Lecture 39: 04/29/09

- Angular momentum states of central potentials
- Rigid Rotator
- Spin

Recap

→ Simultaneous sets of eigenfunctions of $\hat{L}^2, \hat{L}_x, \hat{L}_y, \hat{L}_z$:

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$
$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$
$$[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$

$\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$ are incompatible!

$\Rightarrow$ no complete set of simultaneous eigenfunctions

$\Rightarrow$ uncertainty principle

$\Rightarrow$ can only have definite L_x <u>or</u> L_y <u>or</u> L_z

$$[\hat{L}^2, \hat{L}_x] = 0$$
$$[\hat{L}^2, \hat{L}_y] = 0$$
$$[\hat{L}^2, \hat{L}_z] = 0$$

$\hat{L}^2$ is compatible with each component of $\hat{L}$

$\Rightarrow$ can find complete set of simultaneous eigenfunctions of <u>$\hat{L}^2$</u> <u>and</u> (for example) <u>$\hat{L}_z$</u>

$\Rightarrow$ can label all simultaneous eigenstates $F(\theta, \phi)$ by their eigenvalues L^2 and L_z

Recap

→ Spherical Harmonics

complete set of functions of θ, ϕ:

$$F(\theta,\phi) = Y_\ell^m(\theta,\phi) \propto \underbrace{P_\ell^m(\cos\theta)}_{\text{Legendre functions}} e^{im\phi}$$

→ are eigenfunctions of $\hat{L}^2$:

$$\hat{L}^2 Y_\ell^m(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_\ell^m(\theta,\phi)$$

with $\ell = 0, 1, 2, \dots$

quantized!

