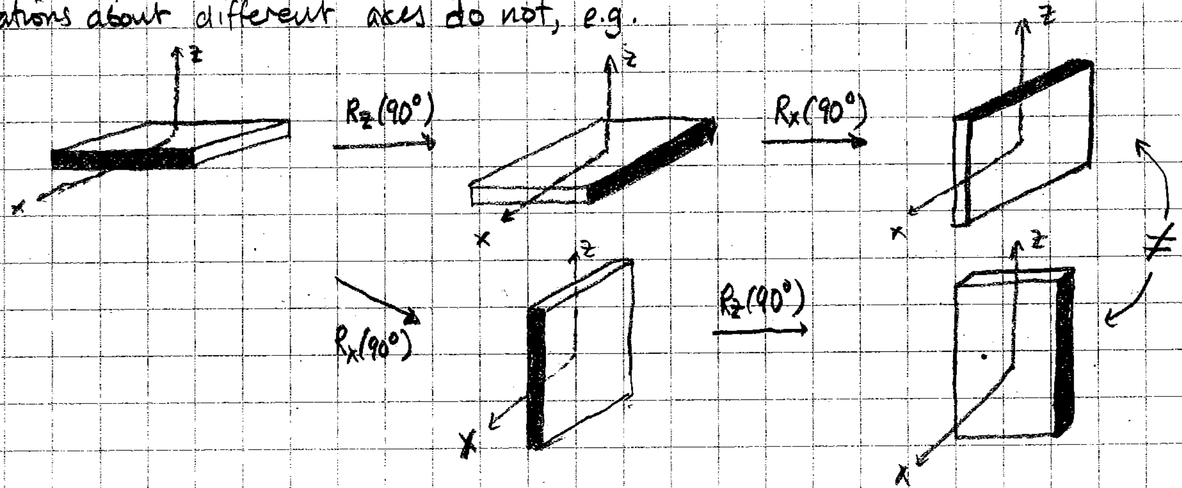
8. ROTATIONS IN THREE-DIMENSIONS & THE THEORY OF ANGULAR MOMENTUM

Classically we know that while rotations about the same axis commute (rotate by $60°$ about $\hat{z}$ then by $30°$ about $\hat{z}$ is the same as $30°$ about $\hat{z}$ followed by $60°$ about $\hat{z}$), rotations about different axes do not, e.g.



Representing the rotation of a vector in 3-D is rather simple - we use a matrix multiplication:

$$\begin{bmatrix} V_x' \\ V_y' \\ V_z' \end{bmatrix} = \begin{bmatrix} R_{x'x} & R_{x'y} & R_{x'z} \\ R_{y'x} & R_{y'y} & R_{y'z} \\ R_{z'x} & R_{z'y} & R_{z'z} \end{bmatrix} \begin{bmatrix} V_x \\ V_y \\ V_z \end{bmatrix} \qquad \underline{V}' = \underline{\underline{R}}\,\underline{V}$$

In order that the length of the vector not be changed under rotation we require $V_x'^2 + V_y'^2 + V_z'^2 = V_x^2 + V_y^2 + V_z^2$

$$\underline{V}'^T \cdot \underline{V}' = \underline{V}^T \underline{V} \quad \Rightarrow \quad \underline{V}^T \underline{\underline{R}}^T \underline{\underline{R}}\, \underline{V} = \underline{V}^T \underline{V} \quad \Rightarrow \underline{\underline{R}}^T \underline{\underline{R}} = \underline{\underline{1}}$$

so $\underline{\underline{R}}$ must be an orthogonal matrix.

For example, suppose we wish to rotate a vector by an angle ϕ about the fixed z-axis, the appropriate matrix would be
$$\underline{\underline{R}}_z(\phi) = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Suppose that we only wish to rotate by an infinitesimal angle $\phi = \varepsilon$, then for rotations about the x, y, z axes we'd have

$$\underline{\underline{R}}_x(\varepsilon) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1-\varepsilon^2/2 & -\varepsilon \\ 0 & \varepsilon & 1-\varepsilon^2/2 \end{bmatrix} ; \; \underline{\underline{R}}_y(\varepsilon) = \begin{bmatrix} 1-\varepsilon^2/2 & 0 & \varepsilon \\ 0 & 1 & 0 \\ -\varepsilon & 0 & 1-\varepsilon^2/2 \end{bmatrix} ; \; \underline{\underline{R}}_z(\varepsilon) = \begin{bmatrix} 1-\varepsilon^2/2 & -\varepsilon & 0 \\ \varepsilon & 1-\varepsilon^2/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

including terms up to $O(\varepsilon^2)$.

