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Lec 34. Orbital A.M. Eigenfunctions – Spherical Harmonics

Given

$$\left.\begin{aligned} x &= r\sin\theta\cos\varphi \\ y &= r\sin\theta\sin\varphi \\ z &= r\cos\theta \end{aligned}\right\} \quad \text{—(1)}$$

and

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} \quad \text{—(2)}$$

we can derive the position space representation of $\hat{L}_x$ & $\hat{L}_y$ as (H.W.)

$$\text{(36)}\left\{\begin{aligned} \hat{L}_x &\rightarrow i\hbar\left(\sin\varphi\frac{\partial}{\partial\varphi} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right) \\ \hat{L}_y &\rightarrow -i\hbar\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right) \end{aligned}\right.$$

From these we get

$$\hat{L}_{\pm} \rightarrow -i\hbar\, e^{\pm i\varphi}\left\{\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\varphi}\right\} \quad \text{—(3)}$$

and,

$$\hat{L}^2 \rightarrow -\hbar^2 \left\{ \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) \right\} \quad -④$$

Note that all the operators depend only on $(\theta, \varphi) \equiv \Omega$ and not on r.

This is because these operators effect rotation which preserve r.

This means that the simultaneous eigenfunctions of $\hat{L}^2, \hat{L}_z$ will only depend on (θ, φ).

Let $\Psi_{l m_l}(\theta, \varphi)$ be the eigenfunctions

$$\Rightarrow \quad \hat{L}^2 \Psi_{l m_l} = l(l+1)\hbar^2 \Psi_{l m_l} \quad -⑤$$

$$\hat{L}_z \Psi_{l m_l} = m_l \hbar \Psi_{l m_l} \quad -⑥$$

But we know that eigenfunction of $\hat{L}_z$ is $\Phi_{m_l}(\varphi)$ and it's only dependent on φ. $\therefore$ $\Psi_{lm_l}(\Omega)$ must be separable in θ & φ terms.

Let $\Psi_{l,m_l}(\theta,\varphi) = \Theta_{lm_l}(\theta)\, \Phi_{m_l}(\varphi)$ — (7)

Now,

$$\hat{L}_+ |ll\rangle = 0 \quad \text{— (8)}$$

$$\Rightarrow \langle r\theta\varphi|\hat{L}_+|ll\rangle = 0 \quad \text{— (9)}$$

Using (3),

$$i \frac{\partial}{\partial\theta} \Psi_{ll}(\theta,\Omega) - \cot\theta \frac{\partial}{\partial\varphi} \Psi_{ll}(\theta,\Omega) = 0 \quad \text{— (10)}$$

$$\Psi_{ll}(\theta,\varphi) = \Theta_{ll}(\theta)\, \Phi_l(\varphi) \quad \text{— (11)}$$

$$\Rightarrow \quad i\, \Phi_l(\theta) \frac{\partial}{\partial\theta} \Theta_{ll}(\theta) - \cot\theta\, \Theta_{ll}(\theta) (il)\, \Phi_l(\varphi) = 0 \quad \text{(12) —}$$

Eliminating $\Phi_l(\varphi)$ we get

$$\frac{d\,\Theta_{ll}(\theta)}{\Theta_{ll}(\theta)} = l \cot\theta \, d\theta \quad — (13)$$

Integration yields.

$$\ln \Theta_{ll}(\theta) = l \ln(\sin\theta) + C \quad — (14)$$

$$\Rightarrow \quad \Theta_{ll}(\theta) = \underset{(\hookrightarrow e^{C})}{A} \sin^{l}\theta \quad — (15)$$

Normalization can determine A.
While doing so let us recall that the integration over θ involves the factor $\sin\theta \, d\theta$

$$dx\,dy\,dz = r^2 \underbrace{\sin\theta \, d\theta}\, d\varphi \quad — (16)$$

$$\therefore \int_0^{\pi} |\Theta_{\ell\ell}(\theta)|^2 \sin\theta \, d\theta = 1 \quad \text{— (17)}$$

is the normalization condition

$$\Rightarrow |A|^2 \int_0^{\pi} \sin^{2\ell}\theta \sin\theta \, d\theta$$

$$= |A|^2 \int_0^{\pi} (1-\cos^2\theta)^{\ell} \sin\theta \, d\theta \quad \text{— (18)}$$