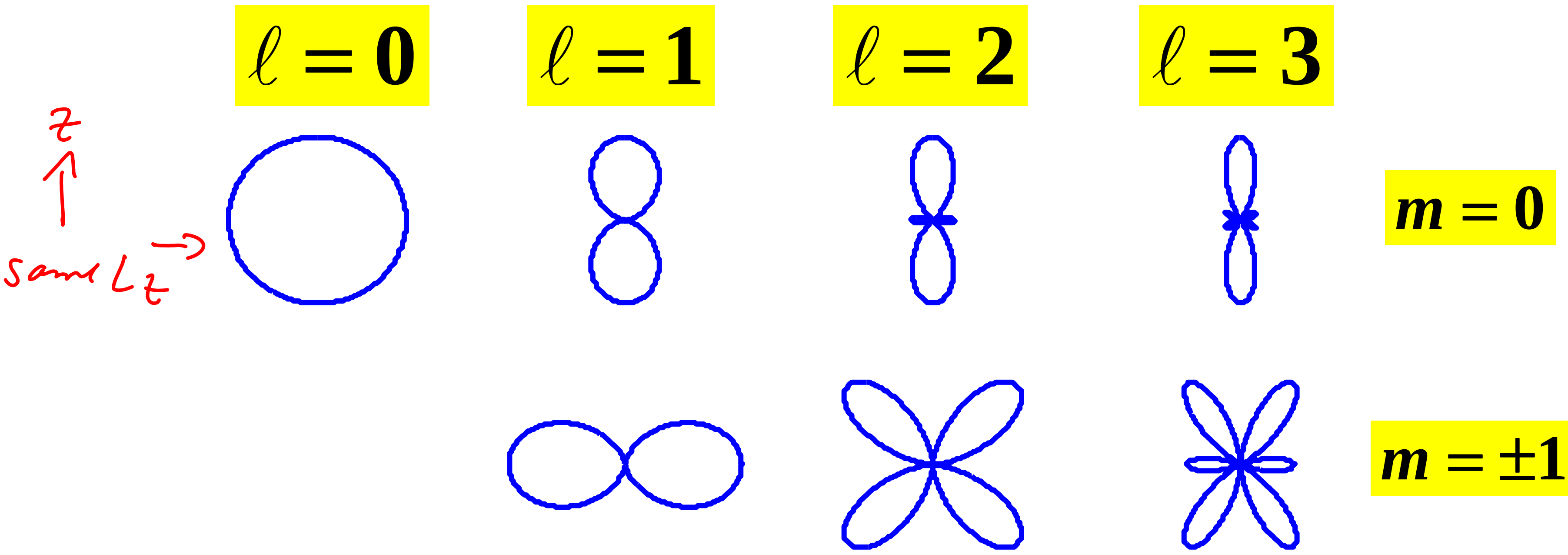
ℓ, m: quantum numbers

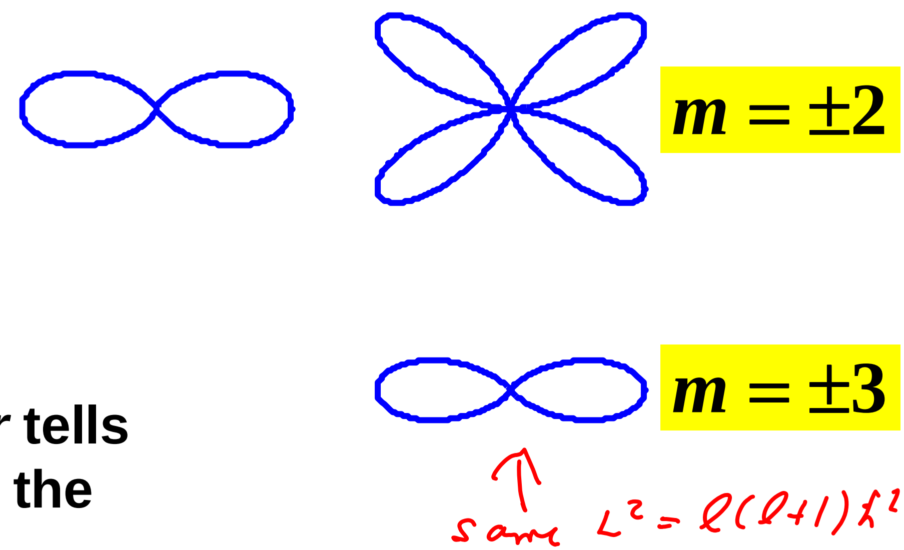
→ and are eigenfunctions of $\hat{L}_z$:

$$\hat{L}_z Y_\ell^m(\theta,\phi) = m\hbar\, Y_\ell^m(\theta,\phi)$$

with $m = -\ell, -\ell+1, \dots, \ell-1, \ell$

→ but: do not have determinate L_x and L_y values!