By matrix multiplication we find that:

$$\underline{\underline{R}}_x(\varepsilon)\underline{\underline{R}}_y(\varepsilon) = \begin{bmatrix} 1-\varepsilon^2/2 & 0 & \varepsilon \\ \varepsilon^2 & 1-\varepsilon^2/2 & -\varepsilon \\ -\varepsilon & \varepsilon & 1-\varepsilon^2 \end{bmatrix} \quad \& \quad \underline{\underline{R}}_y(\varepsilon)\underline{\underline{R}}_x(\varepsilon) = \begin{bmatrix} 1-\varepsilon^2/2 & \varepsilon^2 & \varepsilon \\ 0 & 1-\varepsilon^2/2 & -\varepsilon \\ -\varepsilon & \varepsilon & 1-\varepsilon^2 \end{bmatrix}$$

so that

$$\underline{\underline{R}}_x(\varepsilon)\underline{\underline{R}}_y(\varepsilon) - \underline{\underline{R}}_y(\varepsilon)\underline{\underline{R}}_x(\varepsilon) = \begin{bmatrix} 0 & -\varepsilon^2 & 0 \\ \varepsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \neq \underline{0}$$

demonstrating explicitly that even infinitesimal rotations do not commute.

Note that

$$\underline{\underline{R}}_z(\varepsilon^2) - \underline{\underline{R}}_z(0) = \begin{bmatrix} 0 & -\varepsilon^2 & 0 \\ \varepsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \Rightarrow \underline{[\underline{\underline{R}}_x(\varepsilon), \underline{\underline{R}}_y(\varepsilon)] = \underline{\underline{R}}_z(\varepsilon^2) - \underline{\underline{R}}_z(0)} \quad (A)$$

So we know how classical vectors transform under rotations – the question now is how do <u>state vectors</u>, or <u>kets</u>, transform under rotations? This will be the core of a quantum-mechanical understanding of rotations.

$$|\alpha\rangle_R = \mathcal{D}(\underline{\underline{R}})|\alpha\rangle$$

$\mathcal{D}(\underline{\underline{R}})$ is a rotation <u>operator</u> in the space of kets $|\alpha\rangle$.

We've done this kind of construction before – recall infinitesimal translations, where $\vec{x} \to \vec{x} + d\vec{x}$. We represented this in the space of kets by the operator $T(d\vec{x}) = 1 - \frac{i}{\hbar}\hat{\vec{p}}\cdot d\vec{x}$. Similarly translations in time, $t \to t + dt$ were represented by $\mathcal{U}(dt) = 1 - \frac{i}{\hbar}\hat{H}dt$.

Following this pattern we'll propose $\mathcal{D}(\underline{\underline{R}}_k(\varepsilon)) = 1 - \frac{i}{\hbar}\hat{J}_k\varepsilon$

where $\hat{J}_k$ is a Hermitian operator, forcing $\mathcal{D}$ to be unitary. For a rotation about a general direction $\hat{\underline{n}}$ we'd use

$$\mathcal{D}(\hat{n}, d\phi) = 1 - \tfrac{i}{\hbar}\,\hat{\underline{n}}\cdot\hat{\underline{J}}\,d\phi$$

As before we can build a rotation through a finite angle out of an infinite number of infinitesimal rotations

$$\text{e.g. } \mathcal{D}_z(\phi) = \lim_{N\to\infty}\left[1 - \tfrac{i}{\hbar}\hat{J}_z(\phi/N)\right]^N \longrightarrow e^{-\frac{i}{\hbar}\hat{J}_k\phi}$$

We will insist that the operators $\mathcal{D}$ satisfy the same group properties as the rotation matrices $\underline{\underline{R}}$: e.g.

$$\underline{\underline{R}}_1\underline{\underline{R}}_2 = \underline{\underline{R}}_3 \longrightarrow \mathcal{D}(\underline{\underline{R}}_1)\mathcal{D}(\underline{\underline{R}}_2) = \mathcal{D}(\underline{\underline{R}}_3)$$

$$\underline{\underline{R}}^{-1}\underline{\underline{R}} = \underline{\underline{1}} \longrightarrow \mathcal{D}^{-1}(\underline{\underline{R}})\mathcal{D}(\underline{\underline{R}}) = 1$$

then the operator analogue of (A) would be $D_x(\varepsilon)D_y(\varepsilon) - D_y(\varepsilon)D_x(\varepsilon) = D_z(\varepsilon^2) - D_z(0)$

