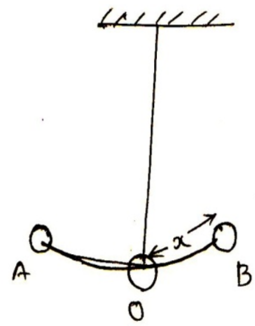
B. Sc. (Semester -6)
Subject : Physics
Course : US06CPHY01
Title : Quantum Mechanics

Unit : 4 – Exactly Soluble Eigen value Problem

The simple Harmonic Oscillator

* The Schrodinger equation and energy eigenvalues :-

Q- Set up the schrodinger equation for simple harmonic oscillator and obtain it's eigen value.



Force acting on the pendulum is proportional to the displacement x. Then the motion of $\bar{e}$ is known as simple harmonic oscillator.

$$\therefore \quad F \propto x$$

$$F = -kx$$

where k is force const

but $F = -\frac{\partial v}{\partial x}$

$$\therefore \quad -\frac{\partial v}{\partial x} = -kx$$

integrating on both the sides w.r.t x we get

$$\therefore \quad -\int \frac{dv}{dx} = -\int kx\, dx$$

$$\therefore \quad \boxed{v = \frac{1}{2}kx^2} \quad \text{——— (1)}$$

where force constant $k = m\omega^2$.

Now, Hamiltonian operator is

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

$$= \frac{1}{2}mv^2 + \frac{1}{2}kx^2$$

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

$$\therefore \boxed{H = -\frac{\hbar^2\nabla^2}{2m} + \frac{1}{2}m\omega^2x^2} \longrightarrow (2)$$

because $\vec{p} \to -i\hbar\vec{\nabla}$ and $k = m\omega^2$.

The stationary state energies E_n & wave function $\psi_n(x)$ are the solution of time independent schrodinger equation. The wave eqn is given by

$$H\psi_n(x) = E\psi(x)$$

using eqn ② we can write

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2x^2\right]\psi(x) = E.\psi(x)$$

For one-dimensional we get

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right]\psi(x) = E\psi(x)$$

multiplying both sides by $-\frac{2m}{\hbar^2}$

$$\therefore \frac{d^2\psi}{dx^2} - \frac{m^2\omega^2}{\hbar^2}x^2\psi(x) = -E\psi\frac{2m}{\hbar^2}$$

$$\therefore \boxed{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\omega^2x^2\right]\psi = 0} \longrightarrow (3)$$

This is the schrodinger equation for S.H.O.

Now take $x = \rho/\alpha$, were $\alpha = \sqrt{\frac{m\omega}{\hbar}}$

substituting this value in above eqn we get

$$\frac{d^2\psi}{d\rho^2}.\alpha^2 + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\omega^2\frac{\rho^2}{\alpha^2}\right]\psi = 0$$

$$\therefore \frac{d^2\psi}{d\rho^2}.\alpha^2 + \frac{2mE}{\hbar^2}\psi - \frac{m^2\omega^2\rho^2}{\hbar^2\alpha^2}.\psi = 0$$

$$\therefore \frac{d^2u}{d\xi^2} + \frac{2mE}{\alpha^2\hbar^2}\cdot u - \frac{m^2\omega^2}{\hbar^2}\cdot\frac{\xi^2}{\alpha^4}u = 0$$

$$\therefore \frac{d^2u}{d\xi^2} + \frac{2mE}{\frac{m\omega}{\hbar}\cdot\hbar^2}\cdot u - \frac{m^2\omega^2}{\hbar^2}\cdot\frac{\xi^2}{\frac{m^2\omega^2}{\hbar^2}}\cdot u = 0 \qquad \left[\because \alpha = \sqrt{\frac{m\omega}{\hbar}}\right]$$

$$\therefore \frac{d^2u}{d\xi^2} + \frac{2Eu}{\hbar\omega} - \xi^2 u = 0$$

$$\left\{\because E = h\nu = \frac{h}{2\pi}\cdot 2\pi\nu = \hbar\omega\right.$$

(dim. less)

define $\frac{2E}{\hbar\omega} = \lambda$, we get

$$\boxed{\frac{d^2u}{d\xi^2} + [\lambda - \xi^2]u = 0} \qquad \text{--- (3)}$$

This is the dimension less schrodinger eqn.

* To examine the asymptotic behaviour of wave function $u(x)$ $[x = \pm\infty]$:-

Asymptotic behaviour means the behaviour of wave function for large value of x.

For simplicity put $\xi = x$

$$\therefore \frac{d^2u}{dx^2} + [\lambda - x^2]u = 0$$

The soln of this eqn is $u(x) = e^{-x^2/2}$.

Another soln is

$$u(x) = e^{x^2/2} \to \infty \quad \text{when } x \to \infty$$

$\therefore$ we will interpolate in the solution

$$\therefore \boxed{u(x) = e^{-x^2/2}\cdot\phi(x)} \qquad \text{--- (4)}$$

Substituting this soln in eqn (3).

Here $\phi(x)$ is unknown polynomials.

$$\therefore \quad \frac{d^2}{dx^2}\left[e^{-x^2/2}\phi(x)\right] + \left[\lambda - x^2\right]\left[e^{-x^2/2}\cdot\phi(x)\right] = 0$$

$$\therefore \quad \frac{d}{dx}\left[e^{-x^2/2}\frac{d\phi(x)}{dx} + \phi(x)\,e^{-x^2/2}\left(-\frac{1}{\cancel{2}}\cdot\cancel{2}x\right)\right] +$$

$$\left[\lambda - x^2\right] e^{-x^2/2}\cdot\phi(x) = 0$$

$$\therefore \quad e^{-x^2/2}\cdot\frac{d^2\phi}{dx^2} + e^{-x^2/2}(-x)\cdot\frac{d\phi}{dx} - \frac{d\phi}{dx}\cdot x\cdot e^{-x^2/2} - \phi(x)\,e^{-x^2/2} +$$

$$x^2\,\phi(x)\,e^{-x^2/2} + (\lambda - x^2)\left(e^{-x^2/2}\phi(x)\right) = 0$$

$$\therefore \quad \frac{d^2\phi}{dx^2} - 2x\frac{d\phi}{dx} + (\lambda - 1)\phi(x) = 0$$

$$\therefore \quad \boxed{\phi''(x) - 2x\,\phi'(x) + (\lambda-1)\,\phi(x) = 0} \quad \text{——} \quad (5)$$

⇒ Series solution:

let us now obtain the series sol^n of eq^n (5). Suppose its series sol^n is given by

$$\phi(x) = \sum_{n=0}^{\infty} a_n\, x^{n+s} \quad \text{——} \quad (6)$$

$$\therefore \quad \phi'(x) = \sum_{n=0}^{\infty} a_n\,(n+s)\,x^{n+s-1}$$

$$\text{and,} \quad \phi''(x) = \sum_{n=0}^{\infty} a_n\,(n+s)(n+s-1)\,x^{n+s-2}$$

Substituting these values in eq^n (5) we get

$$\sum_{n=0}^{\infty}\left[(n+s)(n+s-1)\,x^{n+s-2} - 2x\,(n+s)\,x^{n+s} + (\lambda-1)\,x^{n+s}\right]a_n = 0.$$

$$\therefore \quad \sum_{n=0}^{\infty}\left[(n+s)(n+s-1)\,x^{n+s-2} - 2\,(n+s)\,x^{n+s} + (\lambda-1)\,x^{n+s}\right]a_n = 0 \quad \text{——} \quad (7)$$

Now equating the lowest power of x to zero by putting $n=0$,

$$s(s-1)\,a_0 = 0$$

but $a_0 \neq 0$ $\therefore$ $s(s-1) = 0$

$$\therefore \boxed{s=0 \text{ or } s=1}$$

Now put $s=0$ in eq^n (7),

$$\therefore \sum_{n=0}^{\infty}\left[n(n-1)x^{n-2} - 2n\,x^n + (\lambda-1)x^n\right]a_n = 0 \quad \text{— (8)}$$

Now equating the general coefficient of x^n to zero

$$\therefore (n+2)(n+1)a_{n+2} - \left[2n-(\lambda-1)\right]a_n = 0$$

$$\therefore (n+1)(n+2)a_{n+2} = \left[2n-\lambda+1\right]a_n$$

$$\therefore \boxed{\frac{a_{n+2}}{a_n} = \frac{2n-(\lambda-1)}{(n+2)(n+1)}} \quad \text{— (9)}$$

This formula is known as recurrence formula.

