

### 3D Rigid rotor

$$\left\{ \begin{array}{l} \frac{1}{\Phi} \sin \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Phi}{d\theta} \right) + \beta \sin^2 \theta = m_e^2 \\ \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m_e^2 \\ \Phi_{m_e} = A e^{im_e \phi}, \quad m_e = 0, \pm 1, \pm 2, \dots \quad (\text{but see below}) \end{array} \right.$$

$$\left. \begin{array}{l} \beta = l(l+1), \quad l = 0, 1, 2, \dots \\ m_l = -l, -l+1, \dots 0, \dots, l-1, l \end{array} \right] \text{quantization conditions}$$

$$\left. \begin{array}{l} l=0 \rightarrow m_l=0 \\ l=1 \rightarrow m_l=-1, 0, 1 \\ l=2 \rightarrow m_l=-2, -1, 0, 1, 2 \end{array} \right| \left. \begin{array}{c} s \\ p \\ d \end{array} \right\} \text{H atom}$$

$$Y(\theta, \phi) = Y_l^{m_e}(\theta, \phi) = \Theta_l^{m_e}(\theta) \Phi_{m_e}(\phi)$$

two boundary conditions  $\rightarrow$  two quantum #'s

$$\beta = \frac{2\mu r_0^2 E}{\hbar^2} = \frac{2I}{\hbar^2} E$$

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

$$\hat{H} Y_l^{m_e} = \frac{\hbar^2}{2I} l(l+1) Y_l^{m_e}$$

↑ degeneracy =  $2l+1$

$$\hat{l}^2 Y_l^{m_e} = \hbar^2 l(l+1) Y_l^{m_e}$$

$\hat{l}^2$ : "angular momentum" operator

$|\vec{l}| = \hbar \sqrt{l(l+1)}$

$\hat{l}^2$  and  $\hat{H}$  obviously commute

components of the angular momentum operator

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$$\hat{l}_x = \frac{\hbar}{i} \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) = \frac{\hbar}{i} \left( -\sin\phi \frac{\partial}{\partial \theta} - \cot\theta \cos\phi \frac{\partial}{\partial \phi} \right)$$

$$\hat{l}_y = \frac{\hbar}{i} \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) = \frac{\hbar}{i} \left( \cos\phi \frac{\partial}{\partial \theta} - \cot\theta \sin\phi \frac{\partial}{\partial \phi} \right)$$

$$\hat{l}_z = \frac{\hbar}{i} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

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

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

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

$$\hat{l}_z Y_e^{me} = m_e \hbar Y_e^{me}$$

Can simultaneously know the magnitude of the angular momentum, and one of its components

### Spherical harmonics

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

spherically symmetric  $\rightarrow S$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$\longrightarrow P_z$

$$Y_1^{\pm 1} = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$$

$\begin{cases} \sqrt{\frac{3}{4\pi}} \sin\theta \cos\phi \longrightarrow P_x \\ \sqrt{\frac{3}{4\pi}} \sin\theta \sin\phi \longrightarrow P_y \end{cases}$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$$

$\longrightarrow d_z^2$

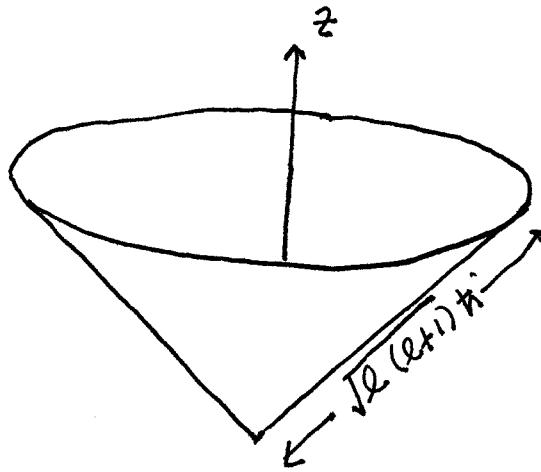
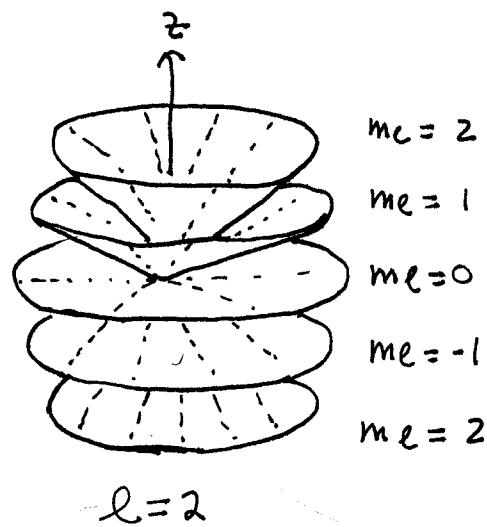
$$Y_2^{\pm 1} = \left(\frac{15}{8\pi}\right)^{1/2} \sin\theta \cos\theta e^{\pm i\phi}$$

$\begin{cases} \sqrt{\frac{15}{4\pi}} \sin\theta \cos\theta \cos\phi \longrightarrow d_{xz} \\ \sqrt{\frac{15}{4\pi}} \sin\theta \cos\theta \sin\phi \longrightarrow d_{yz} \end{cases}$

$$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$$

$\begin{cases} \sqrt{\frac{15}{16\pi}} \sin^2\theta \cos 2\phi \longrightarrow d_{x^2-y^2} \\ \sqrt{\frac{15}{16\pi}} \sin^2\theta \sin 2\phi \longrightarrow d_{xy} \end{cases}$

## Section 7.8



You might find the graphical representations in the supplementary material to be helpful.

Consider a sphere of radius  $\sqrt{l(l+1)}\hbar$

Further suppose  $l=2$ . Then the allowed solutions can be represented as five cones (actually, four cones and one disk).

You can immediately see from this picture that although the  $z$  component of the angular momentum is specified for each cone, the  $x$  and  $y$  components can take on any value.