* Lecture 15 * A. AIELLO-FAU
IK-1 SS2017

- Orbital angular momentum -

Consider again the operator

$$\hat{\underline{L}} = \hat{\underline{r}} \times \hat{\underline{p}}$$

$$= -i\hbar\, \underline{r} \times \vec{\nabla} \quad \text{in position representation.}$$

In spherical coordinates (r, θ, ϕ) with:

$$0 \leq r < \infty; \quad 0 \leq \theta \leq \pi; \quad 0 \leq \phi < 2\pi$$

we have:

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta$$

and
$$\vec{\nabla\psi} = \vec{e}_r \frac{\partial\psi}{\partial r} + \vec{e}_\theta \frac{1}{r}\frac{\partial\psi}{\partial\theta} + \vec{e}_\phi \frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}$$

$$\underline{r} = r\vec{e}_r$$

Then
$$\underline{r} \times \vec{\nabla\psi} = r(\vec{e}_r \times \vec{\nabla}\psi)$$

$$= \cancel{r}\frac{1}{\cancel{r}}\frac{\partial\psi}{\partial\theta}(\vec{e}_r \times \vec{e}_\theta) + \cancel{r}\frac{1}{\cancel{r}\sin\theta}\frac{\partial\psi}{\partial\phi}(\vec{e}_r \times \vec{e}_\phi)$$

where
$$\begin{cases} \vec{e}_r = \dfrac{\partial\vec{r}}{\partial r} = \vec{e}_1\sin\theta\cos\phi + \vec{e}_2\sin\theta\sin\phi + \vec{e}_3\cos\theta \\ \vec{e}_\theta = \dfrac{1}{r}\dfrac{\partial\vec{r}}{\partial\theta} = \vec{e}_1\cos\theta\cos\phi + \vec{e}_2\cos\theta\sin\phi - \vec{e}_3\sin\theta \\ \vec{e}_\phi = \dfrac{1}{r\sin\theta}\dfrac{\partial\vec{r}}{\partial\phi} = -\vec{e}_1\sin\phi + \vec{e}_2\cos\phi \end{cases}$$

Therefore

$$\vec{e}_r \times \vec{e}_\theta = (\vec{e}_1 \sin\theta\cos\phi + \vec{e}_2 \sin\theta\sin\phi + \vec{e}_3 \cos\theta) \times$$

$$\times (\vec{e}_1 \cos\theta\cos\phi + \vec{e}_2 \cos\theta\sin\phi - \vec{e}_3 \sin\theta)$$

$$= \cancel{\vec{e}_3 \sin\theta\cos\theta\sin\phi\cos\phi} + \vec{e}_2 \sin^2\theta\cos\phi +$$

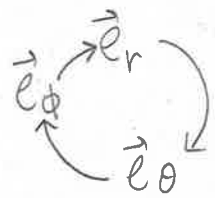
$$\cancel{- \vec{e}_3 \sin\theta\cos\theta\sin\phi\cos\phi} - \vec{e}_1 \sin^2\theta\sin\phi +$$

$$+ \vec{e}_2 \cos^2\theta\cos\phi - \vec{e}_1 \cos^2\theta\sin\phi$$

$$= \vec{e}_2 \cos\phi - \vec{e}_1 \sin\phi = \vec{e}_\phi$$

Similarly:

$$\vec{e}_r \times \vec{e}_\phi = -\vec{e}_\theta$$



← cyclic property

and

$$\vec{r} \times \vec{\nabla}\psi = \vec{e}_\phi \frac{\partial\psi}{\partial\theta} - \frac{1}{\sin\theta}\frac{\partial\psi}{\partial\phi}\vec{e}_\theta$$

So, there is no radial component as expected

Replacing back $\vec{e}_\phi$ and $\vec{e}_\theta$ we get:

$$\vec{r} \times \vec{\nabla}\psi = (-\vec{e}_1 \sin\phi + \vec{e}_2 \cos\phi)\frac{\partial\psi}{\partial\theta} - (\vec{e}_1 \cos\theta\cos\phi + \vec{e}_2 \cos\theta\sin\phi +$$

$$- \vec{e}_3 \sin\theta)\frac{1}{\sin\theta}\frac{\partial\psi}{\partial\phi}$$

$$= \vec{e}_1\left(-\sin\phi\frac{\partial\psi}{\partial\theta} - \frac{\cos\theta}{\sin\theta}\cos\phi\frac{\partial\psi}{\partial\phi}\right) + \vec{e}_2\left(\cos\phi\frac{\partial\psi}{\partial\theta} - \frac{\cos\theta}{\sin\theta}\sin\phi\frac{\partial\psi}{\partial\phi}\right)$$

$$+ \vec{e}_3\frac{\partial\psi}{\partial\phi}$$

Therefore:

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

and

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$$

$$= i\hbar\left\{\frac{\partial}{\partial\theta}\underbrace{(\sin\phi \mp i\cos\phi)}_{=\mp i(\cos\phi \pm i\sin\phi)} + \cot\theta\frac{\partial}{\partial\phi}(\cos\phi \pm i\sin\phi)\right\}$$

$$= i\hbar e^{\pm i\phi}\left(\mp i\frac{\partial}{\partial\theta} + \cot\theta\frac{\partial}{\partial\phi}\right)$$

$$= \hbar e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)$$

It should be noticed that

$$\frac{1}{\hbar^2}\hat{L}^2 = (\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2)/\hbar^2$$