For $n\to\infty$, if the ratio of two successive coefficient tends to zero, then the series is called convergent series.

$$\phi(x) = \sum a_n x^n$$

$$= a_0 + a_2x^2 + a_4x^4 + \cdots + a_kx^k + a_{k+2}x^{k+2} + \cdots$$

here k is ∞

$$\therefore \frac{a_{k+2}}{a_k} = \frac{2k}{k^2} = \frac{2}{k} \to 0$$

We know that

$$e^{t} = 1 + t + \frac{t^2}{2!} + \frac{t^3}{3!} + \cdots$$

take $t = x^2$

$$\therefore \quad e^{x^2} = 1 + x^2 + \frac{x^4}{2!} + \frac{x^6}{3!} + \cdots + \frac{x^k}{\left(\frac{k}{2}\right)!} + \frac{x^{k+2}}{\left(\frac{k+2}{2}\right)!} + \cdots$$

The ratio of two successive coefficients is

$$\frac{x^{k+2}}{x^k} = \frac{(k+2/2)!}{(k/2)!} = \frac{2}{k} \to 0 \quad \text{as } k \to \infty$$

The behaviour of the coefficient is series $\phi(x)$ is exactly the same as in the series for e^{x^2}.

$$\therefore \quad \psi(x) = e^{-x^2/2}\,\phi(x)$$

$$= e^{-x^2/2} \cdot e^{x^2}$$

$$= e^{x^2/2} \to \infty \quad \text{when } x \to \infty$$

The above function will be unacceptable wave fn.

In order to avoid this situation the value of λ is choosen in such a way that the power series for $\phi(x)$ gets cut-off after certain no. of terms, there by making $\phi(x)$ a polynomials.

For example,

$$\phi(x) = a_0 + a_2 x^2 + a_4 x^4 + \cdots + a_k x^k + a_{k+2} x^{k+2} + \cdots$$

If we want to terminate the series after three terms, then the coefficients $a_6, a_8, a_{10} \cdots$ should be zero

This could happen only when the numerator in recurrsion relation is zero put

$\therefore$ $n=4$ in recursion relation

$$\frac{a_6}{a_4} = \frac{8-(\lambda-1)}{6\cdot 5} = \frac{8-(\lambda-1)}{30}$$

$$\therefore\ a_6 = \frac{8-(\lambda-1)}{30}\cdot a_4$$

$\therefore$ Numerator $= 8-(\lambda-1) = 0$

$$\Rightarrow \lambda - 1 = 8$$

$$\therefore \boxed{\lambda = 9} \quad \therefore \boxed{\lambda = 2n+1}$$

We can say that, for $\lambda = 9$ the series will terminate after three terms.

The value of λ which make the series to cut-off at n^{th} terms, ~~for~~ is

$$\boxed{\lambda = 2n+1}$$

But, $\lambda = \frac{2E}{\hbar\omega}$

$$\therefore E = \frac{1}{2}\hbar\omega\lambda$$

$$= \frac{1}{2}\hbar\omega(2n+1)$$

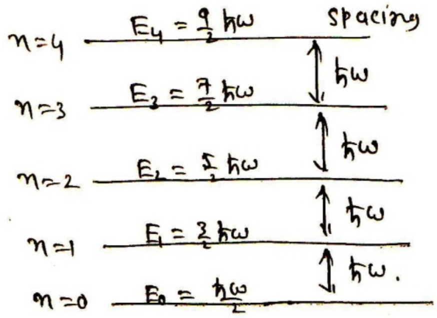
$$\therefore \boxed{E = \hbar\omega(n+1/2)} \qquad \text{——} \ (10)$$

$$n = 0, 1, 2, \ldots$$

This gives energy eigen values of S.H.O.

For $n=0$, $E = \frac{1}{2}\hbar\omega$.

It is known as the zero point energy.



The stationary states of S.H.O are characterized by equally spaced energy levels.

A constant spacing betⁿ successive energy levels is $\hbar\omega = \frac{h}{2\pi} \cdot 2\pi\nu = h\nu$ is exactly what had been postulated by Max plank.

The wave-mechanical treatment gives definite non-zero value for the ground state energy $E_0 = \frac{\hbar\omega}{2}$. This is called zero-point energy.

* Orthonormality: The orthonormal property of the set of functions is

$$(u_m, u_n) = \int u_m^*(x)\, u_n(x)\, dx = \delta_{mn} \quad \text{------} \; (17)$$

To prove this property of the stationary state wave functions $u_n(x)$ we make use of known properties of Hermite polynomials. The generating function $G(s,h)$ of the Hermite polynomials defined as

$$G(s,h) = \sum_{n=0}^{\infty} \frac{1}{n!} H_n(s)\, h^n \quad \text{------} \; (18)$$

$$= e^{(-h^2 + 2sh)} \quad \text{----} \; (19)$$

Here h is a parameter. $H_n(s)$ is the coefficient of $\frac{h^n}{n!}$ in the expansion of $e^{-h^2 + 2sh}$.

Now, consider the integral

$$\int_{-\infty}^{\infty} G(s,h)\, G(s,h')\, e^{-s^2}\, ds \quad \text{-------} \; (20)$$

Now, substituting eqns (18) & (19) in (20) we get

$$\sum_m \sum_n \frac{h^m h'^n}{m!\,n!} \int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \int_{-\infty}^{\infty} e^{-\xi^2} \cdot e^{-h^2+2\xi h} \cdot e^{-h'^2+2\xi h'} d\xi$$

$$= \int_{-\infty}^{\infty} e^{-\xi^2+2\xi(h+h')-(h^2+h'^2)} d\xi \quad \text{----- (21)}$$

$$= \sqrt{\pi} \sum_m \sum_n \frac{2^n h^m h'^n}{n!} \delta_{mn} \quad \text{---- (22)}$$

Now, equating the coefficient of $h^m h'^n$ on both the sides we get

$$\int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \sqrt{\pi}\, 2^n m!$$

$$= \sqrt{\pi}\, 2^n n!\, \delta_{mn} \quad \text{------- (23)}.$$

* <u>Properties of stationary states:</u>

The stationary states of the simple harmonic oscillato are characterized by the energy levels $E_n = (n+\frac{1}{2})\hbar\omega_c$ and the wave function

$$u_n(x) = N_n e^{-\xi^2/2} H_n(\xi).$$

The lowest energy $E_0 = \frac{1}{2}\hbar\omega_c$ is called zero-point energy. The oscillator potential and the first three eigenfunctions are shown in fig (a).

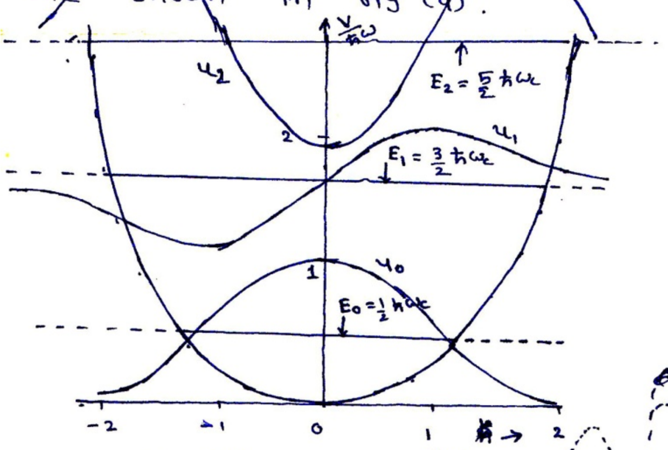
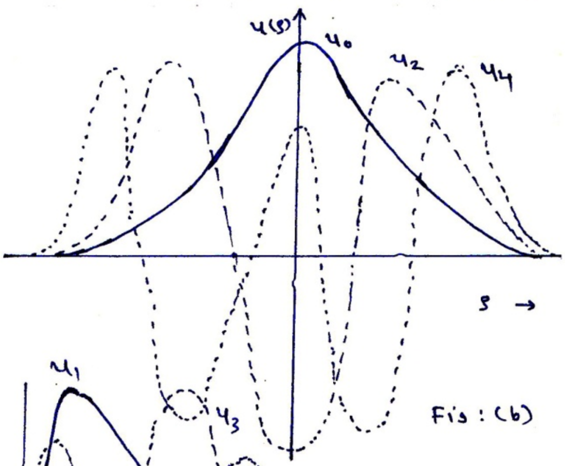


Fig: (a)

$\rho \rightarrow$



Fis: (b)

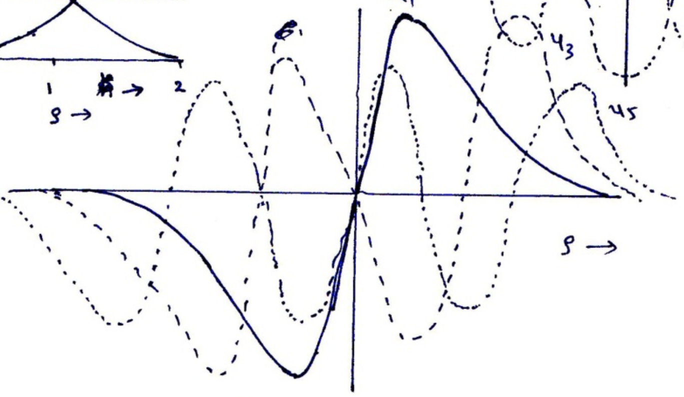


Fig: (c)

Fig (b) & (c) shows the even and odd parity wave functions. The ground state wave function $u_0(x)$ is given by

$$u_0(x) = \left(\alpha^2/\pi\right)^{1/4} e^{-\frac{1}{2}\alpha^2 x^2}.$$

The ground state of the harmonic oscillator is a minimum uncertainty state.

