & \frac{1}{\alpha^2} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{2\mu}{\hbar^2} \left[E \frac{1}{\alpha^2} + \frac{Ze^2}{r} \frac{1}{\alpha^2} - \frac{l(l+1)\hbar^2}{2\mu r^2} \frac{1}{\alpha^2} \right] R(r) = 0 \\ \therefore & \frac{1}{\alpha^2} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \left[\frac{2\mu E}{\hbar^2} \left(-\frac{\hbar^2}{8\mu E} \right) + \frac{2\mu Ze^2}{\hbar^2} \frac{1}{r} \frac{1}{\alpha^2} - \frac{2\mu l(l+1)\hbar^2}{2\mu r^2} \frac{1}{\alpha^2} \right] R(r) = 0 \\ \therefore & \frac{1}{\alpha^2} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \left[-\frac{1}{4} + \frac{2\mu Ze^2}{\hbar^2} \frac{1}{r} \frac{1}{\alpha^2} - \frac{l(l+1)}{r^2} \frac{1}{\alpha^2} \right] R(r) = 0 \\ \therefore & \frac{1}{\alpha^2 r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \left[-\frac{1}{4} + \frac{2\mu Ze^2}{\alpha \hbar^2} \left(\frac{1}{r\alpha} \right) - \frac{l(l+1)}{\alpha^2 r^2} \right] R(r) = 0 \\ \therefore & \frac{1}{\alpha^2 r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \left[-\frac{1}{4} + \frac{\lambda}{\alpha r} - \frac{l(l+1)}{\alpha^2 r^2} \right] R(r) = 0 \quad \dots (4.91) \end{aligned}$$

Since α has unit of distance -inverse. We define dimensionless variables $\rho = \alpha r$ and the radial function $R(r) = R(\rho)$

We have,

$$\begin{aligned} \rho &= \alpha r \\ \therefore d\rho &= \alpha dr \\ \therefore \frac{d}{dr} &= \alpha \frac{d}{d\rho} \end{aligned}$$

With this substitution, equation (4.91) becomes

$$\begin{aligned} & \frac{1}{\rho^2} \alpha \frac{d}{d\rho} \left(r^2 \alpha \frac{d}{d\rho} R(\rho) \right) + \left[-\frac{1}{4} + \frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2} \right] R(\rho) = 0 \\ \therefore & \frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dR(\rho)}{d\rho} \right) + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \right] R(\rho) = 0 \\ \therefore & \frac{1}{\rho^2} \left[2\rho \frac{dR(\rho)}{d\rho} + \rho^2 \frac{d^2 R(\rho)}{d\rho^2} \right] + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \right] R(\rho) = 0 \\ \therefore & \frac{d^2 R(\rho)}{d\rho^2} + \frac{2}{\rho} \frac{dR(\rho)}{d\rho} + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \right] R(\rho) = 0 \quad \dots (4.92) \end{aligned}$$

This is dimensionless radial wave equation for H-atom.

Equation (9) is second order linear differential equation. We can get the series solution.

We examine first the behavior of $R(\rho)$ in asymptotic region.

- (i) When $\rho \rightarrow \infty$, then equation (4.92) becomes

$$\frac{d^2 R(\rho)}{d\rho^2} - \frac{R(\rho)}{4} = 0 \quad \dots (4.93)$$

In equation (4.92) all other terms have ρ - in denominator. Hence, other terms vanish.

The solution of equation (4.93) is

$$R \sim e^{\pm \frac{1}{2}\rho} \quad \dots (4.94)$$

As $\rho \rightarrow \infty$, $R \sim e^{+\frac{1}{2}\rho} \rightarrow \infty$ (the series solution becomes diverging which is not suitable) and $R \sim e^{-\frac{1}{2}\rho} \rightarrow 0$, (the series converging which is suitable). Hence, series solution must have a factor $e^{-\frac{1}{2}\rho}$ in it. Let it be written as a power factor of ρ .

$$R(\rho) = \rho^l e^{-\frac{1}{2}\rho} L(\rho) \quad \dots (4.95)$$

Here,

$\rho^l \rightarrow$ power term

$e^{-\frac{1}{2}\rho} \rightarrow$ take care of asymptotic behavior

$L(\rho) \rightarrow$ series which is to be found

(ii) At $r \rightarrow 0$ (at the nucleus), i.e. $\rho \rightarrow 0$. Hence, from equation (4.95), $R \rightarrow 0$

As $R \rightarrow 0$, $u(r, \theta, \phi) \equiv R(r)Y_{lm}(\theta, \phi) \rightarrow 0$

Hence the probability density $|u|^2 \rightarrow 0$, as expected due to fact that e^- – can not be found at the nucleus.

