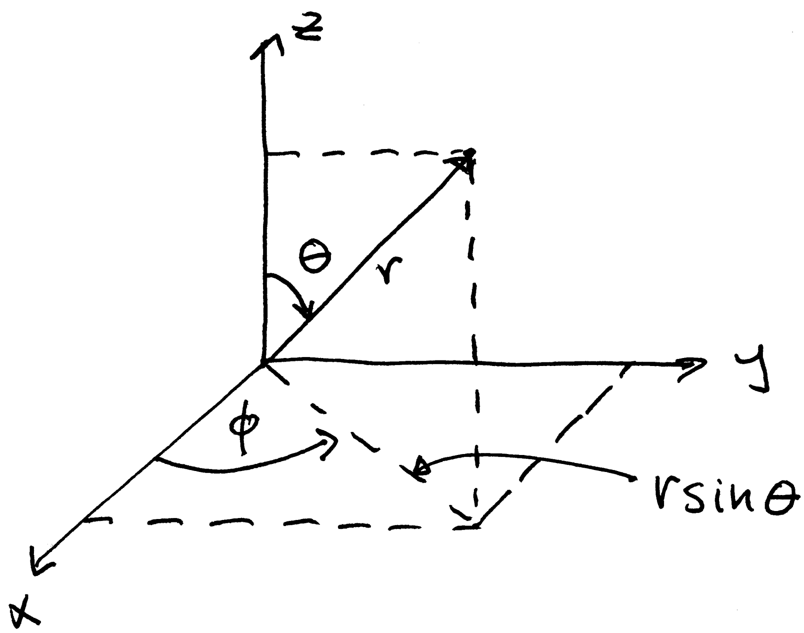
NOTICE THE SPHERICAL SYMMETRY OF THE POTENTIAL V_0

THEREFORE, WE USE SPHERICAL COORDINATES (MATHCHAPTER D)

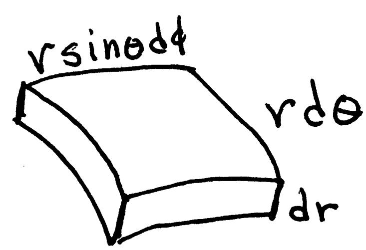


$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$

$$dV = dx\,dy\,dz = r^2\sin\theta\,d\phi\,d\theta\,dr$$



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

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

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

$$\hat{L}^2 Y_J^m(\theta,\phi) = +\hbar^2 J(J+1)\, Y_J^m(\theta,\varphi)$$

$Y_J^m(\theta,\phi)$ SPHERICAL HARMONIC

$$Y_J^m(\theta,\varphi) = \sqrt{\frac{(2J+1)}{4\pi}\frac{(J-|m|)!}{(J+|m|)!}}\; P_J^{|m|}(\cos\theta)\, e^{im\phi}$$

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

$P_J^{|m|}(\cos\theta)$ LEGENDRE POLYNOMIALS

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

$$= \frac{\hat{L}^2}{2I}$$

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

$$\hat{H}\, Y_l^m(\theta,\varphi) = E_{l,m}\, Y_l^m(\theta,\varphi)$$

$$E_{l,m} = \frac{\hbar^2}{2I}\, l(l+1)$$

USE IN PHYSICS l, AND IN CHEMISTRY J.

$$E_J = \frac{\hbar^2}{2I}\, J(J+1) \qquad J = 0, 1, 2, 3, \ldots$$

$$Y_J^m(\theta,\varphi)$$

$$\hat{L}_z Y_J^m(\theta,\varphi) = m\hbar\, Y_J^m(\theta,\varphi)$$

Y_J^m EIGENFUNCTIONS OF $\hat{L}^2$, $\hat{L}_z$

THEREFORE

$$[\hat{L}^2, \hat{L}_z]\, Y_J^m(\theta,\varphi) = 0 \cdot Y_J^m(\theta,\varphi) = 0$$