$$\Rightarrow \left[1 - \frac{i}{\hbar}\hat{J}_x\varepsilon - \frac{1}{\hbar^2}\hat{J}_x^2\varepsilon^2\right]\left[1 - \frac{i}{\hbar}\hat{J}_y\varepsilon - \frac{1}{\hbar^2}\hat{J}_y^2\varepsilon^2\right] - \left[1 - \frac{i}{\hbar}\hat{J}_y\varepsilon - \frac{1}{\hbar^2}\hat{J}_y^2\varepsilon^2\right]\left[1 - \frac{i}{\hbar}\hat{J}_x\varepsilon - \frac{1}{\hbar^2}\hat{J}_x^2\varepsilon^2\right] = 1 - \frac{i}{\hbar}\hat{J}_z\varepsilon^2 - 1$$

terms of $O(\varepsilon^2)$ $\longrightarrow$ $\underline{[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z}$

in general $\boxed{[\hat{J}_i, \hat{J}_j] = i\hbar\,\epsilon_{ijk}\hat{J}_k}$ commutation relation of angular momentum*

[I'll forget about the hats from now on]

We can define an operator $J^2 = J_xJ_x + J_yJ_y + J_zJ_z$ which commutes with all of J_x, J_y, J_z, e.g.

$$\begin{aligned}[J^2, J_z] &= [J_xJ_x, J_z] + [J_yJ_y, J_z] + [J_zJ_z, J_z] \\ &= J_x[J_x, J_z] + [J_x, J_z]J_x \\ &\quad + J_y[J_y, J_z] + [J_y, J_z]J_y \\ &= J_x(-i\hbar J_y) + (-i\hbar J_y)J_x + J_y(+i\hbar J_x) + (+i\hbar J_x)J_y = \underline{0}\end{aligned}$$

$\Rightarrow$ we can have simultaneous eigenstates of J^2 & one of J_x, J_y, J_z - we'll choose J_z:

$$J^2|a,b\rangle = a|a,b\rangle$$
$$J_z|a,b\rangle = b|a,b\rangle$$

now consider operators $J_\pm \equiv J_x \pm iJ_y$ then $[J_+, J_-] = 2\hbar J_z$
& $[J_z, J_\pm] = \pm\hbar J_\pm$
& $[J^2, J_\pm] = 0$

consider the state $J_\pm|a,b\rangle$

$$J_z(J_\pm|a,b\rangle) = ([J_z, J_\pm] + J_\pm J_z)|a,b\rangle = (\pm\hbar J_\pm + bJ_\pm)|a,b\rangle = (b\pm\hbar)(J_\pm|a,b\rangle)$$

$$J^2(J_\pm|a,b\rangle) = J_\pm a|a,b\rangle = a(J_\pm|a,b\rangle)$$

$$\Rightarrow J_\pm|a,b\rangle = c_\pm|a, b\pm\hbar\rangle$$

so $J_\pm$ are "ladder" operators, raising or lowering b by $\hbar$ with each application.

Can we keep applying the raising operator ad infinitum, generating more & more eigenstates of J_z? It turns out that we cannot for a given value of a, there is a maximum value of b, $b^2 \leq a$. The proof is as follows:

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*We'll see that this can be the quantum analogue of $\vec{x}\times\vec{p}$ a little later.

$J^2 - J_z^2 = J_x^2 + J_y^2 = \frac{1}{2}(J_+ J_- + J_- J_+) = \frac{1}{2}(J_+ J_+^\dagger + J_+^\dagger J_+)$ since $J_\pm = J_x \pm i J_y$ & $J_\pm^\dagger = J_\mp$

so $\langle a,b | J^2 - J_z^2 | a,b \rangle = \frac{1}{2} \langle a,b | J_+ J_+^\dagger | a,b \rangle + \frac{1}{2} \langle a,b | J_+^\dagger J_+ | a,b \rangle$

$$= \frac{1}{2} \left(J_+^\dagger |a,b\rangle \right)^\dagger \left(J_+^\dagger |a,b\rangle \right) + \frac{1}{2} \left(J_+ |a,b\rangle \right)^\dagger \left(J_+ |a,b\rangle \right)$$
$$\geq 0$$

$\Rightarrow \langle a,b | a - b^2 | a,b \rangle \geq 0 \quad \Rightarrow \underline{a \geq b^2}$ then $\underline{J_+ |a, b_{max}\rangle = 0}$ to ensure this.

then $J_- J_+ |a, b_{max}\rangle = 0$, but $J_- J_+ = J^2 - J_z^2 - \hbar J_z$

so $(J^2 - J_z^2 - \hbar J_z) |a, b_{max}\rangle = 0 \quad \Rightarrow \quad a - b_{max}^2 - \hbar b_{max} = 0$.
$$a = b_{max}(b_{max} + \hbar)$$