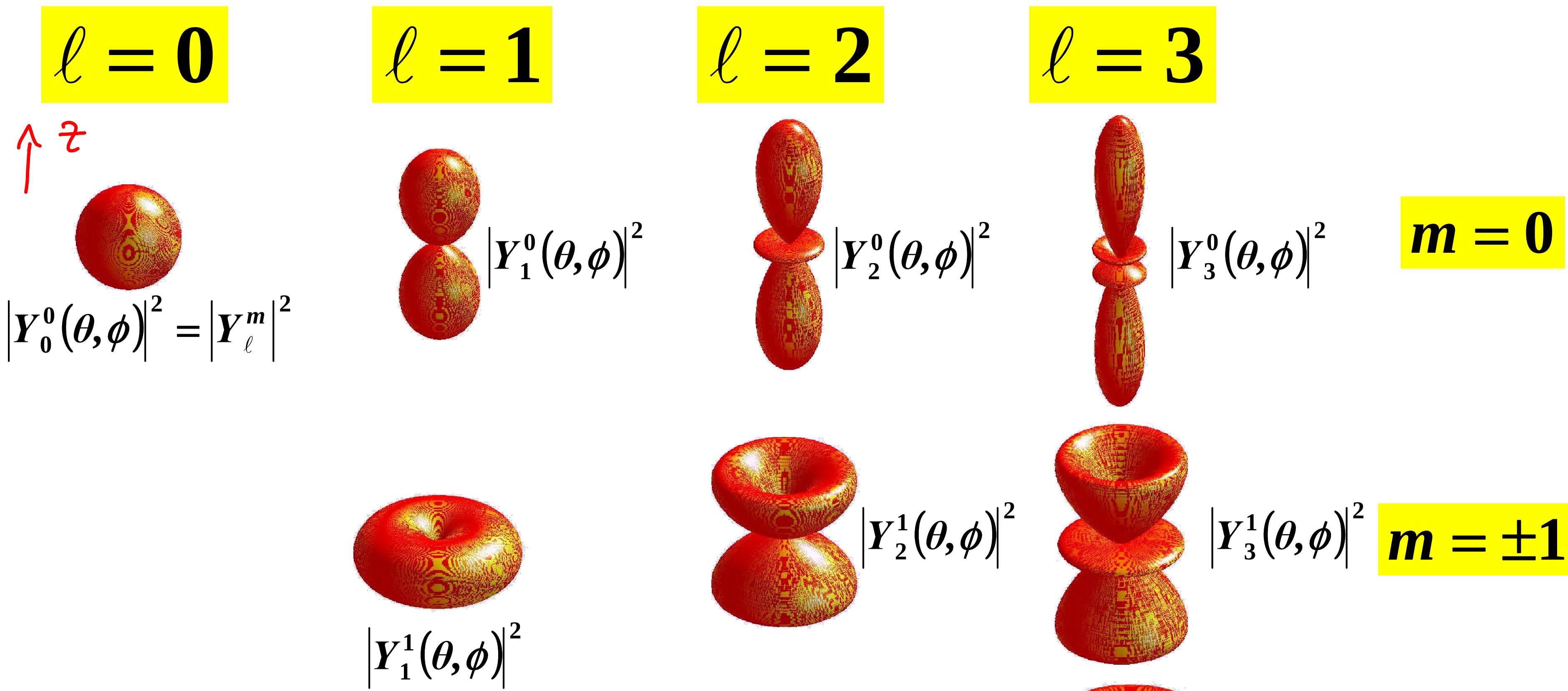


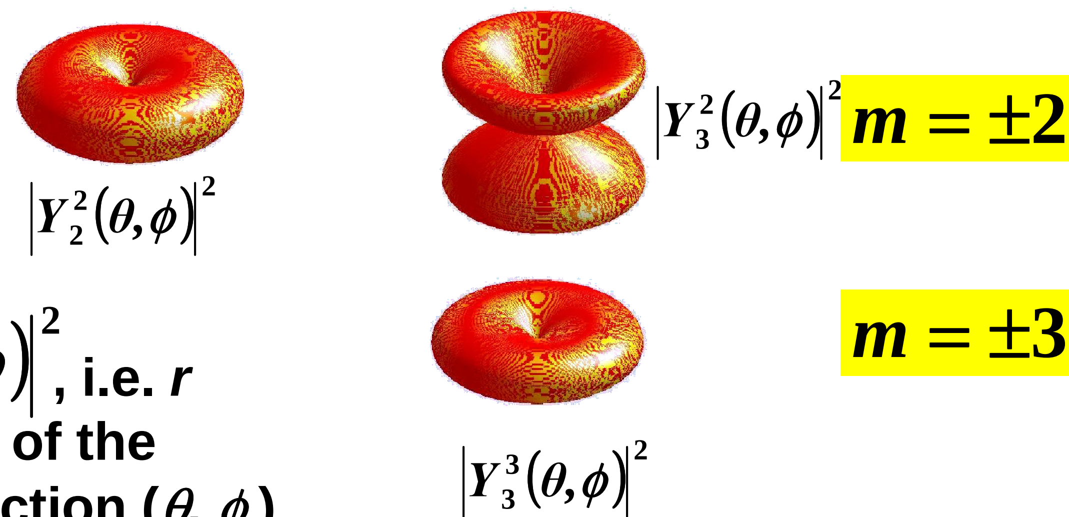


Legendre functions

$$P_\ell^m(\cos\theta)$$

Graphs show $r = P_\ell^m(\cos\theta)$ **, i.e.** r **tells you the magnitude of the function in the direction** θ





Spherical harmonics

$$|Y_\ell^m(\theta,\phi)|^2$$

3-D graphs show $r = |Y_\ell^m(\theta,\phi)|^2$**, i.e.** r **tells you the magnitude square of the spherical harmonics in the direction (**θ, ϕ**)**

- can get complete set Y_ℓ^m from subset $Y_\ell^{m=\ell}(\theta,\phi)$

$$Y_\ell^{m=\ell-j} \propto e^{i\phi}\left[\frac{\partial}{\partial\theta} - i\,\frac{\cos\theta}{\sin\theta}\,\frac{\partial}{\partial\phi}\right]^j Y_\ell^{m=\ell}(\theta,\phi)$$

<u>Note:</u> The set functions $\{Y_\ell^m\}$ is <u>complete</u> and orthonormal, i.e. one can expand <u>any</u> function of θ,ϕ in terms of these functions!