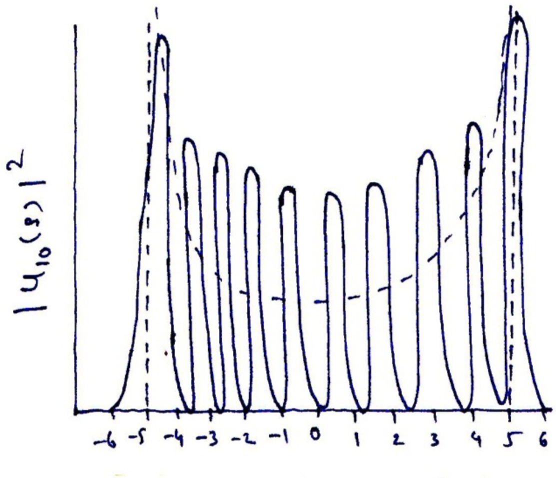


Fig: (d)

$\rho \rightarrow$

Fig: (d) shows the position probability density $|u_n|^2$ for $n = 10$ plotted as a function of $\rho = \alpha x$. The dotted curve represents the classical oscillator. This classical curve is seen to agree well with the average behavior of the quantum mechanical curve.

The Abstract Operator method:

The harmonic oscillator problem can also be solved by abstract operator method. It is said to be ladder (or Raising and Lowering) operators. The pair of operators are

$$a = \left(\frac{m\omega_c}{2\hbar}\right)^{1/2} x + i\left(\frac{1}{2m\hbar\omega_c}\right)^{1/2} p \quad \text{---- (1)}$$

and its adjoint

$$a^{+} = \left(\frac{m\omega_c}{2\hbar}\right)^{1/2} x - i\left(\frac{1}{2m\hbar\omega_c}\right)^{1/2} p \quad \text{---- (2)}$$

It has the property $[a, a^{+}] = 1$ ---- (3)

Taking the product of $a^{+}a$, we find

$$\left.\begin{aligned} a^{+}a &= \frac{p^2}{2m\hbar\omega_c} + \frac{m\omega_c}{2\hbar}x^2 - \frac{1}{2} \\ &= \frac{H}{\hbar\omega_c} - \frac{1}{2} \end{aligned}\right\} \quad \text{---- (4)}$$

where H is the Hamiltonian of the harmonic oscillator.

Thus, $H = (a^{+}a + \frac{1}{2})\hbar\omega_c$ -------- (5)

The eigenvalues of $a^{+}a$ are integers n $(n = 0, 1, 2 \ldots)$

$$\therefore H = (n + \tfrac{1}{2})\hbar\omega_c \quad \text{---- (6)}$$

Coherent States:

The eigenstates of lowering operator a can be expressed in terms of the stationary states u_n of the harmonic oscillator in the form

$$\phi_{\mu} = \sum_{n=0}^{\infty} e^{-\frac{1}{2}|\mu|^2} \cdot \frac{\mu^n}{\sqrt{n!}} u_n \quad \text{---- (1)}$$

The eigenvalue eq^n is

$$a\phi_u = u\phi_u \quad \text{-----} (2)$$

The orthonormality of a given eigenfunction is given by

$$\int \phi_u^* \phi_{u'}\, dx = \int \left(\sum_{m=0}^{\infty} e^{-\frac{1}{2}|u|^2} \frac{(u^*)^m}{\sqrt{m!}} u_m^* \right)\left(\sum_{n=0}^{\infty} e^{-\frac{1}{2}|u'|^2} \frac{(u')^n}{\sqrt{n!}} u_n \right) dx$$

$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} e^{-\frac{1}{2}|u|^2 - \frac{1}{2}|u'|^2} \frac{(u^*)^m (u')^n}{(m!\,n!)^{1/2}} \delta_{mn}$$

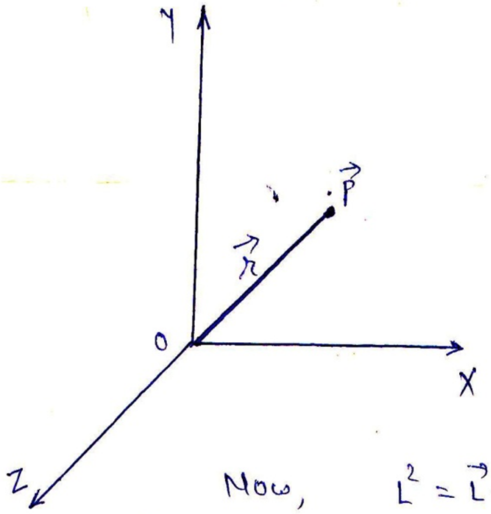
$$= e^{-\frac{1}{2}|u|^2 - \frac{1}{2}|u'|^2} \cdot e^{u^* u'} \quad \text{-------} (3)$$

Thus the eigenfunctions $\phi_u, \phi_{u'}$ are not orthogonal for $u \neq u'$. For $u = u'$ eq^n. (3) reduces to unity, Thus ϕ_u is normalized.

The position probability density of given function $|\phi_u(x,t)|^2$ gives the Gaussian function centred about the point x which oscillates in simple harmonic fashion. The function has no other time dependence. Hence, ϕ_u represents a wave packet which executes simple harmonic oscillations, moving as a whole without any change of shape. Because of this property the state represented by ϕ_u is called a coherent state. The motion of a coherent wave packet is exactly the same as that of a classical oscillator.

* The Angular Momentum Operators:

Q: What is angular momentum ? Write the components of angular momentum in cartesian coordinates. Convert them into spherical polar coordinates (r, θ, ϕ). Hence obtain the expression for L^2 operator in spherical polar coordinates.



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

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

where $\vec{r}(x, y, z)$, $\vec{P}(p_x, p_y, p_z)$

Now,

$$
\begin{aligned}
L^2 &= \vec{L} \cdot \vec{L} \\
&= (\vec{r} \times \vec{P}) \cdot \vec{L} \\
&= \vec{r} \cdot (\vec{P} \times \vec{L}) \\
&= \vec{r} \cdot [\vec{P} \times (\vec{r} \times \vec{P})] \\
&= \vec{r} \cdot [\vec{r}(\vec{P} \cdot \vec{P}) - \vec{P}(\vec{P} \cdot \vec{r})] \\
&= \vec{r} \cdot \vec{r}\,(\vec{P} \cdot \vec{P}) - \vec{r} \cdot \vec{P}\,(\vec{P} \cdot \vec{r}) \\
&= r^2 p^2 - (\vec{r} \cdot \vec{P})(\vec{P} \cdot \vec{r}) \qquad \text{--- (1)}
\end{aligned}
$$

but, $[\vec{r}, \vec{P}] = i\hbar$

$\therefore \vec{r} \cdot \vec{P} - \vec{P} \cdot \vec{r} = i\hbar \qquad \therefore \vec{P} \cdot \vec{r} = \vec{r} \cdot \vec{P} - i\hbar$

$\therefore$ Eq^n (1) becomes

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

$$\therefore \boxed{L^2 = r^2 p^2 - (\vec{r}\cdot\vec{p})^2 + i\hbar\,(\vec{r}\cdot\vec{p})} \quad \text{--- (2)}$$

Component of angular momentum in cartesian coordinates are $\vec{L} = \vec{r} \times \vec{p}$

$$\begin{bmatrix} L_x \\ L_y \\ L_z \end{bmatrix} = \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{bmatrix}$$

$$\left.\begin{aligned} L_x &= y p_z - z p_y \\ L_y &= z p_x - x p_z \\ L_z &= x p_y - y p_x \end{aligned}\right\} \quad \text{--- (3)}$$

But $p_x \rightarrow -i\hbar \frac{\partial}{\partial x}$, $p_y \rightarrow -i\hbar \frac{\partial}{\partial y}$, $p_z \rightarrow -i\hbar \frac{\partial}{\partial z}$

$$\therefore L_x = -y\, i\hbar \frac{\partial}{\partial z} + z\, i\hbar \frac{\partial}{\partial y}$$

$$= i\hbar \left[z \frac{\partial}{\partial y} - y \frac{\partial}{\partial z} \right] \quad \text{--- (4)}$$

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

$$= i\hbar \left[x \frac{\partial}{\partial z} - z \frac{\partial}{\partial x} \right] \quad \text{--- (5)}$$

& $$L_z = i\hbar \left[y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right] \quad \text{--- (6)}$$

Transformations eq^{ns} are given by

$$\left.\begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned}\right\} \quad \text{--- (7)}$$

$$\frac{y}{x} = \tan\phi \qquad \therefore \boxed{\phi = \tan^{-1}\frac{y}{x}}$$

and, $z = r\cos\theta \Rightarrow \cos\theta = \frac{z}{r} \qquad \therefore \boxed{\theta = \cos^{-1}\left(\frac{z}{r}\right)}$

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

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

$$\therefore \boxed{\theta = \cos^{-1}\frac{z}{(x^2+y^2+z^2)^{1/2}}}$$

Now,

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi} \quad \text{——— (8)}$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi} \quad \text{——— (9)}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial z}\frac{\partial}{\partial \phi} \quad \text{——— (10)}$$