Similarly using J_- we can prove $J_- |a, b_{min}\rangle = 0$ & $a = b_{min}(b_{min} - \hbar)$

& hence $b_{max}(b_{max} + \hbar) = b_{min}(b_{min} - \hbar) \quad \Rightarrow \quad \underline{b_{min} = -b_{max}}$

So the allowed values of b are $-b_{max} \leq b \leq b_{max}$. Starting with $|a, -b_{max}\rangle$ we can repeated apply J_+ to get states $b = -b_{max} + n\hbar$ until we hit b_{max} $\Rightarrow$
$$b_{max} = -b_{max} + n\hbar \quad \Rightarrow \quad b_{max} = n \hbar/2 \text{ for integer } n.$$

we define $j = \frac{b_{max}}{\hbar}$ & we see that j can be <u>integral or half-integral only</u>.

Since $a = b_{max}(b_{max} + \hbar)$, we have $a = \hbar^2 j(j+1)$, so that if we say that $b = m\hbar$, our eigenstates are $|j,m\rangle$

$$\boxed{\begin{aligned} J^2 |j,m\rangle &= \hbar^2 j(j+1) |j,m\rangle \\ J_z |j,m\rangle &= \hbar m |j,m\rangle \end{aligned}} \qquad m = \underbrace{-j, -j+1, -j+2 \ldots j-2, j-1, j}_{2j+1 \text{ states}}$$

So in quantum mechanics the angular momentum is quantised - this followed only from the properties of rotations as applied to quantum mechanical states, ie. the commutation relations for the operators J_k.

$J_+ |j,m\rangle = C_+(j,m) |j,m+1\rangle \quad : \quad \langle j,m | J_+^\dagger J_+ |j,m\rangle = |C_+(j,m)|^2 \langle j,m+1 | j,m+1\rangle = |C_+(j,m)|^2$

$$= \langle j,m | J^2 - J_z^2 - \hbar J_z | j,m \rangle = \hbar^2 (j(j+1) - m(m+1))$$

$\Rightarrow C_+(j,m) = \hbar \sqrt{(j-m)(j+m+1)}$ up to an irrelevant phase.

We will return later in the course to the explicit form of the representations of the rotation operator, $D(\underline{R})$ in the $|j,m\rangle$ basis. Right now we'll consider a realisation of J_k that is familiar from classical mechanics,

"orbital angular momentum" $\vec{L} = \vec{x} \times \vec{p}$ or $L_i = \epsilon_{ijk} x_j p_k$

we can easily show that L_i satisfies the commutation relation for angular momentum, $[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$

$$[L_x, L_y] = [yp_z - zp_y, zp_x - xp_z] = [yp_z, zp_x] - [zp_y, zp_x] - [yp_z, xp_z] + [zp_y, xp_z]$$

$$= [yp_z, zp_x] + [zp_y, xp_z] = yp_x[p_z, z] + p_y x[z, p_z] = [z, p_z](p_y x - y p_x)$$

$$= i\hbar(xp_y - yp_x) = \underline{i\hbar L_z}$$

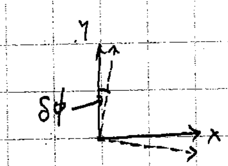
We found that the operator for infinitesimal rotations about the z-axis in the space of kets is $1 - \frac{i}{\hbar} J_z \delta\phi$,

if $J_z = L_z$ & we act on a position eigenket $|x, y, z\rangle$ we see that

$$\left(1 - \frac{i}{\hbar} L_z \delta\phi\right)|x,y,z\rangle = \left(1 - \frac{i}{\hbar}\delta\phi(xp_y - yp_x)\right)|x,y,z\rangle$$

$$= \underbrace{\left(1 - \frac{i}{\hbar}(x\delta\phi)p_y - \frac{i}{\hbar}(-y\delta\phi)p_x\right)}_{\substack{\text{translation by } x\delta\phi \text{ in the } y\text{-direction} \\ \& \text{ by } -y\delta\phi \text{ in the } x\text{-direction}}}|x,y,z\rangle$$

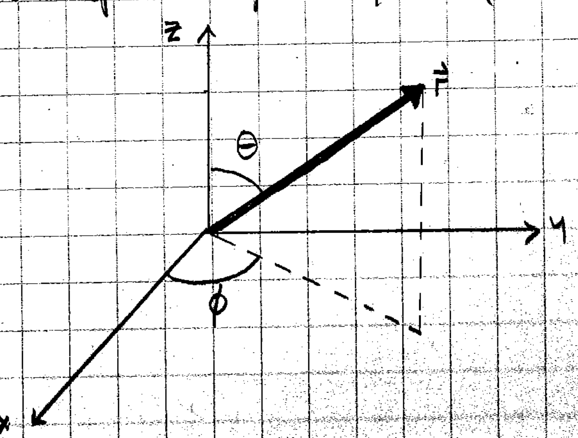
$$= |x - y\delta\phi, y + x\delta\phi, z\rangle$$



So indeed L_k are the generators of rotation in position space.