Using equation (4.95) in (4.92), we have

$$\begin{aligned} & \therefore \frac{d^2}{d\rho^2} \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) + \frac{2}{\rho} \frac{d}{d\rho} \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \right] \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) \\ & = 0 \quad \dots (4.96) \end{aligned}$$

Now, we compute each term separately as follows:

First Term:

$$\begin{aligned} \frac{d^2}{d\rho^2} \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) &= \frac{d}{d\rho} \left[\frac{d}{d\rho} \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) \right] \\ &= \frac{d}{d\rho} \left[l \rho^{l-1} L e^{-\frac{1}{2}\rho} + \rho^l \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} - \frac{1}{2} \rho^l L e^{-\frac{1}{2}\rho} \right] \\ &= \left\{ l(l-1) \rho^{l-2} L e^{-\frac{1}{2}\rho} + l \rho^{l-1} \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} - \frac{1}{2} l \rho^{l-1} L e^{-\frac{1}{2}\rho} \right\} \\ &+ \left\{ l \rho^{l-1} \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} + \rho^l \frac{d^2 L}{d\rho^2} e^{-\frac{1}{2}\rho} - \frac{1}{2} \rho^l \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} \right\} \\ &- \frac{1}{2} \left\{ l \rho^{l-1} L e^{-\frac{1}{2}\rho} + \rho^l \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} - \frac{1}{2} \rho^l L e^{-\frac{1}{2}\rho} \right\} \\ &\therefore \frac{d^2}{d\rho^2} \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) \\ &= \left[\rho^l \frac{d^2 L}{d\rho^2} + 2l \rho^{l-1} \frac{dL}{d\rho} - \rho^l \frac{dL}{d\rho} + \frac{1}{4} \rho^l L - l \rho^{l-1} L + l^2 \rho^{l-2} L \right. \\ &\quad \left. - l \rho^{l-2} L \right] e^{-\frac{1}{2}\rho} \quad \dots (4.97) \end{aligned}$$

Second Term:

$$\frac{2}{\rho} \frac{d}{d\rho} \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) = \left[2l \rho^{l-2} L + 2\rho^{l-1} \frac{dL}{d\rho} - \rho^{l-1} L \right] e^{-\frac{1}{2}\rho} \quad \dots (4.98)$$

Third Term:

$$\begin{aligned} & \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \right] \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) \\ &= \left[\lambda \rho^{l-1} L - \frac{1}{4} \rho^l L - l^2 \rho^{l-2} L - l \rho^{l-2} L \right] e^{-\frac{1}{2}\rho} \quad \dots (16.4.99) \end{aligned}$$

Adding equations (4.97), (4.98) & (4.99)

$$\begin{aligned} & \left\{ l(l-1) \rho^{l-2} L e^{-\frac{1}{2}\rho} + l \rho^{l-1} \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} - \frac{1}{2} l \rho^{l-1} L e^{-\frac{1}{2}\rho} \right\} \\ & + \left\{ l \rho^{l-1} \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} + \rho^l \frac{d^2 L}{d\rho^2} e^{-\frac{1}{2}\rho} - \frac{1}{2} \rho^l \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} \right\} \\ & - \frac{1}{2} \left\{ l \rho^{l-1} L e^{-\frac{1}{2}\rho} + \rho^l \frac{dL}{d\rho} e^{-\frac{1}{2}\rho} - \frac{1}{2} \rho^l L e^{-\frac{1}{2}\rho} \right\} + \frac{2}{\rho} \frac{d}{d\rho} \left(\rho^l e^{-\frac{1}{2}\rho} L(\rho) \right) \\ &= \left[2l \rho^{l-2} L + 2\rho^{l-1} \frac{dL}{d\rho} - \rho^{l-1} L \right] e^{-\frac{1}{2}\rho} \\ & + \left[\lambda \rho^{l-1} L - \frac{1}{4} \rho^l L - l^2 \rho^{l-2} L - l \rho^{l-2} L \right] e^{-\frac{1}{2}\rho} \\ \therefore \rho^l \frac{d^2 L}{d\rho^2} + \left[(2l+1) \rho^{l-1} \frac{dL}{d\rho} \right] - \rho^l \frac{dL}{d\rho} - l \rho^{l-1} L - 2l \rho^{l-2} L + 2l \rho^{l-2} L - \rho^{l-1} L + \lambda \rho^{l-1} L \\ &= 0 \end{aligned}$$