$\hat{L}^2$ AND $\hat{L}_z$ COMMUTE

$J = 0, 1, 2, 3, 4, 5, \ldots$

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

CONSIDER Y_1^m

$$\hat{L}^2 Y_1^m = 2\hbar^2 Y_1^m$$

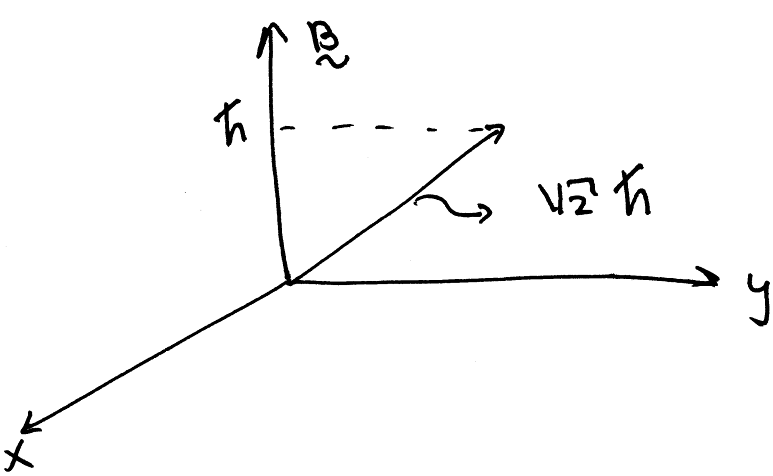
$$\hat{L}_z Y_1^m = m\hbar Y_1^m$$

$$m = -1, 0, 1$$

FOR $J = 1$ $\quad Y_1^{-1}, \; Y_1^{0}, \; Y_1^{-1}$

ARE LINERLY INDEPENDENT WITH THE SAME EIGEN VALUE WITH RESPECT TO $\hat{L}^2$. BUT $\hat{L}_z$ DISTINGUISHES BETWEEN EIGEN FUNCTIONS OF $\hat{L}^2$.

$\hat{L}_z$ IS RELATED TO THE PROJECTION OF THE ANGULAR MOMENTUM $\hat{\underset{\sim}{L}}$ ON A PREFERENCIAL DIRECTION (Z-AXIS) WITH THE HELD OF A MAGNETIC FIELD



$$\hat{L}^2 Y_\ell^m = \hbar^2 \ell(\ell+1) Y_\ell^m$$ ①

CLASSICAL

$$\underset{\sim}{L} = \underset{\sim}{r} \times \underset{\sim}{p}$$

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$
$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$
$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$
$$\hat{p}_y = -i\hbar \frac{\partial}{\partial y}$$
$$\hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

SPHERICAL COORDINATES

$$\hat{L}_x = -i\hbar\left(-\sin\phi \frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$
$$\hat{L}_y = -i\hbar\left(\cos\phi \frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$
$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$\hat{L}_z Y_\ell^m = i\hbar m Y_\ell^m$$

$$\Rightarrow \quad [\hat{L}^2, \hat{L}_z] = 0$$

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

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

$$= \hat{L}_x[\hat{L}_x, \hat{L}_z] + [\hat{L}_x, \hat{L}_z]L_x +$$

$$\hat{L}_y[\hat{L}_y,\hat{L}_z] + [\hat{L}_y,\hat{L}_z]\hat{L}_y$$

WE CAN PROVE THAT

$$[\hat{L}_x,\hat{L}_y] = i\hbar\hat{L}_z$$
$$[\hat{L}_y,\hat{L}_z] = i\hbar\hat{L}_x$$
$$[\hat{L}_{\cancel{y}z},\hat{L}_x] = i\hbar L_y$$

VERY IMPORTANT PROPERTY

$$[\hat{L}^2,\hat{L}_z] = -i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_x\hat{L}_y = 0$$

$$[\hat{L}^2,\hat{L}_x] = [\hat{L}^2,\hat{L}_y] = 0$$

WE HAVE $\{\hat{L}_x,\hat{L}_y,\hat{L}_z\}$ A SET OF 3 OPERATORS AND $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ SUCH THAT

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

<u>DEF</u> OF A LIE ALGEBRA

THEREFORE

$\hat{L}_{\pm} Y_{\ell}^{m}$ IS AN EIGENFUNCTION OF $\hat{L}_z$ WITH EIGENVALUE $(m+1)\hbar$

$$\hat{L}_{\pm} Y_{\ell}^{m} = A_{\ell m}^{\pm} Y_{\ell}^{m+1}$$

$\hat{L}_{\pm}$ STEP OR LADDER OPERATORS

SINCE $m = 0, \pm 1, \pm 2, \ldots, \pm \ell$

$$\left.\begin{aligned} \hat{L}_{+} Y_{\ell}^{\ell} &= 0 \\ \hat{L}_{-} Y_{\ell}^{-\ell} &= 0 \end{aligned}\right\}$$

Spin $\rightarrow \{\hat{S}_x, \hat{S}_y, \hat{S}_z\}$

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