A more useful co-ordinate system is the spherical polar system (r, θ, ϕ)

$x = r\sin\theta\cos\phi$	$r^2 = x^2 + y^2 + z^2$
$y = r\sin\theta\sin\phi$	$\cot\theta = z/\sqrt{x^2+y^2}$
$z = r\cos\theta$	$\tan\phi = y/x$



Suppose we begin with an abitrary state $|\alpha\rangle$ & perform an infinitesimal rotation about the z-axis - the rotated state is

$$\left(1 - \frac{i}{\hbar} L_z \delta\phi\right)|\alpha\rangle$$

which in the position space representation can be expressed

$$\langle x, y, z | \left(1 - \frac{i}{\hbar} L_z \delta\phi\right)|\alpha\rangle = \langle x + y\delta\phi, y - x\delta\phi, z | \alpha\rangle$$

this assumes a simple form in spherical polar co-ordinates:

$$x + y\delta\phi = r\sin\theta(\cos\phi + \sin\phi . \delta\phi) = r\sin\theta(\cos\phi . \cos\delta\phi + \sin\phi . \sin\delta\phi) \quad \text{to first order in } \delta\phi.$$
$$= r\sin\theta\cos(\phi - \delta\phi)$$

$$y - x\delta\phi = r\sin\theta(\sin\phi - \cos\phi\,\delta\phi) = r\sin\theta(\sin\phi\cos\delta\phi - \cos\phi\sin\delta\phi)$$
$$= r\sin\theta\sin(\phi - \delta\phi)$$

$\Rightarrow$ the rotation takes $\phi \to \phi - \delta\phi$ & $\langle r\theta\phi | \left[1 - \frac{i}{\hbar}\delta\phi L_z\right] |\alpha\rangle = \langle r\theta, \phi - \delta\phi | \alpha\rangle$

$$= \langle r\theta\phi|\alpha\rangle - \delta\phi \frac{\partial}{\partial\phi}\langle r\theta\phi|\alpha\rangle \quad \left(\text{performing a Taylor series}\right)$$

thus $\langle \vec{x} | L_z | \alpha\rangle = -i\hbar \frac{\partial}{\partial\phi}\langle \vec{x}|\alpha\rangle$

or $\langle \vec{x} | L_z | \vec{x}'\rangle = \delta^{(3)}(\vec{x} - \vec{x}')\left(-i\hbar\frac{\partial}{\partial\phi}\right)$ (can also obtain this by representing $\vec{p}$ in position space by $\langle \vec{x} | \vec{p} | \vec{x}'\rangle = \delta^{(3)}(\vec{x} - \vec{x}')(-i\hbar\vec{\nabla})$)

The other elements of $\vec{L}$ follow from considering $\vec{x} \times \vec{p}$ in spherical polar co-ordinates

$$\hat{r} = \sin\theta\cos\phi\,\hat{\imath} + \sin\theta\sin\phi\,\hat{\jmath} + \cos\theta\,\hat{k}$$
$$\hat{\phi} = -\sin\phi\,\hat{\imath} + \cos\phi\,\hat{\jmath} \qquad [\hat{\imath} \times \hat{\jmath} = \hat{k}]$$
$$\hat{\theta} = \cos\theta\cos\phi\,\hat{\imath} + \cos\theta\sin\phi\,\hat{\jmath} - \sin\theta\,\hat{k}$$

as a shorthand, I won't explicitly show that the operators are in the position basis

$$\vec{x} \times \vec{p} = -i\hbar\,\vec{x} \times \vec{\nabla} \qquad \vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}$$

$$\vec{L} = \vec{x} \times \vec{p} = -i\hbar\, r\hat{r} \times \vec{\nabla} = -i\hbar r\left[\hat{r} \times \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} + \hat{r} \times \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}\right]$$

$$= -i\hbar\left[\hat{r} \times \hat{\phi}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \hat{r} \times \hat{\theta}\frac{\partial}{\partial\theta}\right]$$

$$L_z = -i\hbar\left[\hat{k}\cdot\hat{r}\times\hat{\phi}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \hat{k}\cdot\hat{r}\times\hat{\theta}\frac{\partial}{\partial\theta}\right]$$

$$= -i\hbar\Big[\hat{k}\cdot\left(\sin\theta\cos^2\phi\,\hat{i}\times\hat{j} - \sin\theta\sin^2\phi\,\hat{j}\times\hat{i}\right)\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}$$
$$+\hat{k}\cdot\left(\sin\theta\cos\theta\sin\phi\cos\phi\,\hat{i}\times\hat{j} + \sin\theta\cos\theta\sin\phi\cos\phi\,\hat{j}\times\hat{i}\right)\frac{\partial}{\partial\theta}\Big]$$