Dividing throughout by ρ^{l-1} ,

$$\rho \frac{d^2 L}{d\rho^2} + [l(l+1) - \rho] \frac{dL}{d\rho} + [\lambda - (l+1)] L(\rho) = 0 \quad \dots (4.100)$$

To solve this equation, let us assume a solution for $L(\rho)$ in the series form:

$$L(\rho) = c_0 + c_1 \rho + c_2 \rho^2 + \dots = \sum_{s=0}^{\infty} c_s \rho^s \quad \dots (4.101)$$

Since we know that $R(\rho)$ behaves like ρ^l for small ρ , $L(\rho)$ must tend to a constant as $\rho \rightarrow 0$, according to equation (12). This why the series has been taken to start with a constant term. c_0 takes care of divergence issue at $\rho \rightarrow 0$ along with ρ^l term in equation (4.95)

Using equation (4.101) in (4.100), we have

$$\begin{aligned} & \sum_{s=0}^{\infty} \rho s(s-1) c_s \rho^{s-2} + \sum_{s=0}^{\infty} [2(l+1) - \rho] c_s s \rho^{s-1} + \sum_{s=0}^{\infty} [\lambda - (l+1)] c_s \rho^s = 0 \\ & \sum_{s=0}^{\infty} c_s s(s-1) \rho^{s-1} + \sum_{s=0}^{\infty} c_s s \rho^{s-1} (2l+1) - \sum_{s=0}^{\infty} c_s s \rho^s + \sum_{s=0}^{\infty} [\lambda - (l+1)] c_s \rho^s = 0 \end{aligned}$$

Since 's' is dummy, replace $s \rightarrow (s+1)$ in first two-terms

$$\therefore \sum_{s=0}^{\infty} [c_{s+1} s \rho^s + c_{s+1} (s+1)(2l+1) \rho^s] + \sum_{s=0}^{\infty} c_s [-s + (\lambda - (l+1))] \rho^s = 0$$

Now, equating the coefficient of ρ^s to zero, we have

$$c_{s+1} \{s(s+1) + (s+1)(2l+1)\} + c_s \{-s + \lambda - l(l+1)\} = 0$$

$$\begin{aligned}\therefore c_{s+1}\{(s+1)(s+2l+1)\} + c_s\{(s+l+1) - \lambda\} &= 0 \\ \therefore \frac{c_{s+1}}{c_s} &= \frac{(s+l+1) - \lambda}{(s+1)(s+2l+1)}\end{aligned}\quad \dots (4.102)$$

This is recurrence relation between the coefficient c_s . i.e. $c_0 \rightarrow c_1 \rightarrow c_2 \rightarrow \dots$

In order to have finite (non-diverging series), series equation (18), higher order co-efficient (c_s) should be progressively small and should become zero after some order. Let at $s = s_{max} = n'$, series (19) becomes zero. (i.e. higher terms will be automatically zero)

Thus, $(s+l+1) - \lambda = 0$, when $s = n'$

$$\therefore (n' + l + 1) = \lambda$$

Since n' , l and 1 are integer. λ will also be integer, say n .

$$\therefore n' + l + 1 = \lambda \equiv n$$

$$\therefore n' = n - l - 1$$

But,

$$\begin{aligned}\lambda \equiv n &= \frac{Ze^2}{\hbar} \left(\frac{\mu}{-2E} \right)^{\frac{1}{2}} \\ \therefore n^2 &= -\frac{Z^2 e^4 \mu}{\hbar^2 2E} \\ \therefore E &= -\frac{Z^2 e^4 \mu}{2\hbar^2 n^2}\end{aligned}\quad \dots (4.103)$$

The Anisotropic Oscillator:

Consider the harmonic oscillator in three dimensions with the Hamiltonian

$$H = K.E + P.E$$

$$\begin{aligned}\therefore H &= \frac{p^2}{2m} + \frac{1}{2}m\omega_1^2 x^2 + \frac{1}{2}m\omega_2^2 y^2 + \frac{1}{2}m\omega_3^2 z^2 \\ \therefore H &= \frac{p^2}{2m} + \frac{1}{2}m[\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2]\end{aligned}\quad \dots (4.104)$$

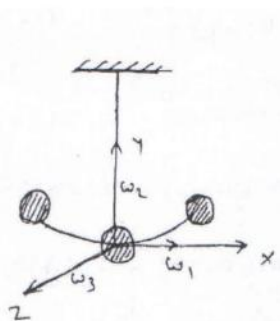


Fig: 4.3

This Hamiltonian can be broken up into a sum $H^{(1)} + H^{(2)} + H^{(3)}$ of Hamiltonians of 3 independent simple harmonic oscillator.

$$\begin{aligned}\therefore H &= \left(\frac{p_x^2}{2m} + \frac{1}{2}m\omega_1^2 x^2 \right) + \left(\frac{p_y^2}{2m} + \frac{1}{2}m\omega_2^2 y^2 \right) + \left(\frac{p_z^2}{2m} + \frac{1}{2}m\omega_3^2 z^2 \right) \\ \therefore H &= H^{(1)} + H^{(2)} + H^{(3)}\end{aligned}\quad \dots (4.105)$$

The time independent Schrodinger equation is

$$\begin{aligned}
 Hu &= Eu \\
 \therefore \left[\frac{p^2}{2m} + V(r) \right] u &= Eu \\
 \therefore \left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] u &= Eu
 \end{aligned}$$

Multiplying on both the sides by $-\frac{2m}{\hbar^2}$

$$\nabla^2 u + \frac{2m}{\hbar^2} [E - V(r)] u = 0 \quad \dots (4.106)$$

This is the Schrodinger equation of simple harmonic oscillator.

Splitting this equation in three parts.

(i)

$$\begin{aligned}
 \frac{d^2 u}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] u &= 0 \\
 \therefore \frac{d^2 u}{dx^2} + \frac{2m}{\hbar^2} \left[E - \frac{1}{2} m \omega_1^2 x^2 \right] u &= 0 \quad \dots (4.107)
 \end{aligned}$$

Now, normalized energy eigen function for simple harmonic oscillator is

$$u_{n_1}^{(1)}(x) = \frac{1}{\sqrt{2^n n!} \sqrt{\pi}} e^{-x^2/2} H_n(x) \quad \dots (4.108)$$

And,

$$E_n^{(1)} = \left(n_1 + \frac{1}{2} \right) \hbar \omega_1 \quad \dots (4.109)$$

(ii)

$$\begin{aligned}
 \frac{d^2 u}{dy^2} + \frac{2m}{\hbar^2} [E - V(y)] u &= 0 \\
 \therefore \frac{d^2 u}{dy^2} + \frac{2m}{\hbar^2} \left[E - \frac{1}{2} m \omega_2^2 y^2 \right] u &= 0 \quad \dots (4.110)
 \end{aligned}$$

$$u_{n_2}^{(2)}(y) = \frac{1}{\sqrt{2^n n!} \sqrt{\pi}} e^{-y^2/2} H_n(y) \quad \dots (4.111)$$

\therefore The normalized energy eigen value is

$$E_n^{(2)} = \left(n_2 + \frac{1}{2} \right) \hbar \omega_2 \quad \dots (4.112)$$

(iii)

$$\therefore \frac{d^2 u}{dz^2} + \frac{2m}{\hbar^2} \left[E - \frac{1}{2} m \omega_3^2 z^2 \right] u = 0 \quad \dots (4.113)$$

\therefore The normalized energy eigen function is

$$u_{n_3}^{(3)}(z) = \frac{1}{\sqrt{2^n n!} \sqrt{\pi}} e^{-z^2/2} H_n(z) \quad \dots (4.114)$$

And, normalized energy eigen value is

$$E_n^{(3)} = \left(n_3 + \frac{1}{2} \right) \hbar \omega_3 \quad \dots (4.115)$$

A complete set of eigen functions of H may be found in the form

$$u_{n_1 n_2 n_3}(x, y, z) = u_{n_1}^{(1)}(x) + u_{n_2}^{(2)}(y) + u_{n_3}^{(3)}(z)$$

Putting equations (4.108), (4.111) & (4.114), we get

$$\therefore u_{n_1 n_2 n_3}(x, y, z) = \frac{1}{(2^n n! \sqrt{\pi})^{3/2}} e^{-r^2/2} H_n(x) H_n(y) H_n(z) \quad \dots (4.116)$$

$u_{n_1}^{(1)}(x), u_{n_2}^{(1)}(y), u_{n_3}^{(1)}(z)$ are eigen functions of three different oscillators given by above equations.