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

$$2r\frac{dr}{dx} = 2x$$

$$\therefore \frac{dr}{dx} = \frac{x}{r} = \frac{r\sin\theta\cos\phi}{r} = \sin\theta\cos\phi$$

$$\text{llly} \quad \boxed{\frac{dr}{dy} = \frac{y}{r} = \sin\theta\sin\phi}$$

$$\boxed{\frac{dr}{dz} = \frac{z}{r} = \cos\theta}$$

Now, $\theta = \cos^{-1}\left(\frac{z}{\sqrt{x^2+y^2+z^2}}\right)$

$$\therefore \frac{d\theta}{dx} = -\frac{1}{\sqrt{1-\frac{z^2}{x^2+y^2+z^2}}} \cdot \frac{z\cdot\left(-\frac{1}{2}\right)}{(x^2+y^2+z^2)^{3/2}}\cdot 2x$$

$$= \frac{z\cdot x\,(x^2+y^2+z^2)^{1/2}}{\sqrt{x^2+y^2}} \cdot \frac{1}{(x^2+y^2+z^2)^{3/2}}$$

$$\therefore \frac{d\theta}{dx} = \frac{z \cdot x}{\sqrt{x^2+y^2}} \cdot \frac{1}{(x^2+y^2+z^2)} = \frac{\cancel{r}\cos\theta \cdot r\cancel{\sin\theta}\cos\phi}{r\cancel{\sin\theta} \cdot \cancel{r}^2}$$

$$= \frac{\cos\theta \cos\phi}{r}$$

similarly $\boxed{\frac{\partial\theta}{\partial y} = \frac{\cos\theta \sin\phi}{r}}$

and, $\boxed{\frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r}}$

$$\phi = \tan^{-1}\left(\frac{y}{x}\right) \quad \therefore \frac{\partial\phi}{\partial x} = \frac{1}{1+\frac{y^2}{x^2}} \cdot y\left(-\frac{1}{x^2}\right) = -\frac{y}{x^2+y^2}$$

$$= -\frac{r\sin\theta \sin\phi}{r^2 \sin^2\theta}$$

$$\boxed{\frac{\partial\phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta}}$$

llly, $\boxed{\frac{\partial\phi}{\partial y} = \frac{\cos\phi}{r\sin\theta}}$ and $\boxed{\frac{\partial\phi}{\partial z} = 0}$

put all these values in eqn (8), (9) & (10)

$$\Rightarrow \frac{\partial}{\partial x} = \sin\theta\cos\phi \frac{\partial}{\partial r} + \cos\theta\cos\phi \frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \quad \text{—— (11)}$$

$$\frac{\partial}{\partial y} = \sin\theta \sin\phi \frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \quad \text{—— (12)}$$

$$\frac{\partial}{\partial z} = \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta} \quad \text{—— (13)}$$

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

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

$$\therefore L_x = -i\hbar \left[r\sin\theta \sin\phi \cancel{\cos\theta} \frac{\partial}{\partial r} - \sin^2\theta \sin\phi \frac{\partial}{\partial\theta} - r\sin\theta \cancel{\cos\theta} \sin\phi \frac{\partial}{\partial r} - \cos^2\theta \sin\phi \frac{\partial}{\partial\theta} - \frac{\cos\theta\cos\phi}{\sin\theta} \frac{\partial}{\partial\phi} \right]$$

$$= -i\hbar \left[-\sin\phi \frac{\partial}{\partial\theta} - \cos\phi \cot\theta \frac{\partial}{\partial\phi} \right]$$

$$\therefore L_x = i\hbar \left[\sin\phi \frac{\partial}{\partial\theta} + \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right] \quad \text{—— (14)}$$

lly, $$L_y = i\hbar \left[-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right] \quad \text{—— (15)}$$

$$L_z = -i\hbar \frac{\partial}{\partial\phi} \quad \text{—— (16)}$$

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, $$\vec{r}\cdot\vec{P} = \vec{r}\cdot(-i\hbar\vec{\nabla}) = -i\hbar(\vec{r}\cdot\vec{\nabla}) \quad \text{—— (16)}$$

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

$$2r\frac{\partial}{\partial r} = 2x\frac{\partial}{\partial x} + 2y\frac{\partial}{\partial y} + 2z\frac{\partial}{\partial z}$$

$$\therefore r\frac{\partial}{\partial r} = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z} = \vec{r}\cdot\vec{\nabla}$$

$\therefore$ Eq^n (16) becomes $\vec{r}\cdot\vec{P} = -i\hbar r\frac{\partial}{\partial r}$

$$(\vec{r}\cdot\vec{P})^2 = (\vec{r}\cdot\vec{P}) * (\vec{r}\cdot\vec{P})$$

$$= \left(-i\hbar r\frac{\partial}{\partial r}\right)\left(-i\hbar r\frac{\partial}{\partial r}\right)$$

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

$$= -\hbar^2 r^2 \frac{\partial^2}{\partial r^2} - \hbar^2 r\frac{\partial}{\partial r}$$

Hence operator L^2 can be written as

$$L^2 = -r^2\hbar^2\nabla^2 + \hbar^2 r^2 \frac{\partial^2}{\partial r^2} + \hbar^2 r \frac{\partial}{\partial r} + \hbar^2 r \frac{\partial}{\partial r}$$

$$= -r^2\hbar^2\nabla^2 + \hbar^2 r^2 \frac{\partial^2}{\partial r^2} + 2\hbar^2 r \frac{\partial}{\partial r}$$

$$= -r^2\hbar^2\nabla^2 + \hbar^2 \frac{\partial}{\partial r}\left[r^2 \frac{\partial}{\partial r}\right]$$

$$= -\hbar^2\left[r^2\nabla^2 - \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right]$$

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

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

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

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

* The Eigenvalue Equation for L^2; Separation of Variables :-

The eigenvalue eqn is given by

$A\phi_a = a\phi_a$ where
$A \rightarrow$ operator
$\phi_a \rightarrow$ Eigen fn
$a \rightarrow$ Eigen value.

Here,

$$L^2 v(\theta,\phi) = \lambda\hbar^2 v(\theta,\phi) \qquad \text{—— (1)}$$

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

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

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

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

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

To solve eigen value eq^n L^2 we use the method of separation of variable.

let $$v(\theta,\phi) = \Theta(\theta)\cdot\Phi(\phi) \quad \text{--- (3)}$$

$\therefore$ Eq^n (2) becomes

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

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

Multiplying both sides by $\dfrac{\sin^2\theta}{\Theta(\theta)\Phi(\phi)}$

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

$$\therefore -\frac{1}{\Phi(\phi)}\frac{\partial^2}{\partial\phi^2}\Phi(\phi) = \lambda\sin^2\theta + \frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\Theta(\theta)\right] \quad \text{--- (4)}$$

The L.H.S of this eq^n 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

$$\therefore \frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \lambda\sin^2\theta = m^2 \quad \text{--- (5)}$$

and, $$-\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2} = m^2 \quad \text{--- (6)}$$

Multiplying eq^n (5) by $\dfrac{\Theta(\theta)}{\sin^2\theta}$ we get

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \left[\lambda - \frac{m^2}{\sin^2\theta}\right]\Theta(\theta) = 0 \quad \text{--- (7)}$$

* Admissibility Conditions on Solutions; Eigenvalues :-

We know that

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

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

There are two sol^{ns} of eq^n (1)

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

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

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

$$\text{i.e.} \quad e^{im2\pi} = 1 \quad \text{—— (2)}$$

$$\therefore \cos(2m\pi) + i\sin(2\pi m) = 1 \quad \text{—— (3)}$$

when $2\pi m = 0, 2\pi, 4\pi, \ldots$ eq^n will be satisfy.

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

these are the possible values of m.

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

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

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

Substituting these values in above eq^n

$$\therefore \int_0^{2\pi} A^* e^{-im\phi} A e^{im\phi} d\phi = 1$$

$$\therefore |A|^2 \int_0^{2\pi} d\phi = 1$$

$$\therefore |A|^2 \cdot 2\pi = 1 \qquad \therefore \boxed{A = \frac{1}{\sqrt{2\pi}}} \quad \text{—— (4)}$$

$\therefore$ The normalized eqn Φ is given by

$$\boxed{\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}} \quad \text{—— (5)}$$

$\Theta(\theta)$ eqn is given by

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + \left(\lambda - \frac{m^2}{\sin^2\theta}\right)\Theta(\theta) = 0 \quad \text{—— (6)}$$

To solve $\Theta(\theta)$ eqn suppose $\cos\theta = \omega$

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

$$\therefore \frac{d}{d\theta} = \frac{d}{d\omega}\cdot\frac{d\omega}{d\theta}$$

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

$$\therefore \boxed{\frac{1}{\sin\theta}\frac{d}{d\theta} = -\frac{d}{d\omega}.}$$

Now, $\cos\theta = \omega$

$$\sin^2\theta = 1 - \cos^2\theta$$

$$= 1 - \omega^2$$

Substituting these values in eqn (6) we get

$$-\frac{d}{d\omega}\left[\sqrt{1-\omega^2}\left(-\sin\theta \frac{d\Theta}{d}\right)\right] + \left[\lambda - \frac{m^2}{1-\omega^2}\right]\Theta(\theta) = 0$$

