

where $R(r)$ obeys the radial equation

$$\left(\frac{-\hbar^2}{2m}\right) \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} R(r) \right) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \right] R(r) = ER(r).$$

3.3. Orbital Angular Momentum

In classical mechanics the Hamiltonian for the central potential problem can be written as

$$H = \frac{p_r^2}{2m} + \frac{\vec{L}^2}{2mr^2} + V(r)$$

with p_r the momentum conjugate to r , $p_r = \frac{\partial \mathcal{L}}{\partial \dot{r}} = m\dot{r}$,
 while $\vec{L} = \vec{r} \times \vec{p}$ is the ^{orbital} angular momentum.
 Comparing this to the quantum mechanical Hamiltonian

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

we identify the radial component of the momentum squared with

$$P_r^2 = -\hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \text{ and}$$

with the orbital angular momentum squared given by

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

$$\left. + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

which is just $(-\hbar^2 r^2)$ times the angular part of the Laplacian ∇^2 . Further, since

$$H \psi_{lm}(r, \theta, \phi) = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \psi_{lm}(r, \theta, \phi) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \right] \psi_{lm}(r, \theta, \phi)$$

$$= E \psi_{lm}(r, \theta, \phi),$$

we see that the $Y_l^m(\theta, \phi)$ are eigenfunctions of L^2

$$L^2 Y_l^m(\theta, \phi) = \hbar^2 l(l+1) Y_l^m(\theta, \phi),$$

with the orbital angular momentum eigenvalues given by $\hbar^2 l(l+1)$, $l=0, 1, 2, \dots$.

To show that the spherical harmonics are indeed the eigenfunctions of L^2 and L_z more rigorously. Recall the definition of the orbital angular momentum

$$\vec{L} = \vec{r} \times \vec{p} = -i\hbar \vec{r} \times \vec{\nabla},$$

thus in components we have

with
$$L_i = \epsilon_{ijk} x_j p_k = \frac{\hbar}{i} \epsilon_{ijk} x_j \frac{\partial}{\partial x_k}$$

 ϵ_{ijk} the anti-symmetric (Levi-Civita) tensor (permutation tensor)

$$\epsilon_{ijk} = \begin{cases} +1 & , i,j,k \text{ is an even permutation of } 1,2,3 \\ -1 & , i,j,k \text{ is an odd permutation of } 1,2,3 \\ 0 & \text{otherwise i.e. any } i,j \text{ or } k \text{ are equal.} \end{cases}$$

that is
$$L_1 = x_2 p_3 - x_3 p_2 = \frac{\hbar}{i} (x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2})$$

$$L_2 = x_3 p_1 - x_1 p_3 = \frac{\hbar}{i} (x_3 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3})$$

$$L_3 = x_1 p_2 - x_2 p_1 = \frac{\hbar}{i} (x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1}).$$

(with $x_1 = x, x_2 = y, x_3 = z$ and $p_1 = p_x, p_2 = p_y, p_3 = p_z$)

Using the canonical commutation relations

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

$$[x_i, x_j] = 0 = [p_i, p_j]$$

we find that

$$\begin{aligned}
[L_1, L_2] &= \left(\frac{\hbar}{i}\right)^2 \left[x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2}, x_3 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3} \right] \\
&= -\hbar^2 \left(x_2 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_2} \right) \\
&= -\hbar^2 \frac{-i}{\hbar} L_3 = i\hbar L_3
\end{aligned}$$

Thus

$[L_1, L_2] = i\hbar L_3$ plus cyclic permutations of the components 1, 2, 3.

In general

$$\begin{aligned}
[L_i, L_j] &= [\epsilon_{ike} x_k p_e, \epsilon_{jmn} x_m p_n] \\
&= \epsilon_{ike} \epsilon_{jmn} [x_k p_e, x_m p_n]
\end{aligned}$$

Now use the identity

$$\begin{aligned}
[A, BC] &= ABC - BCA + BAC - BAC \\
&= B[A, C] + [A, B]C
\end{aligned}$$

to write

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$$\begin{aligned} [x_k p_l, x_m p_n] &= x_m [x_k p_l, p_n] + [x_k p_l, x_m] p_n \\ &= x_m x_k [p_l, p_n] + x_m [x_k, p_n] p_l \\ &\quad + x_k [p_l, x_m] p_n + [x_k, x_m] p_l p_n \\ &= i\hbar (x_m p_l \delta_{kn} - x_k p_n \delta_{lm}) \end{aligned}$$

