(4)

The expectation value of L_z in spherical Polar coordinates is:

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

$$= -i\hbar\left[\cancel{r\sin\theta}\, x\left(\frac{\partial r}{\partial y}\cdot\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\cdot\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial y}\cdot\frac{\partial}{\partial\phi}\right) - y\left(\frac{\partial r}{\partial x}\cdot\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\cdot\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\cdot\frac{\partial}{\partial\phi}\right)\right]$$

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

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

$$= -i\hbar\left[\cos^2\phi + \sin^2\phi\right]\frac{\partial}{\partial\phi}$$

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

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Similarly

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

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

Assignment

Prove that

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

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

Now.

$$L_+ = L_x + i L_y$$

$$= i\hbar\left[\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\right.$$

$$+ i\left(\cot\right.$$

$$L_x^2 =$$

Now

$$L_{+} = L_x + i L_y$$

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

$$= \hbar \left[i \sin\phi \frac{\partial}{\partial\theta} + \underset{\substack{\downarrow \\ \text{Multiply and divided by } i}}{i} \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right]$$

$$= \hbar \left[i \sin\phi \frac{\partial}{\partial\theta} - \frac{1}{i} \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right]$$

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

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

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

multiply and divide by "i" 2nd term.

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

then.

$$L_+ = \hbar\left[(\cos\phi + i\sin\phi)\frac{\partial}{\partial\theta} - (\cos\phi + i\sin\phi)\frac{1}{i}\cot\theta\frac{\partial}{\partial\phi}\right]$$

$$= \hbar\left[e^{i\phi}\frac{\partial}{\partial\theta} - \frac{1}{i}e^{i\phi}\cot\theta\frac{\partial}{\partial\phi}\right]$$

$$\boxed{L_+ = \hbar e^{i\phi}\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]}$$

Similarly $L_- = L_x - iL_y$

$$\boxed{L_- = -\hbar e^{-i\phi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi}\right)}$$

Eigenfunctions of L_z and L^2.

As the operators $\hat{L}_z$ and $\hat{L}^2$ depend only on "θ" and "ϕ", since their eigenstates depends only on "θ" and "ϕ", therfore we write a function for both operators as

$$\Psi_{lm}(\theta, \phi)$$

where $\psi_{\ell m}(\theta,\phi)$ are the Continuous ~~Eigen~~ Eigen fn of θ, ϕ, Hence

$$\hat{L}^2 \psi_{\ell m}(\theta,\phi) = \ell(\ell+1)\hbar^2 \cdot \psi_{\ell m}(\theta,\phi)$$

and.

$$\hat{L}_z \psi_{\ell m}(\theta,\phi) = m\hbar\, \psi_{\ell m}(\theta,\phi)$$

As we know, $\hat{L}_z$ depends only on ϕ, so ~~the~~ we can separate the eigen fn. as.

$$\psi_{\ell m}(\theta,\phi) = G'_{\ell m}(\theta).\ \Phi_{\ell m}(\phi).$$

<u>Eigenfunction of and Eigen value of $\hat{L}_z$,</u>

Since

$$\hat{L}_z \psi_{\ell m}(\theta,\phi) = m\hbar\, \psi_{\ell m}(\theta,\phi)$$

as $\hat{L}_z = -i\hbar \frac{\partial}{\partial\phi}$

So,

$$-i\hbar \frac{\partial}{\partial\phi}\left[\cancel{G'_{\ell m}(\theta)}\,\Phi_{\ell m}(\phi)\right] = m\hbar\, \cancel{G'_{\ell m}(\theta)}\,\Phi_{\ell m}$$

$$-i\frac{\partial}{\partial\phi}\Phi_m(\phi) = m\,\Phi_m(\phi)$$

because. ℓm does not depe...

The sol. of the equ is.

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

where $\frac{1}{\sqrt{2\pi}}$ is the normalization.