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

$$= \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - r^2\nabla_r^2$$

expressed in spherical coordinates

- eigenfunctions of $\hat{L}_z$.

$$\hat{L}_z \psi = \lambda \psi \Leftrightarrow -i\hbar \frac{\partial \psi}{\partial \phi} = \lambda \psi \Rightarrow$$

$$\Rightarrow \psi(r,\theta,\phi) = f(r,\theta) \exp\left(i \frac{\lambda}{\hbar} \phi\right)$$

with $f(r,\theta)$ arbitrary:
The function $\psi(r,\theta,\phi)$ is single-valued only if it is periodic in ϕ. This implies that:

$$\frac{\lambda}{\hbar} = \text{integer}$$

We call $m = 0, \pm 1, \pm 2, \ldots$ such integer, so $\lambda = m\hbar$

and
$$\boxed{\psi(r,\theta,\phi) = f(r,\theta) \exp(im\phi)}$$

If we define
$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} \exp(im\phi)$$

Then
$$\int_0^{2\pi} \Phi_m^*(\phi) \Phi_{m'}(\phi)\, d\phi = \delta_{mm'}$$

Now we want to determine $f(r,\theta)$ for

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

Then

$$\hat{L}^2\psi(r,\theta,\phi) = -\hbar^2\left[\frac{1}{\sin^2\theta}(-m^2)f(r,\theta)\,e^{im\phi} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f(r,\theta)}{\partial\theta}\right)e^{im\phi}\right]$$

Since the variable r does not appear, we can write:

$$f(r,\theta) = R(r)\,\Theta(\theta)$$

and disregard $R(r)$ (it amounts to a simply multiplicative factor)

Then, the equation $\hat{L}^2\psi = \hbar^2 l(l+1)\psi$

becomes:

$$\boxed{\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\Theta(\theta) + l(l+1)\Theta = 0}$$

This equation is well-know. The solutions are the so-called ASSOCIATED LEGENDRE Polynomial $P_l^m(\cos\theta)$:

If we choose to normalize the function $\Theta(\theta)$ according to

$$\int_0^\pi |\Theta|^2 \sin\theta\, d\theta = 1$$

We obtain

$$\Theta_{\ell m}(\theta) = (-1)^m \sqrt{\frac{2\ell+1}{2}\,\frac{(\ell-m)!}{(\ell+m)!}}\; P_\ell^m(\cos\theta) \qquad \text{for } m \geq 0$$

Here we wrote $\Theta_{\ell m}(\theta)$ instead of $\Theta(\theta)$ to indicate the dependence from the labels ℓ and m

If $m < 0$ we use the properties of $P_\ell^m(\cos\theta)$

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(x)$$

to write

$$\Theta_{\ell m}(\theta)\Big|_{m<0} = \Theta_{\ell,-|m|}(\theta) = (-1)^m \Theta_{\ell |m|}$$

The functions

$$Y_{\ell m}(\theta, \phi) = \Theta_{\ell m}(\theta)\, \Phi_m(\phi)$$

$$= (-1)^m \sqrt{\frac{2\ell+1}{4\pi}\,\frac{(\ell-m)!}{(\ell+m)!}}\; P_\ell^m(\cos\theta)\, e^{im\phi}, \quad m \geq 0$$

are called SPHERICAL HARMONICS

It is easy to verify that:

$$Y_{\ell,-m}(\theta,\phi) = (-1)^m Y_{\ell m}^*(\theta,\phi)$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, Y^*_{\ell'm'}(\theta,\phi)\, Y_{\ell m}(\theta,\phi)\, d\theta = \delta_{\ell\ell'}\,\delta_{mm'}$$

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta',\phi')\, Y_{\ell m}(\theta,\phi) = \delta(\phi-\phi')\,\delta(\cos\theta-\cos\theta')$$

$$\sum_{m=-\ell}^{\ell} |Y_{\ell m}(\theta,\phi)|^2 = \frac{2\ell+1}{4\pi}$$

Where

$$\delta(\underline{r}-\underline{r}') = \frac{1}{r}\delta(r-r')\,\delta(\phi-\phi')\,\delta(\cos\theta-\cos\theta')$$

$$= \frac{1}{r\sin\theta}\delta(r-r')\,\delta(\phi-\phi')\,\delta(\theta-\theta')$$

-Some values-

$\ell=0$ $\quad Y_{00} = \frac{1}{4\pi}$

$$\ell=1 \quad \begin{cases} Y_{11} = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi} \\ Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta \end{cases}$$

$$\ell=2 \quad \begin{cases} Y_{22} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi} \\ Y_{21} = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi} \\ Y_{20} = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right) \end{cases}$$

It is also useful to notice that:

$$x \pm iy = r\sin\theta\cos\phi \pm i r\sin\theta\sin\phi$$

$$= r\sin\theta\, e^{\pm i\phi}$$

$$= \mp\sqrt{\frac{8\pi}{3}}\, Y_{1,\pm 1}(\theta,\phi)\cdot r$$

An arbitrary function $g(\theta,\phi)$ can be expanded in spherical harmonics.

$$g(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} A_{\ell m} Y_{\ell m}(\theta,\phi)$$

where

$$A_{\ell m} = \int \sin\theta\, d\theta\, d\phi\, Y^{*}_{\ell m}(\theta,\phi)\, g(\theta,\phi)$$