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

$$L_x = -i\hbar\left[\hat{i}\cdot\hat{r}\times\hat{\phi}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \hat{i}\cdot\hat{r}\times\hat{\theta}\frac{\partial}{\partial\theta}\right]$$
$$= -i\hbar\left[\cos\theta\cos\phi\,\hat{i}\cdot\hat{k}\times\hat{j}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \left(\cos^2\theta\sin\phi\,\hat{i}\cdot\hat{k}\times\hat{j} - \sin^2\theta\sin\phi\,\hat{i}\cdot\hat{j}\times\hat{k}\right)\frac{\partial}{\partial\theta}\right]$$

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

$$L_y = -i\hbar\left[\hat{j}\cdot\hat{r}\times\hat{\phi}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \hat{j}\cdot\hat{r}\times\hat{\theta}\frac{\partial}{\partial\theta}\right]$$

$$= -i\hbar\left[-\cos\theta\sin\phi\,\hat{j}\cdot\hat{k}\times\hat{i}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \left(\cos^2\theta\cos\phi\,\hat{j}\cdot\hat{k}\times\hat{i} - \sin^2\theta\cos\phi\,\hat{j}\cdot\hat{j}\times\hat{i}\right)\frac{\partial}{\partial\theta}\right]$$

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

Raising & lowering operators follow as $L_\pm = L_x \pm iL_y$

$$L_\pm = -i\hbar\left[-\cot\theta\cdot e^{\pm i\phi}\frac{\partial}{\partial\phi} \pm i e^{\pm i\phi}\frac{\partial}{\partial\theta}\right] = \underline{-i\hbar e^{\pm i\phi}\left[\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right]}$$

$$L^2 = L_x^2 + L_y^2 + L_z^2 = L_z^2 + \frac{1}{2}\left(L_+L_- + L_-L_+\right)$$

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

The importance of L^2 becomes clear if we consider the Hamiltonian for a particle moving in three-dimensions

$$\underline{H = \vec{P}^2/2m}$$

r^2

firstly let's derive an operator equation $\vec{L}^2 = \vec{x}^2\vec{p}^2 - (\vec{x}.\vec{p})^2 + i\hbar\vec{x}.\vec{p}$:

(remember $[x_i, p_j] = i\hbar\delta_{ij}$)

$$\vec{L}^2 \equiv \vec{L}\cdot\vec{L} = (\vec{x}\times\vec{p}).(\vec{x}\times\vec{p}) \equiv \sum_{ijklm} \epsilon_{ijk} x_j p_k \, \epsilon_{ilm} x_l p_m$$

$$= \sum_{ijklm} \epsilon_{ijk}\epsilon_{ilm} \, x_j p_k x_l p_m = \sum_{jklm} (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}) x_j p_k x_l p_m$$

$\sum \epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$
e.g. $j=2, k=3$, $l=2, m=3$: LHS $=1$, RHS $=1$
$j=2, k=3$, $l=3, m=2$: LHS $=-1$, RHS $=-1$

$$= \sum_{jk} x_j p_k x_j p_k - \sum_j x_j \sum_k p_k x_k p_j$$

$$= \sum_{jk} x_j \left(-[x_j, p_k] + x_j p_k\right) p_k - \sum_{jk} x_j p_k \left([x_k, p_j] + p_j x_k\right)$$

$$= \sum_{jk} x_j (-i\hbar\delta_{jk} + x_j p_k) p_k - \sum_{jk} x_j p_k (i\hbar\delta_{kj} + p_j x_k)$$

$$= -i\hbar\vec{x}.\vec{p} + \vec{x}^2\vec{p}^2 - i\hbar\vec{x}.\vec{p} - \sum_{jk} x_j p_j p_k x_k$$

$$= -2i\hbar\vec{x}.\vec{p} + \vec{x}^2\vec{p}^2 - \vec{x}.\vec{p}\sum_k \left(-[x_k, p_k] + x_k p_k\right)$$

$$= -2i\hbar\vec{x}.\vec{p} + \vec{x}^2\vec{p}^2 + \vec{x}.\vec{p}\sum_k i\hbar\delta_{kk} - (\vec{x}.\vec{p})^2$$

$$= -2i\hbar\vec{x}.\vec{p} + \vec{x}^2\vec{p}^2 + 3i\hbar\vec{x}.\vec{p} - (\vec{x}.\vec{p})^2 = \underline{\vec{x}^2\vec{p}^2 - (\vec{x}.\vec{p})^2 + i\hbar\vec{x}.\vec{p}}$$