Constant. can be calculated as.

$$\int_0^{2\pi} \phi_m^* \phi_m \, d\phi = 1. \qquad 0 \leq \phi \leq 2\pi$$

This is the eigenfunction of $\hat{L}_z$ operator. Now calculate the eigen value of this,

$$\hat{L}_z \Phi_m(\phi) = -i\hbar \frac{\partial}{\partial \phi} \Phi_m(\phi)$$

$$= -i\hbar \frac{1}{\sqrt{2\pi}} \frac{\partial}{\partial \phi} e^{im\phi}$$

$$= -i\hbar \, im \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

$$\hat{L}_z \Phi_m(\phi) = m\hbar \frac{1}{\sqrt{2\pi}} e^{im\phi} = m\hbar \, \Phi_m(\phi)$$

This shows that the expectation value of $\hat{L}_z$ has a discrete set of values, which varies from $-l$ to $+l$.

Eigenfunctions of L^2 :-

L^2 depend both on "θ" and "ϕ"

therefore, we choose the Eigenfn.

as $\psi_{lm}(\theta,\phi) = G'(\theta).\, e^{im\phi} \frac{1}{\sqrt{2\pi}}$

$= G(\theta)\, e^{im\phi}$

where $G(\theta) = G'(\theta) \cdot \frac{1}{\sqrt{2\pi}}$

So.

$L^2 \psi_{lm}(\theta,\phi) = \lambda\, \psi_{lm}(\theta,\phi)$

$L^2\, G(\theta).e^{im\phi} = \lambda.\, G(\theta)\, e^{im\phi}$

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

$G(\theta)\, e^{im\phi} = \lambda\, G(\theta)\, e^{im\phi}$

$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta.\frac{\partial G}{\partial\theta}\right]\cancel{e^{im\phi}} - \frac{G m^2}{\sin^2\theta}\cancel{e^{im\phi}} =$

$= -\frac{\lambda}{\hbar^2}\, G\, \cancel{e^{im\phi}}$

or.

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial G}{\partial\theta}\right) - \frac{m^2}{\sin^2\theta}G = -\frac{\lambda}{k^2}G$$

$\Rightarrow$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial G}{\partial\theta}\right) + \left(\frac{\lambda}{k^2} - \frac{m^2}{\sin^2\theta}\right)G = 0 \quad \rightarrow (1)$$

Let us write

$$\cos\theta = \xi \Rightarrow \cos^2\theta = \xi^2$$

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

$$\sin\theta = \sqrt{1-\xi^2}$$

$$\frac{\partial}{\partial\theta} = \frac{\partial}{\partial\xi}\cdot\frac{\partial\xi}{\partial\theta}$$

$$= -\sin\theta\frac{\partial}{\partial\xi}$$

then equ (1) becomes

$$\frac{1}{\sin\theta}\left(-\sin\theta\frac{\partial}{\partial\xi}\right)\left(\sin\theta\cdot\frac{\partial}{\partial\theta}\cdot G\right) + \left[\frac{\lambda}{k^2} - \frac{m^2}{(1-\xi^2)}\right]G = 0$$

put the value of $\frac{\partial}{\partial\theta}$

$$\frac{1}{\sin\theta}\left(-\sin\theta\frac{\partial}{\partial\xi}\right)\left(-\sin^2\theta\frac{\partial G}{\partial\xi}\right) + \left[\frac{\lambda}{k^2} - \frac{m^2}{(1-\xi^2)}\right]G$$

or

$$\frac{\partial}{\partial\xi}\left[\sin^2\theta\frac{\partial G}{\partial\xi}\right] + \left[\frac{\lambda}{k^2} - \frac{m^2}{(1-\xi^2)}\right]G = 0$$

put the value of $\sin^2\theta$

$$\frac{\partial}{\partial\xi}\left[(1-\xi^2)\frac{\partial G}{\partial\xi}\right] + \left[\frac{\lambda}{k^2} - \frac{m^2}{(1-\xi^2)}\right]G = 0$$

differentiate the Ist term w.r.t. ξ.
we will get

$$(1-\xi^2)\frac{\partial^2 G}{\partial \xi^2}-2\xi\frac{\partial G}{\partial \xi}+\left[\frac{\lambda}{k^2}-\frac{m^2}{(1-\xi^2)}\right]G=0$$

for $\lambda = \ell(\ell+1)k^2$, we will get

$$\boxed{(1-\xi^2)\frac{\partial^2 G}{\partial \xi^2}-2\xi\frac{\partial G}{\partial \xi}+\left[\ell(\ell+1)-\frac{m^2}{1-\xi^2}\right]G=0} \quad (*)$$

This is the associated Legender's equ.