So

$$\begin{aligned} [L_i, L_j] &= i\hbar (\epsilon_{ikl} \epsilon_{jmk} x_m p_l - \epsilon_{ikl} \epsilon_{jln} x_k p_n) \\ &\quad \text{(relabelling dummy indices)} \\ &= -i\hbar \epsilon_{ilk} \epsilon_{jmk} (x_m p_l - x_l p_m) \end{aligned}$$

Now $\epsilon_{ilk} \epsilon_{jmk} = \delta_{ij} \delta_{lm} - \delta_{im} \delta_{lj}$

Then

$$\begin{aligned} [L_i, L_j] &= -i\hbar (\delta_{ij} x_m p_m - x_i p_i - \delta_{im} x_j p_j + x_j p_i) \\ &= +i\hbar (x_i p_j - x_j p_i) \\ \text{But } \epsilon_{ijk} L_k &= \epsilon_{ijk} \epsilon_{klm} x_l p_m \\ &= (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) x_l p_m \\ &= x_i p_j - x_j p_i \end{aligned}$$

So
$$[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$$

The components of \vec{L} do not commute with each other. Hence they are not simultaneously diagonalizable i.e. $\Delta L_1, \Delta L_2 \geq \frac{\hbar}{2} |\Delta L_3|$

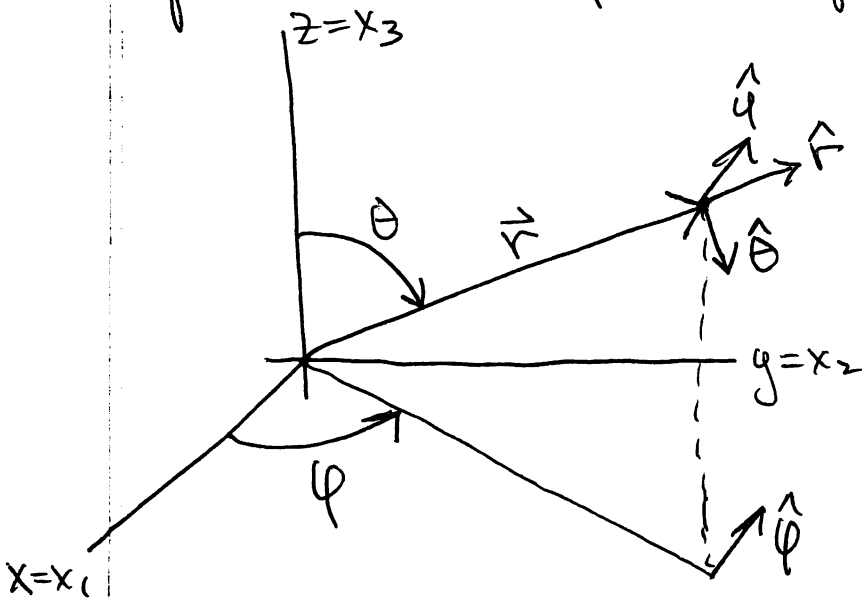
However $\vec{L}^2 = L \cdot L$ commutes with \vec{L} (as we shall see \vec{L} generates spatial rotations, as \vec{p} generates spatial translations, hence, \vec{L}^2 is a scalar dot product and invariant under rotations $[\vec{L}^2, \vec{L}] = 0$)

$$\begin{aligned} [\vec{L}^2, L_j] &= [L_i L_i, L_j] \\ &= L_i [L_i, L_j] + [L_i, L_j] L_i \\ &= i\hbar \epsilon_{ijk} L_i L_k + i\hbar \epsilon_{ijk} L_k L_i \\ &= i\hbar (\epsilon_{ijk} + \underbrace{\epsilon_{kji}}_{=-\epsilon_{ijk}}) L_i L_k \\ &= 0 \end{aligned}$$

change dummy
i, k indices on second
term

Hence we can determine the eigenvalues of \vec{L}^2 and one of the components L_i , say L_3 , simultaneously since $[\vec{L}^2, L_3] = 0$.

