

Angular momentum wavefunctions

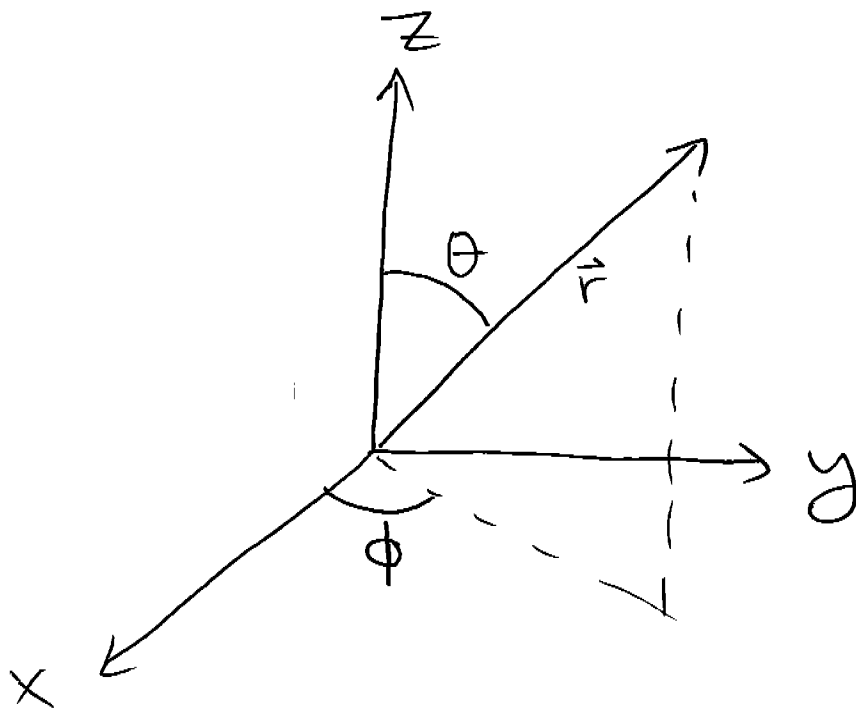
$$\vec{L} = \vec{r} \times \vec{p} = \frac{\hbar}{i} \vec{r} \times \vec{\nabla}$$

It is most convenient to work in spherical polar coordinates:

$$z = r \cos \theta$$

$$y = r \sin \theta \sin \phi$$

$$x = r \sin \theta \cos \phi$$



$$r = |\vec{r}|$$

Expressed in terms of $\theta + \phi$, $\angle 2$
the Cartesian components of \vec{L}
are:

$$L_x = i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right)$$

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

$$L_z = -i\hbar \frac{\partial}{\partial \phi} \quad (\text{c.f. Lecture 7})$$

By convention, the angular momentum
eigenfunctions in polar coordinates
are written

$$\psi_{lm} \equiv Y_{lm}(\theta, \phi).$$

The eigenvalue problem

$$L_z Y_{lm} = m\hbar Y_{lm}$$

can thus be expressed as

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- $$\frac{\hbar}{i} \frac{\partial}{\partial \phi} Y_{lm}(\theta, \phi) = m\hbar Y_{lm}(\theta, \phi)$$

$$\frac{\partial}{\partial \phi} Y_{lm} = im Y_{lm}$$

$$\Rightarrow Y_{lm}(\theta, \phi) = e^{im\phi} Y_{lm}(\theta, 0)$$

- Y_{lm} must be single-valued under $\phi \rightarrow \phi + 2\pi$ in order for the wavefunction to be continuous.

$$\Rightarrow e^{im2\pi} = 1, \quad m \in \mathbb{Z}.$$

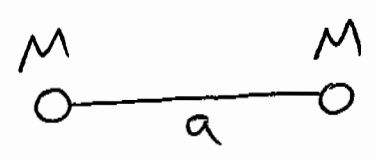
- This implies, in particular,

that $l \equiv m_{\max} \in \mathbb{Z}$. The

orbital angular momentum quantum # is a non-negative integer.

Example: The rigid rotor

Consider a diatomic molecule in the form of two identical atoms of mass M , separated by a rigid rod (bond) of length a .