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

$$\therefore \frac{d}{d\omega}\left[(1-\omega^2)\frac{d\Theta}{d\omega}\right] + \left[\lambda - \frac{m^2}{1-\omega^2}\right]\Theta(\theta) = 0$$

Take the soln $\Theta(\theta) = P(\omega)$

$$\therefore \frac{d}{d\omega}\left[(1-\omega^2)\frac{dP(\omega)}{d\omega}\right] + \left[\lambda - \frac{m^2}{1-\omega^2}\right]P(\omega) = 0$$

$$\therefore \boxed{(1-\omega^2)\frac{d^2P}{d\omega^2} - 2\omega\frac{dP}{d\omega} + \left[\lambda - \frac{m^2}{1-\omega^2}\right]P(\omega) = 0} \quad \text{—— (7)}$$

Sol^n of this polynomial eq^n is

$$P(\omega) = (1-\omega^2)^a \, K(\omega) \quad , \; a > 0 \qquad \text{——— (8)}$$

Diff^n with respect to ω

$$\frac{dP}{d\omega} = (1-\omega^2)^a \frac{dk}{d\omega} + K(\omega)\, a\, (1-\omega^2)^{a-1} (-2\omega)$$

$$= (1-\omega^2)^a \frac{dk}{d\omega} - 2a\omega K(\omega)(1-\omega^2)^{a-1} \qquad \text{——— (9)}$$

$$\frac{d^2P}{d\omega^2} = (1-\omega^2)^a \frac{d^2k}{d\omega^2} + \frac{dk}{d\omega}\, a\, (1-\omega^2)^{a-1}(-2\omega) - 2a\omega K(\omega)(a-1)(1-\omega^2)^{a-2}(-2\omega)$$
$$- 2aK(\omega)(1-\omega^2)^{a-1} - 2a\omega \frac{dk}{d\omega}(1-\omega^2)^{a-1}$$

$$= (1-\omega^2)^a \frac{d^2k}{d\omega^2} - 2a\omega \frac{dk}{d\omega}(1-\omega^2)^{a-1} + 4a(a-1)\omega^2 k(\omega)(1-\omega^2)^{a-2}$$
$$- 2aK(\omega)(1-\omega^2)^{a-1} - 2\omega \frac{dk}{d\omega}\, a\, (1-\omega^2)^{a-1}$$

$$\therefore \frac{d^2P}{d\omega^2} = (1-\omega^2)^a \frac{d^2k}{d\omega^2} - 4a\omega \frac{dk}{d\omega}(1-\omega^2)^{a-1} + 4a(a-1)\omega^2 K(\omega)(1-\omega^2)^{a-2}$$
$$- 2aK(\omega)(1-\omega^2)^{a-1} \qquad \text{——— (10)}$$

Substituting eq^{ns} (8), (9) & (10) in eq^n (7) we get

$$(1-\omega^2)\frac{d^2P}{d\omega^2} - 2\omega \frac{dP}{d\omega} + \left[\lambda - \frac{m^2}{1-\omega^2}\right] P(\omega) = 0$$

$$(1-\omega^2)\Big[(1-\omega^2)^a \frac{d^2k}{d\omega^2} - 4a\omega \frac{dk}{d\omega}(1-\omega^2)^{a-1} + 4a(a-1)\omega^2 K(\omega)(1-\omega^2)^{a-2}$$
$$- 2aK(\omega)(1-\omega^2)^{a-1}\Big] - 2\omega\left[(1-\omega^2)^a \frac{dk}{d\omega} - 2a\omega K(\omega)(1-\omega^2)^{a-1}\right]$$
$$+ \left[\lambda - \frac{m^2}{1-\omega^2}\right](1-\omega^2)^a K(\omega) = 0$$

$$\therefore (1-\omega^2)^{a+1} \frac{d^2k}{d\omega^2} - 4a\omega(1-\omega^2)^a \frac{dk}{d\omega} + 4a(a-1)\omega^2 K(\omega)(1-\omega^2)^{a-1} - 2aK(\omega)(1-\omega^2)^a$$
$$- 2\omega(1-\omega^2)^a \frac{dk}{d\omega} - 4a\omega^2 K(\omega)(1-\omega^2)^{a-1} + \lambda(1-\omega^2)^a K(\omega)$$
$$- \frac{m^2}{1-\omega^2}(1-\omega^2)^a K(\omega) = 0$$

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

$$(1-\omega^2)\frac{d^2k}{d\omega^2} - 4a\omega \frac{dk}{d\omega} + \frac{4a(a-1)\omega^2 K(\omega)}{1-\omega} - 2aK(\omega) - 2\omega \frac{dk}{d\omega} - \frac{4a\omega^2 K(\omega)}{1-\omega}$$
$$+ \lambda K(\omega) - \frac{m^2}{1-\omega^2} K(\omega) = 0$$

$$\therefore (1-\omega^2)\frac{d^2k}{d\omega^2} - 2\omega(2a+1)\frac{dk}{d\omega} + \left[-2a + \frac{4a^2(\omega^2-1)}{1-\omega^2} + \frac{4a^2}{1-\omega^2} - \frac{m^2}{1-\omega^2} + \lambda\right]k(\omega) = 0$$

$$\therefore (1-\omega^2)\frac{d^2k}{d\omega^2} - 2\omega(2a+1)\frac{dk}{d\omega} + \left[-2a - 4a^2 + \frac{4a^2}{1-\omega^2} - \frac{m^2}{1-\omega^2} + \lambda\right]k(\omega) = 0$$

$$\therefore (1-\omega^2)\frac{d^2k}{d\omega^2} - 2\omega(2a+1)\frac{dk}{d\omega} + \left[-2a - 4a^2 + \frac{4a^2 - m^2}{1-\omega^2} + \lambda\right]k(\omega) = 0$$

we assume, $4a^2 = |m|^2 \quad \therefore 2a = |m|$

By putting the above assumption, we get

$$\therefore (1-\omega^2)\frac{d^2k}{d\omega^2} - 2\omega(|m|+1)\frac{dk}{d\omega} + \left[\lambda - |m| - |m|^2\right]k(\omega) = 0 \quad \text{— (ii)}$$

The above eqn can be solved by series method.

The series soln of the above eqn is given by

$$k(\omega) = \sum a_n \omega^{n+s}$$

$$\therefore \frac{dk}{d\omega} = \sum a_n (n+s)\,\omega^{n+s-1}$$

$$\frac{d^2k}{d\omega^2} = \sum a_n (n+s)(n+s-1)\,\omega^{n+s-2}$$

put $s = 0$,

$$k(\omega) = \sum a_n \omega^n$$

$$\frac{dk}{d\omega} = \sum a_n (n)\,\omega^{n-1}$$

$$\frac{d^2k}{d\omega^2} = \sum a_n (n)(n-1)\,\omega^{n-2}$$

substituting these values in eqn (ii) we get

$$(1-\omega^2)\sum a_n n(n-1)\omega^{n-2} - 2\omega(|m|+1)\sum a_n (n)\omega^{n-1} + \left[\lambda - |m| - |m|^2\right]\sum a_n \omega^n = 0$$

$$\therefore \sum a_n n(n-1)\omega^{n-2} - \sum a_n n(n-1)\omega^n - 2(|m|+1)\sum a_n n\,\omega^n + \left[\lambda - |m| - |m|^2\right]\sum a_n \omega^n = 0$$

$$\therefore \sum a_n n(n-1)\omega^{n-2} - \sum a_n\left[n(n-1) + 2(|m|+1)n - (\lambda - |m| - |m|^2)\right]\omega^n = 0$$

Equate the coefficients of ω^r to zero. We substitute $n = r+2$ in first term and $n = r$ in the second term. —— (12)

$$\therefore \; a_{r+2}(r+2)(r+1)\,\omega^r - a_r\left[r(r-1) + 2(|m|+1)r - \lambda + |m| + |m|^2\right]\omega^r = 0$$

$$\therefore \; a_{r+2}(r+2)(r+1) = a_r\left[r(r-1) + 2(|m|+1)r - \lambda + |m| + |m|^2\right]$$

$$\therefore \; \frac{a_{r+2}}{a_r} = \frac{r^2 - r + 2|m|r + 2r - \lambda + |m| + |m|^2}{(r+2)(r+1)}$$

$$\therefore \; \frac{a_{r+2}}{a_r} = -\frac{\lambda - (r+|m|)(r+|m|+1)}{(r+1)(r+2)} \qquad \text{—— (13)}$$

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

$$K(\omega) = \sum a_n \omega^n$$

$$= a_0 + a_2\omega^2 + a_4\omega^4 + \cdots$$

$$a_1 = a_3 = a_5 = \cdots = 0.$$

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

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

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

$$\therefore \; \frac{a_{r+2}}{a_r} = \frac{(r+|m|)(r+|m|+1)}{(r+1)(r+2)}$$

$$= \frac{r^2\left(1 + \frac{|m|}{r}\right)\left(1 + \frac{|m|+1}{r}\right)}{r^2\left(1+\frac{1}{r}\right)\left(1+\frac{2}{r}\right)}$$

$$= \left(1 + \frac{|m|}{r}\right)\left(1 + \frac{|m|+1}{r}\right)\left(1+\frac{1}{r}\right)^{-1}\left(1+\frac{2}{r}\right)^{-1}$$