$\Rightarrow$ orthonormal:

$$\int_0^{2\pi}\int_0^{\pi}\left[Y_\ell^m(\theta,\phi)\right]^*\left[Y_{\ell'}^{m'}(\theta,\phi)\right]\sin\theta\, d\theta\, d\phi$$

$$= \delta_{\ell\ell'}\,\delta_{mm'}$$

- First few spherical harmonics $Y_\ell^m(\theta,\phi)$

	$\ell=0$	$\ell=1$	$\ell=2$
$m=0$	$Y_0^0=\left(\frac{1}{4\pi}\right)^{1/2}$ $\uparrow$ $\sin^0\theta$	$Y_1^0=\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$	$Y_2^0=\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$
$m=\pm1$		$Y_1^{\pm1}=\mp\left(\frac{3}{8\pi}\right)^{1/2}\underline{\sin\theta}\,e^{\pm i\phi}$ $\uparrow$ $\sin^1\theta$	$Y_2^{\pm1}=\mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta\,e^{\pm i\phi}$
$m=\pm2$			$Y_2^{\pm2}=\left(\frac{15}{32\pi}\right)^{1/2}\underline{\sin^2\theta}\,e^{\pm2i\phi}$ $\uparrow$ $\sin^2\theta$

recall $Y_\ell^{m=\pm\ell} \propto \sin^\ell\theta$

Comment 1: • Eigenvalues of $Y_\ell^m(\theta,\phi)$:

→ have eigenvalues of $\hat{L}^2$. $L^2 = \ell(\ell+1)\hbar^2 \geq 0$

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

⇒ quantized

⇒ can only measure these values!

→ eigenvalues of $\hat{L}_z$: $L_z = m\hbar$

Important: for a state of given $L^2 = \ell(\ell+1)\hbar^2$

⇒ L_z can have any value of $m\hbar$, such that $\langle L_z \rangle^2 \leq \langle \hat{L}^2 \rangle$

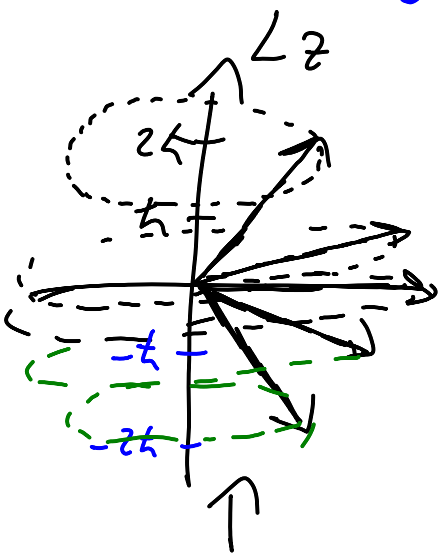
z component of a vector ≤ length of that vector!

⇒ $\hbar^2 m^2 \leq \hbar^2 \ell(\ell+1)$ ⇒ $|m| \leq \sqrt{\ell(\ell+1)}$

⇒ $m = -\ell, -\ell+1, \ldots, 0, \ldots \ell-1, \ell$

but <u>not</u> $|m| = \ell+1$, since $\ell+1 > \sqrt{\ell(\ell+1)}$!

Comment 2: • "vector model" of L (use with care!):



– "vector" length of L

$$L = \sqrt{\ell(\ell+1)}\,\hbar$$

$(= \sqrt{6}\,\hbar$ for $\ell = 2)$

– possible L_z-value

$$-\ell\hbar \le L_z \le \ell\hbar$$

$(L_z = -2\hbar, -\hbar, 0, \hbar, 2\hbar$ here$)$

states do <u>not</u> have a determinate L_x or L_y value ("smeared out vectors")

$\Rightarrow$ $\hat{L}^2$ and $\hat{L}_z$ have definite values for these states, but $\hat{L}_x$ and $\hat{L}_y$ are <u>not</u> definite!