Now consider this in the position representation

$$\vec{L}^2 \rightsquigarrow r^2(-i\hbar\vec{\nabla})^2 - (\vec{r}.(-i\hbar\vec{\nabla}))^2 + i\hbar\,\vec{r}.(-i\hbar\vec{\nabla})$$

$$= -\hbar^2 r^2\nabla^2 + \hbar^2(\vec{r}.\vec{\nabla})(\vec{r}.\vec{\nabla}) + \hbar^2\,\vec{r}.\vec{\nabla} \qquad \vec{r}.\vec{\nabla} = r\frac{\partial}{\partial r}$$

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

& thus $-\hbar^2\nabla^2 = L^2/r^2 - \hbar^2\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial r}\right)$

but recall that

$$H = \frac{1}{2m}\vec{p}^2 \rightsquigarrow \frac{1}{2m}(-i\hbar\vec{\nabla})^2 = -\frac{\hbar^2}{2m}\nabla^2$$

& thus in the position representation $H = -\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial r}\right) + \frac{L^2}{2mr^2}$

where the angular dependence is completely within L^2!

Let's recall that we're often interested in stationary states whose wavefunctions are the eigenfunctions of the Hamiltonian

$$H\,\phi_E(r,\theta,\phi) = E\,\phi_E(r,\theta,\phi).$$

(this is a partial differential eqn)

Suppose that we could express these wavefunctions as a product of a factor depending upon r & a factor depending upon θ,ϕ:

$$\phi_E(r,\theta,\phi) = R(r)\,X(\theta,\phi),$$

then the kinetic energy piece of the Hamiltonian being factored into those two terms is very handy

$$H = f\left(r,\frac{\partial}{\partial r}\right) + \frac{L^2}{2mr^2} \qquad \left(L^2 = fn\left(\theta,\phi,\frac{\partial}{\partial\theta},\frac{\partial}{\partial\phi}\right) \text{ but not } r, \frac{\partial}{\partial r}\,!\right)$$

$$\Rightarrow \quad H\phi_E = E\phi_E \longrightarrow X(\theta,\phi)\, f\left(r,\frac{\partial}{\partial r}\right)R(r) + R(r)\frac{1}{2mr^2}L^2 X(\theta,\phi) = E\,R(r)X(\theta,\phi)$$

if we knew what the eigenfunctions of the L^2 operator were $\left(L^2 X_\lambda(\theta,\phi) = \lambda X_\lambda(\theta,\phi)\right)$ we'd be able to write

$$X_\lambda(\theta,\phi)\left[f\left(r,\frac{\partial}{\partial r}\right)R(r) + \frac{\lambda^2}{2mr^2}R(r) - E R(r) = 0\right]$$

where the object in square brackets is an ordinary differential eqn.

So for solving three-dimensional problems it will pay to know the eigenfunctions of the L^2 operator.

REMEMBER : $\vec{L}$ is just a particular realisation of the generator of rotations, $\vec{J}$. We already know that the eigenstates of J^2 have integral or half-integral eigenvalues and are simultaneously eigenstates of J_z.

eigenequation $\quad L_z X_m(\theta,\phi) = m\hbar\, X_m(\theta,\phi)$

$$-i\hbar\frac{\partial}{\partial\phi}X_m(\theta,\phi) = m\hbar\, X_m(\theta,\phi) \quad \Rightarrow X_m(\theta,\phi) = f(\theta)\,e^{im\phi}$$

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

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

$$\Rightarrow \left[\frac{-m^2}{\sin^2\theta} + \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right) + l(l+1)\right] f_{ml}(\theta) = 0$$ ordinary differential equ