~~for~~ Hence The Legender Polynomials $P_\ell(\xi)$ are the sol. of the following equ. for $m=0$ $(**)$

$$(1-\xi^2)\frac{\partial^2 P_\ell}{\partial \xi^2}-2\xi\frac{\partial P_\ell}{\partial \xi}+\ell(\ell+1)P_\ell=0$$

ℓ is Int

[when $m=0$ and ℓ is integer, the equ$(*)$ is identical to the polynomial (Legender)]

$$(1-x^2)y''-2xy'+\left(\ell(\ell+1)-\frac{m^2}{1-x^2}\right)y=0$$

when $m=0$, $\ell=$ integer.
then the sol. is

$$P_\ell(x)=\frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}\left[(x^2-1)^\ell\right]$$

So in our case the sol will be

$$\boxed{P_\ell(\xi)=\frac{1}{2^\ell \ell!}\frac{d^\ell}{d\xi^\ell}(\xi^2-1)^\ell}$$

This is the Rodrigues formula for Legender polynomial;
for, $l = 0, 1, 2, \cdots$, the values are:

$$P_0(\xi) = 1.$$

$$P_1(\xi) = \cancel{\frac{1}{2}\frac{d}{d\xi}(\xi^2-1)} = \xi$$

$$P_2(\xi) = \cancel{\frac{1}{2}(3\xi^2-1)}$$

Now we are interested in the value of G_1;
differentiating the equ (**) m-times. By applying the Leiebnitz the

$$(1-\xi^2)\frac{d^{m+2}}{d\xi^{m+2}}P_\ell - 2\xi m \frac{d^{m+1}}{d\xi^{m+1}}P_\ell - 2\frac{d^m}{d\xi^m}P_\ell \frac{m(m-1)}{2!} - 2\xi\frac{d^{m+1}}{d\xi^{m+1}}P_\ell - 2m\frac{d^m}{d\xi^m}P_\ell + \ell(\ell+1)\frac{d^m}{d\xi^m}P_\ell = 0.$$

or.

$$(1-\xi^2)\frac{d^{m+2}}{d\xi^{m+2}}P_\ell - 2\xi(m+1)\frac{d^{m+1}}{d\xi^{m+1}}P_\ell + \left[\ell(\ell+1) - m(m-1) - 2m\right]\frac{d^m}{d\xi^m}P_\ell = 0$$

$$\hookrightarrow \left|(f\cdot g)^{(n)} = f^{(n)}\cdot g + \binom{n}{1}f^{(n-1)}\cdot g' + \binom{n}{2}f^{(n-2)}g'' + \cdots + \binom{n}{n}f\cdot g^{(n)}\right.$$

Let us write.

$$u = \frac{d^m}{d\xi^m} P_l$$

So.

$$(1-\xi^2)\frac{d^2u}{d\xi^2} - 2\xi(m+1)\frac{du}{d\xi} + [l(l+1) - m(m+1)] = 0$$

If we make the substitution.

$$u = (1-\xi^2)^{-m/2} v, \quad v = u(1-\xi^2)^{m/2}$$

then

$$\frac{du}{d\xi} = -\frac{m}{2}(1-\xi^2)^{-m/2-1}(-2\xi)v + (1-\xi^2)^{-m/2}\frac{dv}{d\xi}$$

$$= m\xi(1-\xi^2)^{-m/2-1} v + (1-\xi^2)^{-m/2}\frac{dv}{d\xi}$$

$$\frac{d^2u}{d\xi^2} = m(1-\xi^2)^{-m/2-1} v + m\xi(-m/2-1)(1-\xi^2)^{-m/2-2} \times$$

$$(-2\xi)v + m\xi(1-\xi^2)^{-m/2-1}\frac{dv}{d\xi} -$$

$$-m/2(1-\xi^2)^{-m/2-1}(-2\xi)\frac{dv}{d\xi}$$

$$+ (1-\xi^2)^{-m/2}\frac{d^2v}{d\xi^2}$$

by putting the values of $\frac{du}{d\xi}$ and $\frac{d^2u}{d\xi^2}$ in equ above, we will get

$$(1-\xi^2)\frac{d^2v}{d\xi^2} - 2\xi\frac{dv}{d\xi} + \left[l(l+1) - \frac{m^2}{1-\xi^2}\right]v = 0$$

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This is identical to equ. (*), so we can take

$$G \propto V.$$

$$G = C_{lm} V = C_{lm} (1-\xi^2)^{m/2} U.$$

or

$$G = C_{lm} (1-\xi^2)^{m/2} \frac{d^m}{d\xi^m} P_l$$

$$= C_{lm} P_{lm}(\xi)$$

where

$$P_{lm}(\xi) = (1-\xi^2)^{m/2} \frac{d^m}{d\xi^m} \boxed{P_l}$$

is the associated Legender Polynomial and C_{lm} are constant of proportionality.