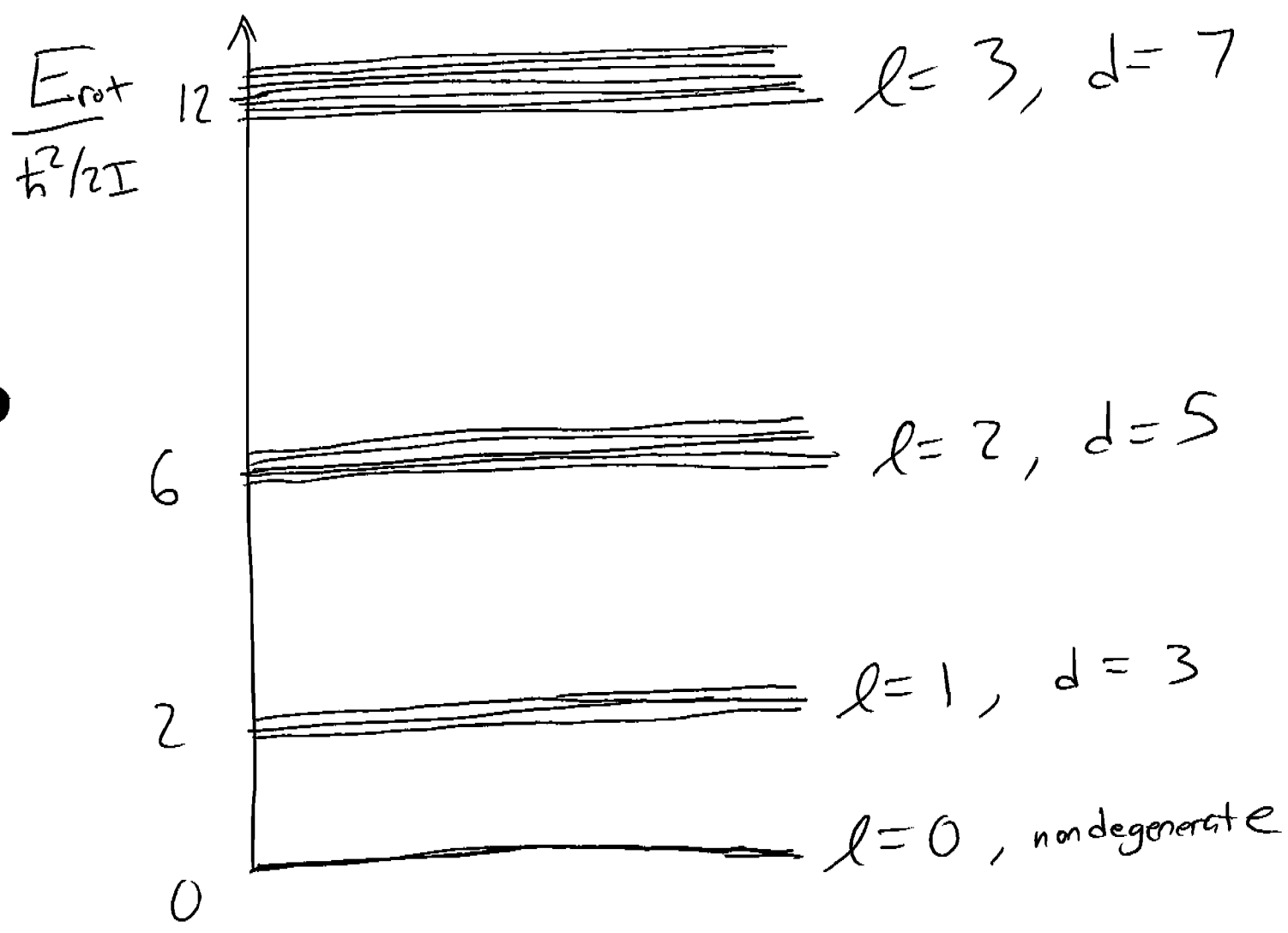


$$I_{cm} = \frac{Ma^2}{2} = I$$

$$\hat{H} = \hat{H}_{cm} + \hat{H}_{rot}, \quad \hat{H}_{rot} = \frac{\hat{L}^2}{2I}$$

$$E_{rot} = \frac{\hbar^2}{2I} l(l+1), \quad l=0, 1, 2, \dots$$

For each value of l , there are $2l+1$ degenerate energy levels $-l \leq m \leq l$:



Now, for the dependence on θ 6

$$L_+ Y_{\ell\ell}(\theta, \phi) = 0$$

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

$$\left(\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) Y_{\ell\ell}(\theta, \phi) = 0$$

$$Y_{\ell\ell}(\theta, \phi) = e^{i\ell\phi} P_{\ell}^{\ell}(\theta),$$

$$\text{where } P_{\ell}^{\ell}(\theta) \equiv Y_{\ell\ell}(\theta, 0)$$

$$\left(\frac{\partial}{\partial \theta} - \ell \cot \theta \right) P_{\ell}^{\ell}(\theta) = 0$$

$$\frac{d P_{\ell}^{\ell}(\theta)}{d\theta} = \ell \cot \theta P_{\ell}^{\ell}(\theta)$$

$$\frac{d P_{\ell}^{\ell}}{P_{\ell}^{\ell}} = \ell \frac{d \sin \theta}{\sin \theta}$$

$$\ln P_l^m = l \ln(\sin \theta) + C'$$

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$$P_l^m(\theta) = C (\sin \theta)^l$$

$$\Rightarrow Y_{lm}(\theta, \phi) = C \sin^l \theta e^{i l \phi}$$

Normalization

$$1 = \langle ll | ll \rangle = \int_0^{2\pi} d\phi \int_0^{\pi} \sin \theta d\theta |Y_{lm}(\theta, \phi)|^2$$

$$= 2\pi |C|^2 \int_0^{\pi} (\sin \theta)^{2l+1} d\theta$$

$$= 2\pi |C|^2 \frac{2^{2l+1} (l!)^2}{(2l+1)!}$$

$$\Rightarrow C = \frac{1}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}}$$

The remaining wavefunctions may be obtained from $Y_{lm}(\theta, \phi)$ using L_{\pm}

$$\bullet L_- = L_x - iL_y = \hbar e^{-i\varphi} \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \varphi} \right) \quad (18)$$

$$Y_{l, l-1}(\theta, \varphi) = \frac{L_- Y_{ll}(\theta, \varphi)}{\hbar \sqrt{l(l+1) - l(l-1)}} = \frac{L_-}{\hbar} \frac{Y_{ll}}{\sqrt{2l}}$$

⋮

$$\bullet Y_{lm} = \left(\frac{1}{\hbar} \right)^{l-m} \sqrt{\frac{(l+m)!}{(2l)! (l-m)!}} L_-^{l-m} Y_{ll}$$

$$Y_{lm}(\theta, \varphi) = \frac{(-1)^m}{2^l l!} \sqrt{\frac{2l+1}{4\pi}} \sqrt{\frac{(l+m)!}{(l-m)!}} P_l^m(\cos \theta) e^{im\varphi}$$

where $P_l^m(\eta)$ is an associated

Legendre function, defined

by $P_l^m(\eta) = (-1)^m \left(\frac{1}{1-\eta^2}\right)^{m/2} \left(\frac{d}{d\eta}\right)^{l-m} (\eta^2-1)^l$ 9

$$P_0^0 = 1$$

$$P_1^0 = 2\cos\theta$$

$$P_1^1 = \sin\theta$$

$$P_2^0 = 4(3\cos^2\theta - 1)$$

$$P_2^1 = 4\sin\theta \cos\theta$$

$$P_2^2 = \sin^2\theta$$

⋮

The first few angular momentum wavefunctions are :

- $Y_{00} = \frac{1}{2\sqrt{\pi}}$

$$Y_{10} = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cos \theta$$

$$Y_{1,\pm 1} = \mp \frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin \theta e^{\pm i\varphi}$$

$$Y_{20} = \frac{1}{4}\sqrt{\frac{5}{\pi}} (3 \cos^2 \theta - 1)$$

- $Y_{2,\pm 1} = \mp \frac{1}{2}\sqrt{\frac{15}{2\pi}} \sin \theta \cos \theta e^{\pm i\varphi}$

$$Y_{2,\pm 2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{\pm 2i\varphi}$$

⋮

- These are known as spherical harmonics.