An easy way to get at the solutions of this equation is to use the ladder operators

$$L_+ |l, m=+l\rangle = 0$$

in the position representation: $-i\hbar\left[-\cot\theta\, e^{i\phi}\frac{\partial}{\partial\phi} + i e^{i\phi}\frac{\partial}{\partial\theta}\right] e^{il\phi} f_{ll}(\theta) = 0$

$$\Rightarrow \left(-il\cot\theta + i\frac{d}{d\theta}\right) f_{ll}(\theta) = 0$$

$$\Rightarrow \left(-l\cos\theta + \sin\theta\frac{d}{d\theta}\right) f_{ll}(\theta) = 0$$

$$\Rightarrow \underline{f_{ll}(\theta) \propto (\sin\theta)^l} \qquad \left[\frac{d}{d\theta}\sin^l\theta = l\sin^{l-1}\theta\cos\theta\right]$$

thus $\langle\theta,\phi|l, m=l\rangle = N e^{il\phi}(\sin\theta)^l$

$$1 = \langle l,m=l|l,m=l\rangle = \int d\Omega\, |N|^2 \sin^{2l}\theta = |N|^2 \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta\, \sin^{2l}\theta = |N|^2 \cdot 2\pi \int_{-1}^{1} d\cos\theta\, (\sin^2\theta)^l$$

$$= |N|^2\, 2\pi \int_{-1}^{1} d\cos\theta\, (1-\cos^2\theta)^l = |N|^2\, 2\pi \int_{-1}^{1} dz\, (1-z^2)^l$$

with some work can determine that $N = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)\,(2l)!}{4\pi}}$

where the $(-1)^l$ factor is a conventional phase choice.

The eigenfunctions for $m<l$ can be obtained by acting with L_-:

in the position representation $L_- = -i\hbar e^{-i\phi}\left[-i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right]$

since $L_-|l,m\rangle = \hbar\sqrt{(l+m)(l-m+1)}\,|l,m-1\rangle$

so $|l,m-1\rangle = \dfrac{L_-}{\hbar\sqrt{(l+m)(l-m+1)}}|l,m\rangle$

& $\langle\theta,\phi|l,m-1\rangle = \dfrac{i e^{-i\phi}}{\sqrt{(l+m)(l-m+1)}}\left[-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]\langle\theta,\phi|l,m\rangle$

e.g. $l=1$: $\langle\theta,\phi|1,+1\rangle = \frac{-1}{2}\sqrt{\frac{3\cdot 2!}{4\pi}}\, e^{i\phi}\sin\theta = \underline{-\sqrt{\frac{3}{8\pi}}\, e^{i\phi}\sin\theta}$

$$\langle\theta,\phi|1,0\rangle = \frac{e^{-i\phi}}{\sqrt{1\cdot 2}}\left[-\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right]\left(-\sqrt{\frac{3}{8\pi}}\, e^{i\phi}\sin\theta\right) = -\frac{\sqrt{3}}{\sqrt{16\pi}}\left[-\cos\theta + i\cos\theta\, i\right.$$

$$\langle\theta,\phi|1,0\rangle = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$\langle\theta,\phi|1,-1\rangle = \frac{e^{-i\phi}}{\sqrt{1\cdot 2}}\left[-\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right]\left(\sqrt{\frac{3}{4\pi}}\cos\theta\right)$$

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

These eigenfunctions are known as the "Spherical Harmonics", for $m \geq 0$ they can be obtained from

$$Y_l^m(\theta,\phi) \equiv \langle\theta,\phi|l,m\rangle = \frac{(-1)^l}{2^l l!}\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l+m)!}{(l-m)!}}\,e^{im\phi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\sin\theta)^{2l}$$

& $Y_l^{-m}(\theta,\phi) = (-1)^m\, Y_l^{m*}(\theta,\phi)$ gives the $m<0$ solutions.

For the few lowest l, the explicit solutions are

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\,z/r$$

$$Y_1^{\pm1} = \mp\sqrt{\frac{3}{8\pi}}\,e^{\pm i\phi}\sin\theta = \mp\sqrt{\frac{3}{8\pi}}\,\frac{x\pm iy}{r}$$

notice that this is like the spherical components of a vector.

$$Y_2^0 = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$$

$$Y_2^{\pm1} = \mp\sqrt{\frac{15}{8\pi}}\,e^{\pm i\phi}\cos\theta\sin\theta$$

$$Y_2^{\pm2} = \sqrt{\frac{15}{32\pi}}\,e^{\pm 2i\phi}\sin^2\theta$$

Remember these functions are the eigenstates of L^2 & L_z in the position basis:

$$L^2\, Y_l^m = l(l+1)\hbar^2 Y_l^m \qquad \& \qquad L_z Y_l^m = m\hbar\, Y_l^m$$

Exercise: convince yourself that these functions can only be wavefunctions of a quantum system if l & m are integers.

as we'd expect of non-degenerate eigenstates of Hermitian operators, they are orthogonal:

$$\delta_{l'l}\,\delta_{m'm} = \langle l',m'|l,m\rangle = \int d\Omega\; Y_{l'}^{m'*}(\theta,\phi)\,Y_l^m(\theta,\phi)$$