The energy eigen values $[E_{n_1 n_2 n_3}]$ to which $u_{n_1 n_2 n_3}$ belongs is given by

$$E_{n_1 n_2 n_3} = E_{n_1}^{(1)} + E_{n_2}^{(2)} + E_{n_3}^{(2)}$$

$$\therefore E_{n_1 n_2 n_3} = \left(n_1 + \frac{1}{2}\right) \hbar \omega_1 + \left(n_2 + \frac{1}{2}\right) \hbar \omega_2 + \left(n_3 + \frac{1}{2}\right) \hbar \omega_3 \quad \dots (4.117)$$

The Isotropic Oscillator:

When the oscillators is isotropic, then $\omega_1 = \omega_2 = \omega_3 = \omega$. Then, the energy eigen values of the isotropic oscillator is given by

$$\begin{aligned} E_{n_1 n_2 n_3} &= \left(n_1 + \frac{1}{2}\right) \hbar \omega + \left(n_2 + \frac{1}{2}\right) \hbar \omega + \left(n_3 + \frac{1}{2}\right) \hbar \omega \\ &= \left[(n_1 + n_2 + n_3) + \frac{3}{2}\right] \hbar \omega \\ \therefore E_{n_1 n_2 n_3} &= \left(n + \frac{3}{2}\right) \hbar \omega \quad \dots (4.118) \end{aligned}$$

Here, $n = n_1 + n_2 + n_3$

Since the energy depends only on the sum $n = n_1 + n_2 + n_3$ in this case, the levels are degenerate.

The potential energy is given by

$$V = \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2) = \frac{1}{2} m \omega^2 r^2 \quad \dots (4.119)$$

The wave function is

$$u_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi)$$

The radial wave equation with

$$V = \frac{1}{2} m \omega^2 r^2$$

In terms of the dimensionless variables $\rho = \alpha r$ with $\alpha = (m\omega/\hbar)^{1/2}$ takes the form

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dR}{d\rho} \right) + \left[\lambda - \rho^2 - \frac{l(l+1)}{\rho^2} \right] R = 0 \quad \dots (4.120)$$

Where,

$$R(\rho) = R(r) \text{ and } \lambda = \frac{2mE}{\hbar^2 \alpha^2} = \frac{2E}{\hbar \omega} \quad \dots (4.121)$$

$R(\rho)$ behaves like ρ^l for small ρ and $e^{-\rho^2/2}$ for large ρ .

$$\therefore R = \rho^l e^{-\frac{1}{2}\rho^2} K \quad \dots (4.122)$$

In terms of K equation (17) is

$$\xi \frac{d^2 K}{d\xi^2} + \left(l + \frac{3}{2} - \xi\right) \frac{dK}{d\xi} + \frac{1}{4}(\lambda - 3 - 2l)K = 0 \quad \dots (4.123)$$

With $\xi = \rho^2$,

$$\lambda = 2n + 3, \quad \eta = l + 2n' \quad \dots (4.124)$$

The energy eigen value is

$$E_n = \left(n + \frac{3}{2}\right) \hbar \omega \quad \dots (4.125)$$

Where, $n = 0, 1, 2, \dots \dots \dots$

Question Bank

Multiple choice questions:

- (1) Force acting on the pendulum is proportional to _____
 (a) Velocity (b) **displacement**
 (c) Time (d) acceleration
- (2) Hamiltonian operator for simple harmonic oscillator is $H =$ _____
 (a) $\frac{p^2}{2m} + \frac{1}{2}kx^2$ (b) $\frac{p^2}{2m}$
 (c) $\frac{1}{2}kx^2$ (d) $\frac{p^2}{2m} + kx$
- (3) Potential of harmonic oscillator is $V =$ _____
 (a) mgh (b) $\frac{1}{2}kx^2$
 (c) $\frac{p^2}{2m}$ (d) kx
- (4) Energy eigen value of simple harmonic oscillator is given by $E =$ _____
 (a) $\hbar v$ (b) $\left(n + \frac{1}{2}\right) \hbar \omega$
 (c) $N \hbar v$ (d) $\hbar \omega$
- (5) The zero point energy for simple harmonic oscillator is $E =$ _____
 (a) $\hbar \omega$ (b) $\frac{1}{2} \hbar \omega$
 (c) $\frac{3}{2} \hbar \omega$ (d) $\frac{5}{2} \hbar \omega$
- (6) The ground state energy for simple harmonic oscillator is $E =$ _____
 (a) $\hbar \omega$ (b) $\frac{1}{2} \hbar \omega$
 (c) $\frac{3}{2} \hbar \omega$ (d) $\frac{5}{2} \hbar \omega$
- (7) Energy eigen value of an isotropic oscillator is given by $E =$ _____
 (a) $\hbar v$ (b) $\hbar \omega$
 (c) $N \hbar v$ (d) $\left(n + \frac{3}{2}\right) \hbar \omega$
- (8) Angular momentum is defined as $L =$ _____
 (a) $\vec{r} \cdot \vec{p}$ (b) $\vec{r} \times \vec{p}$

- (c) $\vec{r} \times \vec{p}$ (d) mv
- (9) In a rigid rotator distance between two particles is _____
 (a) Variable (b) Zero
 (c) Infinite (d) **constant**
- (10) The quantum mechanical energy for a particle in one-dimension square well potential is _____
 (a) $E = \frac{l(l+1)\hbar^2}{I}$ (b) $E = \frac{l(l+1)\hbar^2}{2I}$
 (c) $E = \frac{(l+1)\hbar^2}{I}$ (d) $E = \frac{(l+1)\hbar^2}{2I}$
- (11) Central potential is a function of _____
 (a) r (b) θ
 (c) ϕ (d) **r and θ**
- (12) Energy of an isotropic oscillator is _____
 (a) Continues (b) **Discrete**
 (c) 0 (d) $h\nu$
- (13) For a rigid rotator the differences of energy levels are govern by $\Delta E =$ _____
 (a) $\left(n + \frac{1}{2}\right)\hbar\omega$ (b) $Nh\nu$
 (c) $\left(n + \frac{3}{2}\right)\hbar\omega$ (d) $\frac{\hbar^2}{I}l$
- (14) The energy eigen value for isotropic oscillator is $E =$ _____
 (a) $\left(n + \frac{1}{2}\right)\hbar\omega$ (b) $E = \frac{(l+1)\hbar^2}{2I}$
 (c) $\left(n + \frac{3}{2}\right)\hbar\omega$ (d) $E = \frac{l(l+1)\hbar^2}{2I}$

Short Questions:

- Set up the Hamiltonian for simple harmonic oscillator
- Write the dimension less Schrodinger equation for simple harmonic oscillator
- Draw the energy level diagram of simple harmonic oscillator
- Find the components of angular momentum
- Write down expression for ∇^2 in spherical polar coordinates
- Write the expression of angular momentum operator L^2 in terms of spherical polar coordinates
- What is rigid rotator? State the expression for its energy level separation. What is importance of studying rigid rotator?
- Define central potential? Write down the expression for Hamiltonian of a particle moving in a central potential field
- Write the radial equation for a particle in central potential
- Write the Hamiltonian for anisotropic oscillator
- Write the energy eigen value for anisotropic oscillator
- What is isotropic oscillator? Write down expressions for its energy

Long Questions:

- Derive the dimension less Schrodinger equation for simple harmonic oscillator

2. Set up the Hamiltonian of simple harmonic oscillator and derive the expression of its energy eigen value
3. Derive the expression of angular momentum operator L^2 in terms of spherical polar coordinates
4. Set up the Hamiltonian for a particle in one dimension square well and obtain its energy eigen value
5. What is rigid rotator? Show that the spacing between two energy level is increases with l
6. Derive the radial equation for a particle in central potential
7. Set up the Hamiltonian of anisotropic oscillator and derive its energy eigen value
8. What is an isotropic oscillator? Obtain the expression of its energy eigen value