Let $x = \cos\theta \Rightarrow dx = -\sin\theta \, d\theta$

$$\therefore 1 = |A|^2 \int_{-1}^{1} (1-x^2)^{\ell} \, dx \quad \text{— (19)}$$

We use the identity

$$\int_{-1}^{1} (1-x^2)^{\ell} \, dx = \frac{\ell! \, 2^{\ell+1}}{(2\ell+1)!!} \quad \text{— (20)}$$

$$\therefore \quad A = \sqrt{\frac{(2\ell+1)!!}{\ell!\,2^{\ell+1}}} \qquad -(21)$$

$$\therefore \quad \Theta_{\ell\ell}(\theta) = \sqrt{\frac{(2\ell+1)!!}{\ell!\,2^{\ell+1}}}\,\sin^{\ell}\theta \qquad -(22)$$

and $$\Psi_{\ell\ell}(\theta,\varphi) = \sqrt{\frac{(2\ell+1)!!}{\ell!\,2^{\ell+1}\,2\pi}}\,\sin^{\ell}\theta\, e^{i\ell\varphi} \qquad -(23)$$

The other functions for a given ℓ can be obtained by repeated application of $\hat{L}_-$.

$$\Theta_{\ell\,\ell-1}(\theta) = \frac{-i\hbar}{C^-_{\ell\ell}}\, e^{-i\varphi}\left[-i\frac{\partial \Theta_{\ell\ell}}{\partial\theta} - \ell\cot\theta\,.\,\Theta_{\ell\ell}\right] \qquad -(24)$$

⋮

Overall we find that

$$\boxed{\Theta_{l m_l}(\theta) = \sqrt{\frac{(2l+1)(l-m_l)!}{2(l+m_l)!}}\, P_l^{m_l}(\cos\theta)} \quad \text{— (25)}$$

where,

$$\boxed{P_l^{m}(x) \equiv \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l} \quad \text{(26)}$$

$P_l^m(x)$ are called the associated Legendre polynomials. (26) is the Rodrigues' formula to generate them.

Θ & Φ together form the spherical Harmonics:

$$\boxed{Y_l^{m_l}(\theta,\varphi) = \sqrt{\frac{(2l+1)(l-m_l)!}{4\pi(l+m_l)!}}\, P_l^{m_l}(\cos\theta)\, e^{im_l\varphi}} \quad \text{— (27)}$$

such that

(28) $$\begin{cases} \hat{L}^2 Y_l^{m_l}(\theta,\varphi) = l(l+1)\hbar^2 Y_l^{m_l}(\theta,\varphi) \\ \hat{L}_z Y_l^{m_l}(\theta,\varphi) = m_l \hbar Y_l^{m_l}(\theta,\varphi) \end{cases}$$

with $l = 0, 1, 2, \ldots$

$m_l = 0, \pm 1, \pm 2, \ldots, \pm l$

These have the following properties.

1. $$\left(Y_l^{m_l}(\theta,\varphi)\right)^* = (-1)^{m_l} Y_l^{-m_l}(\theta,\varphi) \quad (29)$$

2. $$\hat{\pi}\, Y_l^{m_l}(\theta,\varphi) = (-1)^l Y_l^{-m}(\theta,\varphi) \quad (30)$$

$\hat{\pi}$ → coordinate inversion

3. $$\int_0^{\pi}\int_0^{2\pi} \underbrace{\sin\theta\, d\theta\, d\varphi}_{d\Omega}\, Y_l^{m_l *}(\Omega)\, Y_{l'}^{m_l'}(\Omega) = \delta_{ll'}\,\delta_{m_l m_l'} \quad (31)$$

Some A.L.P.

$$P_0^0(\cos\theta) = 1 \qquad (r\text{-like}$$

$$P_1^0(\cos\theta) = \cos\theta \qquad (z\text{-like})$$

$$P_1^1(\cos\theta) = -\sin\theta \qquad (x,y\text{-like})$$

(32)

$$P_2^0(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$$

$$P_2^1(\cos\theta) = -3\cos\theta\sin\theta$$

$$P_2^2(\cos\theta) = 3\sin^2\theta$$

It's easy to show using (26) that

$$P_l^{-m_l}(x) = (-1)^{m_l}\frac{(l-m_l)!}{(l+m_l)!}P_l^{m_l}(x) \qquad -(33)$$

So the 2 are proportional. So only one of them is specified in (32).