

PHYS 486: Lecture # 22

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Hydrogen Atom

Connect \hat{L} to the angular equation. Recall that the angular equation is

$$\frac{1}{Y} \left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right\} = l(l+1) \quad (1)$$

Note that

$$\vec{L} = -i\hbar(r \times \nabla) \quad (2)$$

Where ∇ is the gradient operator in spherical coordinates. Although, we cannot solve everything in spherical coordinates since we care about L_z . With $r = r\hat{r} + \dots$, we have that

$$L = -i\hbar \left(r(\hat{r} \times \hat{r})\partial_r + (\hat{r} \times \hat{\theta})\partial_\theta + (\hat{r} \times \hat{\phi}) \frac{1}{\sin \theta} \partial_\phi \right) \quad (3)$$

Note that

$$\hat{r} \times \hat{\theta} = \hat{\phi}, \quad \hat{r} \times \hat{\phi} = -\hat{\theta} \quad (4)$$

In cartesian coordinates, we have

$$\hat{\theta} = \cos \theta \cos \phi \hat{i} + \cos \theta \sin \phi \hat{j} + \sin \theta \hat{k} \quad (5)$$

$$\hat{\phi} = -\sin \phi \hat{i} + \cos \phi \hat{j} \quad (6)$$

Then

$$L_x = -i\hbar(-\sin \phi \partial_\theta - \cos \phi \cot \theta \partial_\phi) \quad (7)$$

$$L_y = -i\hbar(\cos \phi \partial_\theta - \sin \phi \cot \theta \partial_\phi) \quad (8)$$

$$L_z = -i\hbar \partial_\phi \quad (9)$$

Defining the ladder operators, we have that

$$L_{\pm} = L_x \pm iL_y = \pm \hbar \exp(\pm i\phi) (\partial_\theta \pm i \cot \theta \partial_\phi) \quad (10)$$

$$L^2 = L_+ L_- + L_z^2 - \hbar L_z \quad (11)$$

$$\implies -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \partial_\theta) + \frac{1}{\sin^2 \theta} \partial_\phi^2 \right] \quad (12)$$

Thus, our angular equation can be computed as

$$\hbar^2 l(l+1)Y = L^2 Y \quad (13)$$

This is the eigenvalue equation for Y . To solve for $Y(\theta, \phi)$. Let $Y = \Omega(\theta)\Lambda(\phi)$, then we get

$$\frac{1}{\Omega} \left[\sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Omega}{d\theta} + l(l+1) \sin^2 \theta \right) \right] + \underbrace{\frac{1}{\Lambda} \frac{d^2}{d\phi^2} \Lambda}_{=-m^2} = 0 \quad (14)$$

Then we solve

$$d_\phi^2 \Lambda = -m^2 \Lambda \implies \Lambda(\phi) = \exp(im\phi) \quad (15)$$

These are the eigenfunctions of L_z . We have to demand that $\Lambda(\phi) = \Lambda(\phi + 2\pi)$, then we get that m must be an integer. In principle, A.M allows $l = \text{integer or integer } + 1/2$. However, orbital A.M. can only be an integer.

We next solve the θ equation. Note that this solutions are the Legendre Functions, thus,

$$\Omega(\theta) = Ap_l^m(\cos \theta) \quad (16)$$

Such that

$$P_l^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) \quad (17)$$

Where P_l is the l -th legendre polynomial:

$$P_l = \frac{1}{2^l l!} \left(\frac{d}{dx} \right)^l (x^2 - 1)^l \quad (18)$$

With normalization, etc., we get that

$$Y_l^m(\theta, \phi) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} \exp(im\phi) P_l^m(\cos \theta) \quad (19)$$

These are called "spherical harmonics". As well,

$$\langle Y_l^m | Y_{l'}^{m'} \rangle = \delta_{ll'} \delta_{mm'} \quad (20)$$

Summary

$V = V(r)$ (central potential) leads to

$$L^2 Y(\theta, \phi) = \hbar^2 l(l+1) Y(\theta, \phi) \quad (21)$$

$$L_z Y = \hbar m Y \quad (22)$$