Neglect the higher order terms

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

$$= 1 + \frac{2|m|-2}{r}$$

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

$$\frac{a_{r+2}}{a_r} = 1 + \frac{4a-2}{r} + \cdots \qquad —— (14)$$

Since the coefficients tend to equality as $r \to \infty$, the series $K(\omega)$ diverges for $\omega = 1$. In fact, the asymptotic behaviour 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 $(1-\omega^2)^{-2a}$.

$$P(\omega) = (1-\omega^2)^a \; K(\omega)$$
$$= (1-\omega^2)^a \cdot (1-\omega^2)^{-2a}$$
$$= (1-\omega^2)^{-a}.$$

$\omega = \cos\theta \quad \therefore \omega^2 \to 1 \quad \therefore P(\omega) \to \infty.$

Therefore in the neighbourhood 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 $r = t$, $t = 0, 1, 2 \ldots$ where t may have any values $0, 1, \ldots$

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

assume, $t + |m| = l$

$$\therefore \boxed{\lambda = l(l+1)} \qquad —— (15)$$

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

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

$$\boxed{\lambda\hbar^2 = l(l+1)\hbar^2} \qquad —— (16)$$

* 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 $\lambda = l(l+1)$

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

This eq^n is closely related to Legender's $diff^n$ eq^n.

If $m=0$ then it reduces to Legender's equation

$$\therefore (1-\omega^2) K''(\omega) - 2\omega K'(\omega) + l(l+1) K(\omega) = 0 \quad \text{--- (2)}$$

$$\therefore (1-\omega^2) P_l''(\omega) - 2\omega P_l'(\omega) + l(l+1) P_l(\omega) = 0 \quad \text{--- (3)}$$

$P_l(\omega)$ = Legendre polynomials.

Actually eq^n (1) is m^{th} derivatives of eq^n (2).

According to Libnitz theorem

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

Using Libnitz theorem, taking m^{th} derivatives of eq^n (3), we get

$$\text{(i)} \quad \frac{d^m}{dx^m}\left[(1-\omega^2) P_l''(\omega)\right] = (1-\omega^2)\frac{d^{m+2} P_l}{d\omega^{m+2}} + {}^mC_1 (-2\omega) \frac{d^{m+1} P_l}{d\omega^{m+1}} + {}^mC_2 (-2) \frac{d^m P_l}{d\omega^m}$$

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

$$= (1-\omega^2)\frac{d^{m+2} P_l}{d\omega^{m+2}} - 2m\omega \frac{d^{m+1} P_l}{d\omega^{m+1}} - m(m-1)\frac{d^m P_l}{d\omega^m}$$

Similarly m^{th} derivative of the 2^{nd} term is given by

(ii) $\frac{d^m}{d\omega^m}\left[2\omega P_l'\right] = 2\omega \frac{d^{m+1} P_l}{d\omega^{m+1}} + {}^mC_1 \cdot 2 \cdot \frac{d^m P_l}{d\omega^m}$

$$= 2\omega \frac{d^{m+1} P_l}{d\omega^{m+1}} + 2m \frac{d^m P_l}{d\omega^m}$$

(iii) $\frac{d^m}{d\omega^m}\left[l(l+1) P_l(\omega)\right] = l(l+1) \frac{d^m P_l(\omega)}{d\omega^m}$

The m^{th} derivative of Legendre's diffⁿ eqⁿ is

$$(1-\omega^2) \frac{d^{m+2} P_l(\omega)}{d\omega^{m+2}} - 2\omega(|m|+1) \frac{d^{m+1} P_l(\omega)}{d\omega^{m+1}} + \left\{ l(l+1) - |m| - |m|^2 \right\} \frac{d^m P_l(\omega)}{d\omega^m} = 0 \quad \text{--- (4)}$$

Comparing eqⁿˢ (1) & (4)

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

$$K(\omega) = \frac{d^m P_l(\omega)}{d\omega^m} = P_l^m(\omega) \quad \text{--- (5)}$$

The polynomial solⁿ of Θ eqⁿ is

$$\Theta(\theta) = (1-\omega^2)^a K(\omega)$$

$$= (1-\omega^2)^a P_l^m(\omega)$$

Now, $\omega = \cos\theta$

$\therefore 1-\omega^2 = \sin^2\theta$ and, $2a = |m|$

$\therefore a = \frac{|m|}{2}$

$$\therefore \Theta(\theta) = (\sin^2\theta)^{\frac{|m|}{2}} \frac{d^m}{d\omega^m} P_l(\omega)$$

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

$$\therefore \boxed{P_l^m(\omega) = \sin^{|m|}\theta \frac{d^m}{d\omega^m} P_l(\omega)} \quad \text{--- (6)}$$

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

The Orthogonality Property is defined as

$$\int P_l^m(\omega) \cdot P_{l'}^m(\omega)\, d\omega = \frac{2}{2l+1} \cdot \frac{(l+m)!}{(l-m)!}\, \delta_{ll'}$$

$\delta_{ll'} = 1$ for $l = l'$

$= 0$ for $l \neq l'$

If we take $l = l'$, then

$$\int P_l^m(\omega) \cdot P_l^m(\omega)\, d\omega = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!}$$

$$\therefore \int |P_l^m(\omega)|^2 d\omega = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \quad \text{——— (7)}$$

The fuⁿ $\Theta(\theta)$ can now be written as

$$\Theta(\theta) = N \cdot P_l^m(\omega)$$

N is a normalization constant. The orthogonality property for $\Theta(\theta)$ fuⁿ is defined as $\int \Theta_{lm}(\theta)\, \Theta_{lm}(\theta) \sin\theta\, d\theta =$

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

$$\therefore N^2 \int |P_l^m(\omega)|^2 d\omega = 1 \qquad \left(\because \begin{array}{l} \omega = \cos\theta \\ d\omega = -\sin\theta\, d\theta \end{array} \right.$$

The limit of θ is from $0 \to \pi$

$\omega = \cos\theta$ is from -1 to $+1$

Substituting the value of integral from eqⁿ (7), we get

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

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

$\therefore$ The Normalized $\Theta(\theta)$ fuⁿ is given by

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

The complete eigen fn of L^2 operator is

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

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

put $v(\theta,\phi) = Y_{lm}(\theta,\phi)$

$$\therefore \boxed{Y_{lm}(\theta,\phi) = \left[\frac{2l+1}{4\pi}\cdot\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\omega)\, e^{im\phi}\, (-1)^m} \quad -(8)$$

This is the eigen fn for L^2 operator.

⇒ SPHERICAL HARMONICS :

(i) $l = m = 0$

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

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

(ii) $l=1,\ m=0$

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

$$= \left[\frac{3}{4\pi}\right]^{1/2}\cdot\cos\theta$$

(iii) $l=m=1$

$$Y_{11} = \left[\frac{3}{4\pi}\cdot\frac{1}{2}\right]^{1/2}(-1)^1\, P_1^1(\cos\theta)\, e^{i\phi}$$

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

$$= -\left[\frac{3}{8\pi}\right]^{1/2}\sin\theta\, e^{i\phi}$$

(iv) $l=1,\ m=-1$

$$Y_{1,-1} = \left[\frac{3}{8\pi}\right]^{1/2}\sin\theta\, e^{-i\phi}$$

(v) $l=2,\ m=0$

$$Y_{2,0} = \left[\frac{10}{8\pi}\right]^{1/2}\frac{1}{2}\left[3\cos^2\theta-1\right] = \left[\frac{5}{16\pi}\right]^{1/2}(3\cos^2\theta-1)$$

(vi) $l=2,\ m=1$

$$Y_{2,1} = \left[\frac{5}{4\pi}\cdot\frac{1}{6}\right](-1)^1\, P_2^1(\cos\theta)\, e^{i\phi}$$

$$= -\left[\frac{5}{24\pi}\right]^{1/2}\sin\theta\cos\theta\, e^{i\phi}$$

→ Legender polynomial is defined as

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

For $m=0$:

(i). $l=0$; $P_0^0(\omega) = \frac{1}{1} = 1$

(ii) $l=1$, $P_1^0(\omega) = \frac{1}{2} \frac{d}{d\omega} (\omega^2-1)^1 = \frac{1}{2} \cdot 2\omega = \omega = \cos\theta$

(iii) $l=2$, $P_2^0(\omega) = \frac{1}{(2)^2(2)} \frac{d^2}{d\omega^2} (\omega^2-1)^2$

$$= \frac{1}{8} \frac{d^2}{d\omega^2} (\omega^2-1)^2$$

$$= \frac{1}{8} \frac{d^2}{d\omega^2} (\omega^4 - 2\omega^2 + 1)$$

$$= \frac{1}{8} \frac{d}{d\omega} (4\omega^3 - 4\omega)$$

$$= \frac{1}{8} [(4)(3)\omega^2 - 4] = \frac{1}{2} [3\cos^2\theta - 1]$$

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

(i) $l=1$, $m=1$

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

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

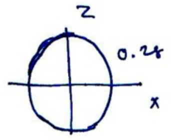
(ii) $l=2$, $m=1$

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

* <u>Polar diagramm:</u> $[\, Y_{lm}(\theta, \phi) \rightarrow \theta \,]$

Polar diagram is a diagram of of spherical harmonic

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



$l=0$, $m=0$

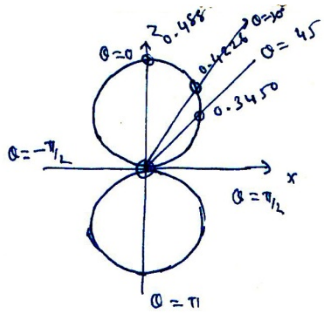
(ii) $Y_{1,0} = \left[\frac{3}{4\pi}\right]^{1/2} \cos\theta$

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

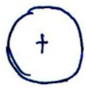
$\theta = 30^\circ$, $Y_{1,0} = \left[\frac{3}{4\pi}\right]^{1/2}(0.8660) = 0.4226$

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

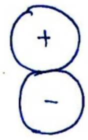
$\theta = 90^\circ$, $\quad Y_{1,0} = 0$



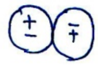
The polar diagrams for the $Y_{lm}(\theta,\phi)$ for points in the x–z plane are shown in below figs.