The Associated Legender Polynomial can be written as by puting P_l value

$$P_{lm}(\xi) = (1-\xi^2)^{m/2} \frac{d^m}{d\xi^m} \left[\frac{1}{2^l l!} \frac{d^l}{d\xi^l} (\xi^2-1)^l \right]$$

$$= (1-\xi^2)^{m/2} \frac{1}{2^l l!} \frac{d^{m+l}}{d\xi^{m+l}} (\xi^2-1)^l$$

$$\boxed{P_{lm} = \frac{(1-\xi^2)^{m/2}}{2^l\, l!} \frac{d^{m+l}}{d\xi^{m+l}} (\xi^2-1)^l}$$

So the simultaneous eigenfns. of L_z and L^2 are

$$\psi_{\ell m}(\theta,\phi) = C_{\ell m} \cdot G(\theta) \cdot e^{im\phi}$$

$$\boxed{\psi_{\ell m}(\theta,\phi) = C_{\ell m} \cdot P_{\ell m}(\xi) \cdot e^{im\phi}}$$

$$\boxed{\psi_{\ell m}(\theta,\phi) = Y_{\ell m}(\theta,\phi)}$$

The functions $Y_{\ell m}$ are called spherical harmonics. So the spherical harmonics are precisely the simultaneous eigenfunctions of L_z and L^2.

we can observe that $P_\ell(\xi)$ is a polynomial in ξ of degree ℓ, but $P_{\ell m}(\xi)$ is not a polynomial in general. For example, when "m" is odd, $P_{\ell m}(\xi)$ will have a function of $\sqrt{1-\xi^2}$,

i.e

$$P_{21}(\xi) = (1-\xi^2)^{1/2} \frac{d}{d\xi}\left(\frac{1}{2}(3\xi^2-1)\right)$$

$$= 3\xi\sqrt{1-\xi^2} \quad \text{- etc.}$$

We therefore write P_{lm} as $P_{lm}(\cos\theta)$
where $\sqrt{1-\cos^2\theta} = \sin\theta$

Some associated Legendre Polynomials are.

$$P_{11} = \sin\theta$$
$$P_{10} = \cos\theta$$
$$P_{22} = 3\sin^2\theta$$
$$P_{21} = 3\sin\theta\cos\theta$$
$$P_{20} = \frac{1}{2}(3\cos^2\theta - 1)$$

The simultaneous eigenfns of L^2 and L_z are

$$Y_{lm}(\theta,\phi) = C_{lm}\, P_{lm}(\cos\theta)\, e^{im\phi}$$

The constant C_{lm} are fixed in such a way that the spherical harmonics are normalized. i.

$$\int \psi^*_{l'm'}(\theta,\phi)\, Y_{lm}(\theta,\phi)\, dv = \delta_{ll'}, \delta_{mm'}$$

Since the integral, ~~over~~ we have spherical angles whose range of integration is.

$$0 \leq \phi \leq 2\pi$$
$$0 \leq \theta \leq \pi$$

So.

$$= \int_0^{\pi} P^{*}_{lm}(\cos\theta)\, P_{lm}(\cos\theta)\, \sin\theta\, d\theta$$
$$\times \int_0^{2\pi} |e^{im\phi}|^2\, d\phi\ |C_{lm}|^2$$

Because the integral over dV is. π.

$$\int dV = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta$$

and.

$$\int_0^{2\pi} |e^{im\phi}|^2\, d\phi = 2\pi$$

Hence, the normalization constants of spherical harmonics are

$$\boxed{C_{lm} = (-1)^m \sqrt{\frac{(2l+1)}{2}\,\frac{(l-m)!}{(l+m)!}}}$$

Assignment.