The spherical harmonics can also be found by solving (1)

the P.D.E.:

$$\nabla^2 Y_{lm}(\theta, \phi) = -l(l+1) Y_{lm}(\theta, \phi)$$

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

$$\left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + l(l+1) \right] Y_{lm}(\theta, \phi) = 0$$

$$0 = \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) - \frac{m^2}{\sin^2\theta} + l(l+1) \right] P_l^m(\cos\theta)$$

$$\frac{d}{du} (1-u^2) \frac{dP_l^m(u)}{du} + \left[l(l+1) - \frac{m^2}{1-u^2} \right] P_l^m(u) = 0$$

Parity of the angular momentum eigenfunctions

$$\vec{L} = \vec{r} \times \vec{p} = \frac{\hbar}{i} (\vec{r} \times \nabla)$$

$$\hat{P} \vec{L} \psi = \frac{\hbar}{i} (-\vec{r} \times \frac{\partial}{\partial (-\vec{r})}) \hat{P} \psi$$

$$= \frac{\hbar}{i} (\vec{r} \times \nabla) \hat{P} \psi$$

$$= \vec{L} \hat{P} \psi$$

$$\Rightarrow [\hat{P}, \vec{L}] = 0$$

$$[\hat{P}, L_{\pm}] = 0, \quad [\hat{P}, L_z] = 0$$

$$[\hat{P}, \vec{L}^2] = 0.$$

These relations imply that the eigenfunctions of \vec{L}^2 are also eigenfunctions of \hat{P} = parity.

Moreover, since L_{\pm} commute

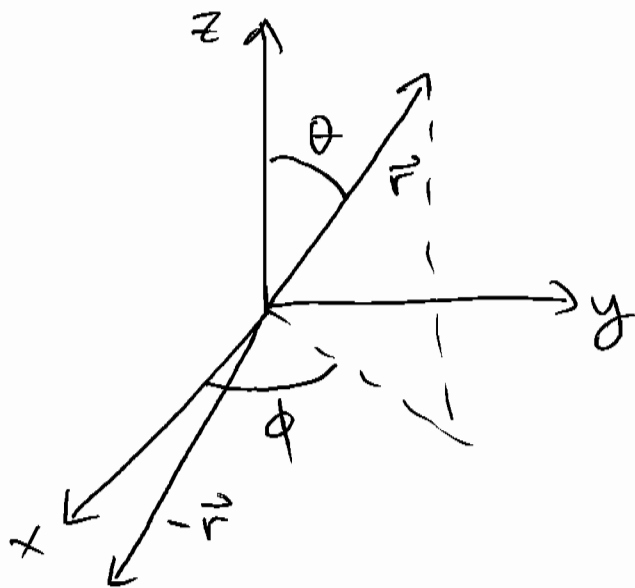
with \hat{P} , the eigenvalue of parity cannot depend on $m = L_z/\hbar$, but only on l , the total angular momentum quantum # \therefore

$$\hat{P} Y_{lm} = P(l) Y_{lm}$$

Now $\hat{P} \psi(\vec{r}) = \psi(-\vec{r})$.

In polar coordinates,

$$\hat{P} \psi(r, \theta, \phi) = \psi(r, \pi - \theta, \phi + \pi)$$



$$\hat{P} \circ \begin{matrix} r \rightarrow r \\ \theta \rightarrow \pi - \theta \\ \phi \rightarrow \phi + \pi \end{matrix}$$

$$\hat{P} Y_{\ell m}(\theta, \phi) = Y_{\ell m}(\pi - \theta, \phi + \pi) \quad \text{14}$$

We can thus determine $P(\ell)$ from

$$Y_{\ell \ell}(\theta, \phi) = C \sin^{\ell} \theta e^{i\ell\phi}$$

$$\sin(\pi - \theta) = \sin \theta, \quad e^{i\ell(\phi + \pi)} = (-1)^{\ell}$$

$$\Rightarrow \boxed{P(\ell) = (-1)^{\ell}}$$