The relevance of all this to our earlier work is that the spherical harmonics $Y_l^m(\theta, \varphi)$ are the simultaneous eigenfunctions of L^2 and L_3 . To see this we next express the orbital angular momentum operator in spherical polar coordinates.



Note:

$$\hat{r} \times \hat{\theta} = \hat{\varphi}$$

$$\hat{\theta} \times \hat{\varphi} = \hat{r}$$

$$\hat{\varphi} \times \hat{r} = \hat{\theta}$$

In spherical polar coordinates the Cartesian coordinates are given by

$$x_1 = r \sin \theta \cos \varphi$$

$$x_2 = r \sin \theta \sin \varphi$$

$$x_3 = r \cos \theta$$

while the spherical coordinate basis vectors $(\hat{r}, \hat{\theta}, \hat{\varphi})$ are given by

$$\hat{r} = \sin\theta \cos\varphi \hat{i} + \sin\theta \sin\varphi \hat{j} + \cos\theta \hat{k}$$

$$\hat{\theta} = \cos\theta \cos\varphi \hat{i} + \cos\theta \sin\varphi \hat{j} - \sin\theta \hat{k}$$

$$\hat{\varphi} = -\sin\varphi \hat{i} + \cos\varphi \hat{j}$$

The gradient operator in spherical coordinates is given as

$$\vec{\nabla} = \hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\varphi} \frac{1}{r \sin\theta} \frac{\partial}{\partial \varphi}$$

hence the orbital angular momentum operator in spherical polar coordinates is

$$\begin{aligned} \vec{L} &= \vec{r} \times \vec{p} = r \hat{r} \times \frac{\hbar}{i} \vec{\nabla} \\ &= \frac{\hbar}{i} \left(\hat{\varphi} \frac{\partial}{\partial \theta} - \hat{\theta} \frac{1}{\sin\theta} \frac{\partial}{\partial \varphi} \right) \end{aligned}$$

Thus the Cartesian components, $L_1 = \hat{i} \cdot \vec{L}$, $L_2 = \hat{j} \cdot \vec{L}$, $L_3 = \hat{k} \cdot \vec{L}$ have easily found in polar coordinates to be

$$L_x = L_1 = \frac{\hbar}{i} \left(-\sin\varphi \frac{\partial}{\partial\theta} - \cot\theta \cos\varphi \frac{\partial}{\partial\varphi} \right)$$

$$L_y = L_2 = \frac{\hbar}{i} \left(\cos\varphi \frac{\partial}{\partial\theta} - \cot\theta \sin\varphi \frac{\partial}{\partial\varphi} \right)$$

$$L_z = L_3 = \frac{\hbar}{i} \frac{\partial}{\partial\varphi}$$

A direct calculation then gives L^2 in terms of spherical polar coordinates

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

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

This differential operator is nothing but the angular part of the Laplacian, thus

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

Indeed, recalling page -203-, the spherical harmonics are the eigenfunctions of the orbital \mathbf{L} momentum squared and its z -component

$$\vec{L}^2 Y_l^m(\theta, \phi) = \hbar^2 l(l+1) Y_l^m(\theta, \phi)$$

$$L_z Y_l^m(\theta, \phi) = m\hbar Y_l^m(\theta, \phi)$$

for $l = 0, 1, 2, \dots; m = -l, -l+1, \dots, 0, \dots, l-1, l$

The orbital angular momentum squared \vec{L}^2 has eigenvalues $l(l+1)\hbar^2$, $l = 0, 1, 2, \dots$ and the third (or z-) component L_z has eigenvalues $m\hbar$, $m = -l, -l+1, \dots, l-1, l$. The angular momentum is said to be "quantized".

Each eigenstate of total orbital angular momentum squared, i.e. for each l , has $(2l+1)$ components, one for each L_z eigenvalue $m\hbar$. The integer $l = 0, 1, 2, \dots$ denotes the orbital angular momentum and according to spectroscopic notation is denoted as S, P, D, F, ... for $l = 0, 1, 2, 3, \dots$ eigenstates while the magnetic quantum number m takes possible values $-l, \dots, +l$.