$\Rightarrow$ complete lack of determination of the azimuthal angle ϕ $\Rightarrow$ $|Y_\ell^m(\theta,\phi)|^2$ does not depend on ϕ!

$\Rightarrow$ $\langle L_x \rangle = 0$ $\quad \langle L_y \rangle = 0$

Note: $\Rightarrow$ could write a state with definite L^2 and definite L_x (for example) as a linear superposition of states of definite L^2 and L_z (Y_ℓ^m)

$\rightarrow$ would need states of of given ℓ-value but several L_z / m-values.

Comment 3: • Degeneracy due to spherical symmetry:

for each ℓ-value: $(2\ell+1)$ states of different m-values

$\Rightarrow$ If the energy operator is spherically symmetric, all of the states with different m-values for a given ℓ-value have the same energy ("multiplet")

recall ~~rad~~ radial eq. ②

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2}+\left\{\frac{\ell(\ell+1)\hbar^2}{2\cdot mass\cdot r^2}+V(r)\right\}u=Eu(r)$$

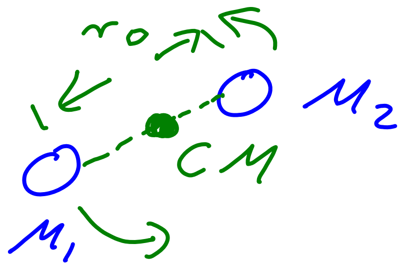
$\Rightarrow$ depends on ℓ, but not on m-quantum #

$\Rightarrow$ factor $(2\ell+1)$ degeneracy for each ℓ!

$\rightarrow$ H-atom has even more degeneracy due to $1/r$ Coulomb potential...

- **Side note: Rigid rotator:**

Example: diatomic molecule



→ assume rigid bound → bound length does not change

→ can rotate:

⇒ only energy from rotation about CoM:

→ energy operator: $\hat{E} = \frac{\hat{p}_t^2}{2\mu}$ ← transverse comp. of linear momentum

μ ← reduced mass $= \frac{m_1 m_2}{m_1 + m_2}$

$$= \frac{\hat{L}^2}{2\mu r_0^2}$$

→ more generally: for any rigid rotator with moment of inertia I: $\hat{E} = \frac{\hat{L}^2}{2I}$

have same eigenfunctions!

$\rightarrow$ already know state of definite $\hat{L}^2$: $Y_\ell^m(\theta, \phi)$

$\Rightarrow$ $L^2 = \ell(\ell+1)\hbar^2$ for these states

$\Rightarrow$ states of definite energy for rotation:

$$\hat{E} Y_\ell^m = \frac{\hat{L}^2}{2I} Y_\ell^m = \frac{\ell(\ell+1)\hbar^2}{2I} Y_\ell^m$$

$$\Rightarrow E = \frac{\ell(\ell+1)\hbar^2}{2I}$$

: energy eigenvalues

$\ell = 0, 1, \ldots$

quantized!

with degeneracy of $\underbrace{2\ell+1}$ for each given ℓ-number!

from allowed range of m-values for given ℓ

- Spin (intrinsic angular momentum):

→ recall Stern-Gerlach experiment: found two levels of definite z-components of the angular momentum for atomic cesium

→ This can not be orbital angular momentum!

of L_z states: $2\ell+1$

if $\ell = 0$ ⇒ 1 $(m=0)$

if $\ell = 1$ ⇒ 3 $(m=-1,0,+1)$

if $\ell = 2$ ⇒ 5 $(m=-2,-1,0,1,2)$

⇒ no way to have splitting into 2 beams!

⇒ Spin: Angular momentum intrinsic to fundamental particles like electrons, ...

→ <u>intrinsic</u>: • not associated with <u>any</u> orbital dynamics

• particle does not rotate about its "center of mass"