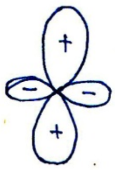
$l=0,\ m=0$



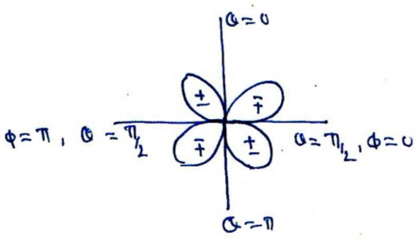
$l=1,\ m=0$



$l=1,\ m=\pm 1$



$l=2,\ m=0$



$l=2,\ m=\pm 1$

$l=2,\ m=\pm 2$

* **Physical Interpretation:**

· The z-component of angular momentum operator is

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

Eigen value eqn for L^2 operator is

$$L^2 v(\theta,\phi) = \lambda\hbar^2 v(\theta,\phi) \quad , \text{ where } \lambda = l(l+1)$$

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

$v(\theta,\phi)$ is eigen fn of L^2.

Spherical Harmonics

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

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

$(-1)^m$ = phase factor.

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

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

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

$$L_z \, Y_{lm}(\theta,\phi) = m\hbar \, Y_{lm}(\theta,\phi) \quad \text{——} \; (2)$$

$$\because \; -i\hbar \frac{\partial}{\partial\phi}\left[\Theta(\theta)\,\Phi(\phi)\right] = -i\hbar\,\Theta(\theta)\frac{\partial}{\partial\phi}\left[\Phi(\phi)\right]$$

$$= -i\hbar\,\Theta(\theta)\frac{\partial}{\partial\phi}\left(e^{im\phi}\right)$$

$$= -i\hbar\,\Theta(\theta)\, im\, e^{im\phi}$$

$$= -i\hbar \cdot im\,\Theta(\theta)\,\Phi(\phi)$$

$$= m\hbar \, Y_{lm}(\theta,\phi)$$

where $m\hbar$ = eigen value of L_z operator. L^2 & L_z have same eigen function. This happens if both the operators 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 quantised. It can take the values

$L_z = m\hbar$, where m = integer and is called magnetic quantum number.

Eqn (2) 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 itself 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 eqn. it follows that all the component of L commute with L^2. , to produce

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

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

Now, $[A, BC] = [A, B]C + B[A, C]$

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

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

$\Rightarrow$ similarly $[L^2, L_z] = 0$ and $[L^2, L_y] = 0$

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

$\Rightarrow [L^2, L_x] = 0 \Rightarrow L^2$ & L_x have simultaneous eigen fun, say

$$\Phi_{lm}(\theta, \phi) \quad \& \quad Y_{lm}(\theta, \phi).$$

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

$\therefore$ Eigen function of $L_x \neq$ Eigen function of L_z.

$\Rightarrow [L^2, L_y] = 0$ & L^2 & L_y have simultaneous eigen functions.

say $\quad f_{lm}(\theta, \phi) = Y_{lm}(\theta, \phi)$

$$[L_y, L_z] = i\hbar x \neq 0.$$

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 $Y_{lm}(\theta,\phi)$.

L_z does not commute with L_x & L_y.

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.

$$\boxed{\Phi_{lm}(\theta,\phi) = a Y_{1,1} + b Y_{1,0} + c Y_{1,-1}.}$$

* **Angular momentum in stationary states of systems 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 K.E of a particle $= \frac{1}{2} m v^2$

$$= \frac{1}{2} I\omega^2 = \frac{I^2\omega^2}{2I} = \frac{L^2}{2I}.$$

If there are no forces effect in the motion then P.E will be zero.

$\therefore$ Total energy $=$ K.E $+$ P.E

$$= \frac{L^2}{2I} + 0 = \frac{L^2}{2I}$$

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

The eigen value eqn for this particle is

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

, H is Hamiltonian operator.

$I = m r_0^2$

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

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

The eigen value eqn for L^2 operator is

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

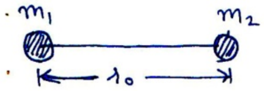
Divide on both the sides by $2I$

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

$\therefore$ The quantum mechanical energy for this particle is

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

* **Rigid Rotator:**



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

$E = \frac{l(l+1)}{2I}\hbar^2$ 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 $\Delta E = E_l - E_{l-1}$

$$= \frac{l(l+1)}{2I}\hbar^2 - \frac{(l-1)l\hbar^2}{2I}$$

$$= \frac{\hbar^2}{2I}\left[l^2 + l - l^2 + l\right]$$

$$= \frac{\hbar^2\, \cancel{2}l}{\cancel{2}I} = \frac{\hbar^2 l}{I}$$

$\therefore$ $\boxed{\Delta E \propto l}$

The levels are not equispaced. The spacing betn two levels is not constant, it increases, with increase 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,

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

$$H = p^2/2m + V(r)$$

For a system of two particles

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

The eigen value eqn is

$$H\psi = E\psi$$

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

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

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

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

$$\nabla^2 u - \frac{2\mu}{\hbar^2}V(r).u = -\frac{2\mu E}{\hbar^2}.u$$

$$\therefore \boxed{\nabla^2 u + \frac{2\mu}{\hbar^2}\left[E - V(r)\right]u = 0} \quad \text{--- (1)}$$

Substituting the value of ∇^2 in spherical polar coordinates

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

$$\therefore \left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\times\frac{\hbar^2}{\hbar^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right]u$$

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

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

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

$$u(r,\theta,\phi) = R(r)\,Y_{lm}(\theta,\phi) \quad \text{--- (3)}$$

$\therefore$ Eq^n (2) becomes

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

$$\Rightarrow Y_{lm}(\theta,\phi)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}R(r)\right) - \frac{R(r)L^2}{\hbar^2 r^2}Y_{lm}(\theta,\phi) +$$

$$\frac{2\mu}{\hbar^2}\left[E - V(r)\right]R(r)\,Y_{lm}(\theta,\phi) = 0$$

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

$$\therefore Y_{lm}(\theta,\phi)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}R(r)\right) - l(l+1)\hbar^2 Y_{lm}(\theta,\phi)\frac{R(r)}{\hbar^2 r^2} +$$

$$\frac{2\mu}{\hbar^2}\left[E - V(r)\right]R(r)\,Y_{lm}(\theta,\phi) = 0$$

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

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

Multiply by $R(r)$

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

$$\therefore \boxed{\frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{dR(r)}{dr}\right) + \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2}\right] R(r) = 0} \quad (4)$$

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

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

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

Now, here $\vec{l} = l \cdot \frac{h}{2\pi}$

In Q.M $\vec{l} = \sqrt{l(l+1)}\,\hbar$. Angular momentum $L^2 = l(l+1)\hbar^2$.

The eigenvalue problem for a spherically symmetric potential thus reduces to determining for what values of E the radial wave eqⁿ (4) has admissible solution and then finding the solutions.

* **The Radial Wave Function:**

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

$$\text{Norm} = \int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} u(r,\theta,\phi)\, u^*(r,\theta,\phi)\, d\tau$$

$$= \int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} R(r)\, Y_{lm}(\theta,\phi)\, R^*(r)\, Y^*_{lm}(\theta,\phi)\, r^2 dr \sin\theta\, d\theta\, d\phi$$

$$= \left[\int_{r=0}^{\infty} R^*(r) R(r) r^2 dr\right]\left[\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} Y_{lm}(\theta,\phi)\, Y^*_{lm}(\theta,\phi) \sin\theta\, d\theta\, d\phi\right]$$

since $Y_{lm}(\theta,\phi)$ is normalised function it has unit norm.

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

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

$$\langle A \rangle = \int \psi^* A \psi\, d\tau$$

$$\therefore \langle A \rangle = \int R^*(r)\, A\, R(r)\, r^2 dr$$

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

$$\therefore \langle A \rangle = \int \frac{\chi^*(r)}{r} A \frac{\chi(r)}{r} r^2 dr$$

$$= \int \chi^*(r)\, A\, \chi(r)\, dr.$$

with this assumption the radial wave function now becomes

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

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

$$\therefore \frac{1}{r^2}\frac{d}{dr}\left[r^2\left(\frac{1}{r}\frac{d\chi}{dr} - \frac{\chi(r)}{r^2}\right)\right] + \left[\qquad '' \qquad\right] = 0$$

$$\therefore \frac{1}{r^2}\frac{d}{dr}\left[r\frac{d\chi}{dr} - \chi(r)\right] + \quad '' \quad = 0$$

$$\therefore \frac{1}{r^2}\left[r\frac{d^2\chi}{dr^2} + \frac{d\chi}{dr} - \frac{d\chi}{dr}\right] + \quad '' \quad = 0$$

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

multiplying by r

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

The behaviour of the wave function near the origin can be seen from this equation.

For any $l \neq 0$, the centrifugal term $\frac{l(l+1)}{r^2}$ diverges (as $r \to 0$) and dominates over the other terms.

$\therefore$ In the neighbourhood of the origin $r=0$, $\frac{2\mu}{\hbar^2}(E - V(r))$ term can be neglected.

$$\therefore \frac{d^2\chi}{dr^2} - \frac{l(l+1)}{r^2}\chi(r) = 0 \qquad \text{as } r \to 0$$

solution of this eqn is given by

$$\chi(r) = \text{const. } r^m$$

$$\frac{d\chi}{dr} = m r^{m-1}, \qquad \frac{d^2\chi}{dr^2} = m(m-1) r^{m-2}$$

substituting in above eqn

$$m(m-1) r^{m-2} - \frac{l(l+1)}{r^2} r^m = 0$$

$$\therefore m(m-1) r^{m-2} - l(l+1) r^{m-2} = 0$$

$$\therefore [m(m-1) - l(l+1)] r^{m-2} = 0$$

$$\therefore m(m-1) - l(l+1) = 0$$

$$m^2 - m - l^2 - l = 0$$

$$\therefore (m^2 - l^2) - (m+l) = 0$$

$$\therefore (m+l)(m-l-1) = 0$$

$$\therefore m+l=0 \quad \text{or} \quad m-l-1=0$$

$$\therefore m = -l, \qquad m = l+1$$

$\therefore$ solution will be

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

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

When we put $r=0$ in (1)

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

$\therefore$ This solution is not acceptable since it make $R(r)$ diverging as $r \to 0$.

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

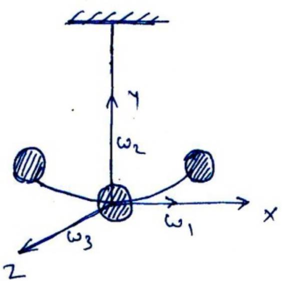
$$\therefore \boxed{R(r) = \text{const.}\ r^{l}}$$

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

* The Anisotropic Oscillator :

Consider the harmonic oscillator in three dimension with the Hamiltonian
$$H = K.E + P.E$$
$$= \frac{p^2}{2m} + \frac{1}{2}m\omega_1^2 x^2 + \frac{1}{2}m\omega_2^2 y^2 + \frac{1}{2}m\omega_3^2 z^2$$

$$\therefore H = \frac{p^2}{2m} + \frac{1}{2}m\left[\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2\right] \quad \text{—— (1)}$$



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

$$\therefore H = \left(\frac{p_x^2}{2m} + \frac{1}{2}m\omega_1^2 x^2\right) + \left(\frac{p_y^2}{2m} + \frac{1}{2}m\omega_2^2 y^2\right) + \left(\frac{p_z^2}{2m} + \frac{1}{2}m\omega_3^2 z^2\right)$$

$$\therefore H = H^{(1)} + H^{(2)} + H^{(3)} \quad \text{—— (2).}$$

The time independent schrodinger eq^n is
$$H\psi = E\psi$$
$$\therefore \left[\frac{p^2}{2m} + V(r)\right]\psi = E\psi$$
$$\therefore \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi$$

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

$$\therefore \boxed{\nabla^2 u + \frac{2m}{\hbar^2}[E - V(r)]u = 0} \quad \text{—— (3)}$$

This is the Schrodinger eqn of S.H.O.

Splitting this eqn in three parts.

(1) $$\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]u = 0 \quad \text{—— (4)}$$

$$\therefore \frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\,\omega_1^2 x^2\right]u = 0$$

Now, normalized energy eigen fn for S.H.O is

$$u_{n_1}^{(1)}(x) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}\, e^{-x^2/2} H_n(x) \quad \text{—— (5)}$$

and, $$E_n^{(1)} = \left(n_1 + \frac{1}{2}\right)\hbar\omega_1 \quad \text{—— (6)}$$

(2) $$\frac{d^2u}{dy^2} + \frac{2m}{\hbar^2}[E - V(y)]u = 0 \quad \text{—— (7)}$$

$$\therefore \frac{d^2u}{dy^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\omega_2^2 y\right]u = 0$$

$$\therefore u_{n_2}^{(2)}(y) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}\, e^{-y^2/2} H_n(y) \quad \text{—— (8)}$$

$\therefore$ Normalized energy eigen value is

$$E_n^{(2)} = \left(n_2 + \frac{1}{2}\right)\hbar\omega_2 \quad \text{—— (9)}$$

(3) $$\frac{d^2u}{dz^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\omega_3^2 z^2\right]u = 0 \quad \text{—— (10)}$$

$\therefore$ Normalized energy eigen fn is

$$u_{n_3}^{(3)}(z) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}\cdot e^{-z^2/2}\cdot H_n(z) \quad \text{—— (11)}$$

and, Normalized energy eigen value is

$$E_n^{(3)} = \left(n_3 + \frac{1}{2}\right)\hbar\omega_3 \quad \text{—— (12).}$$

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

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

putting $e q^n$ (5), (8) & (11) we get,

$$\therefore\ u_{n_1 n_2 n_3}(x, y, z) = \frac{1}{(2^n n! \sqrt{\pi})^{3/2}} e^{-r^2/2} H_n(x) H_n(y) H_n(z) \quad \text{—— (13)}$$

$u^{(1)}_{n_1}(x)$, $u^{(2)}_{n_2}(y)$, $u^{(3)}_{n_3}(z)$ are eigen functions of three different oscillators given by above $e q^{ns}$.

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

$$E_{n_1 n_2 n_3} = E^{(1)}_{n_1} + E^{(2)}_{n_2} + E^{(3)}_{n_3}$$

$$= (n_1 + \tfrac{1}{2})\hbar\omega_1 + (n_2 + \tfrac{1}{2})\hbar\omega_2 + (n_3 + \tfrac{1}{2})\hbar\omega_3$$

* The Isotropic Oscillator:

When the oscillators is isotropic, then $\omega_1 = \omega_2 = \omega_3 = \omega$

Then, the energy eigen values of the isotopic oscillator is given by

$$\therefore\ E_{n_1 n_2 n_3} = (n_1 + \tfrac{1}{2})\hbar\omega + (n_2 + \tfrac{1}{2})\hbar\omega + (n_3 + \tfrac{1}{2})\hbar\omega$$

$$= [(n_1 + n_2 + n_3) + \tfrac{3}{2}]\hbar\omega$$

$$\therefore\ E_{n_1 n_2 n_3} = (n + \tfrac{3}{2})\hbar\omega, \quad n = n_1 + n_2 + n_3 \quad \text{—— (1)}$$

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

$$V = \tfrac{1}{2} m\omega^2 (x^2 + y^2 + z^2) = \tfrac{1}{2} m\omega^2 r^2 \quad \text{—— (2)}$$

The wave $f n^n$ is $\quad u_{nlm}(r, \theta, \phi) = R_{nl}(r)\, Y_{lm}(\theta, \phi)$

The radial wave $e q^n$ with $V = \tfrac{1}{2} m\omega^2 r^2$, in terms of the dimensionless variables $\rho = \alpha r$ with $\alpha = (m\omega/\hbar)^{1/2}$ takes the form

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2 \frac{dR_l}{d\rho}\right) + \left[\lambda - \rho^2 - \frac{l(l+1)}{\rho^2}\right] R = 0 \quad \text{—— (4) (3)}$$

where, $R(\rho) = R(r)$ and $\lambda = \frac{2mE}{\hbar^2 \alpha^2} = \frac{2E}{\hbar\omega}$ —— (4)

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

$$\therefore \quad R = \rho^l e^{-1/2\rho^2} K \quad \text{—— (5)}$$

In terms of K eq^n (3) is $\xi \frac{d^2K}{d\xi^2} + (l + \frac{3}{2} - \xi)\frac{dK}{d\xi} + \frac{1}{4}(\lambda - 3 - 2l)K = 0$ —— (5)

with $\xi = \rho^2$.

$$\lambda = 2n+3, \; n = l + 2n' \quad \text{—— (6)}$$

The energy eigen value is $E_n = (n + \frac{3}{2})\hbar\omega$ —— (6)

$n = 0, 1, 2 \ldots$