Chapter 7, continued **3D Rigid Rotor**

$$\begin{cases} \dfrac{1}{\Theta}\sin\theta\dfrac{d}{d\theta}\left(\sin\theta\dfrac{d\Theta}{d\theta}\right)+\beta\sin^2\theta = m_\ell^2 \\ \dfrac{1}{\Phi}\dfrac{d^2\Phi}{d\phi^2} = -m_\ell^2 \end{cases}$$

$$\Phi_{m_\ell} = Ae^{im_\ell\phi}, \qquad m_\ell = 0, \pm 1, \pm 2, \ldots$$ (but see below)

$$\left.\begin{aligned} &\beta = \ell(\ell+1), \quad \ell = 0,1,2,\ldots \\ &m_\ell = -\ell, -\ell+1, \ldots 0, \ldots, \ell-1, \ell \end{aligned}\right\}$$ quantization conditions

$$\ell = 0 \quad \rightarrow \quad m_\ell = 0$$

$$\ell = 1 \quad \rightarrow \quad m_\ell = -1, 0, 1$$

$$\ell = 2 \quad \rightarrow \quad m_\ell = -2, -1, 0, 1, 2$$

$$\left.\begin{matrix} \text{s} \\ \text{p} \\ \text{d} \end{matrix}\right\} \text{H atom}$$

$$Y(\theta,\phi) = Y_\ell^{m_\ell}(\theta,\phi) = \Theta_\ell^{m_\ell}(\theta)\Phi_{m_\ell}(\phi)$$

two boundary conditions $\rightarrow$ two quantum #s

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

$$E = \frac{\hbar^2}{2I}\ell(\ell+1), \qquad \ell = 0,1,2,\ldots$$

$$\hat{H}Y_\ell^{m_\ell} = \frac{\hbar^2}{2I}\ell(\ell+1)Y_\ell^{m_\ell}$$

degeneracy = $2\ell+1$

$$\hat{\ell}^2 Y_\ell^{m_\ell} = \hbar^2\ell(\ell+1)Y_\ell^{m_\ell}$$

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

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

$$\left|\vec{\ell}\right| = \hbar\sqrt{\ell(\ell+1)}$$

components of the angular momentum operator

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

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

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

$$\left[\hat{\ell}_x, \hat{\ell}_y \right] = i\hbar\hat{\ell}_z$$

$$\left[\hat{\ell}_y, \hat{\ell}_z \right] = i\hbar\hat{\ell}_x$$

$$\left[\hat{\ell}_z, \hat{\ell}_x \right] = i\hbar\hat{\ell}_y$$

$$\hat{\ell}_z Y_\ell^{m\ell} = m_\ell \hbar Y_\ell^{m\ell}$$

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 $\longrightarrow$ s

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

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

$$\left\{\begin{array}{ll} \sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi & \longrightarrow p_x \\ \sqrt{\frac{3}{4\pi}}\sin\theta\sin\phi & \longrightarrow p_y \end{array}\right.$$

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

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

$$\left\{\begin{array}{ll} \sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\cos\phi & \longrightarrow d_{xz} \\ \sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\sin\phi & \longrightarrow d_{yz} \end{array}\right.$$

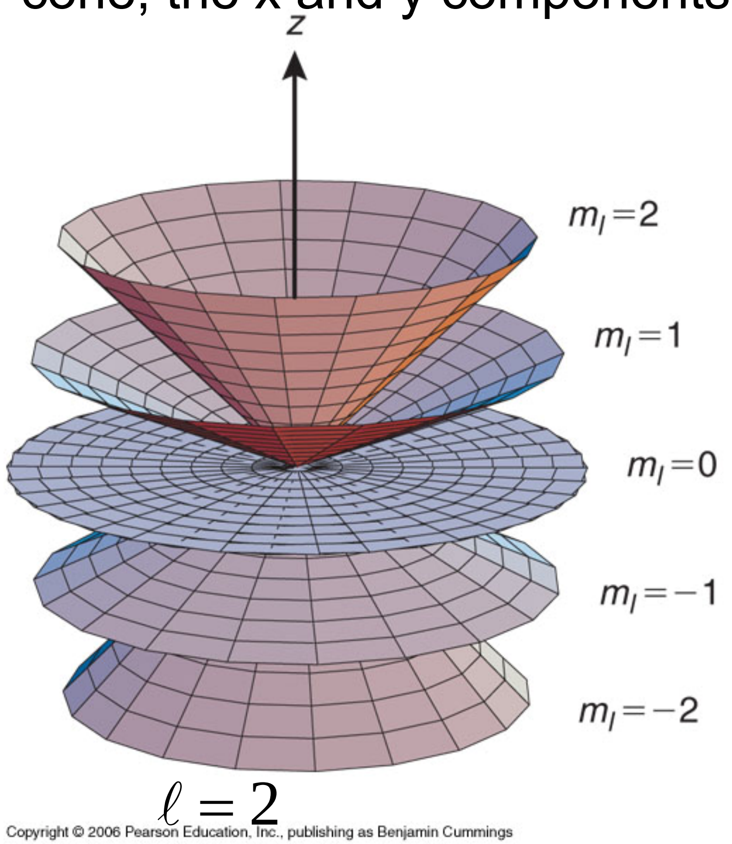
$$Y_2^{\pm 2} \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$$

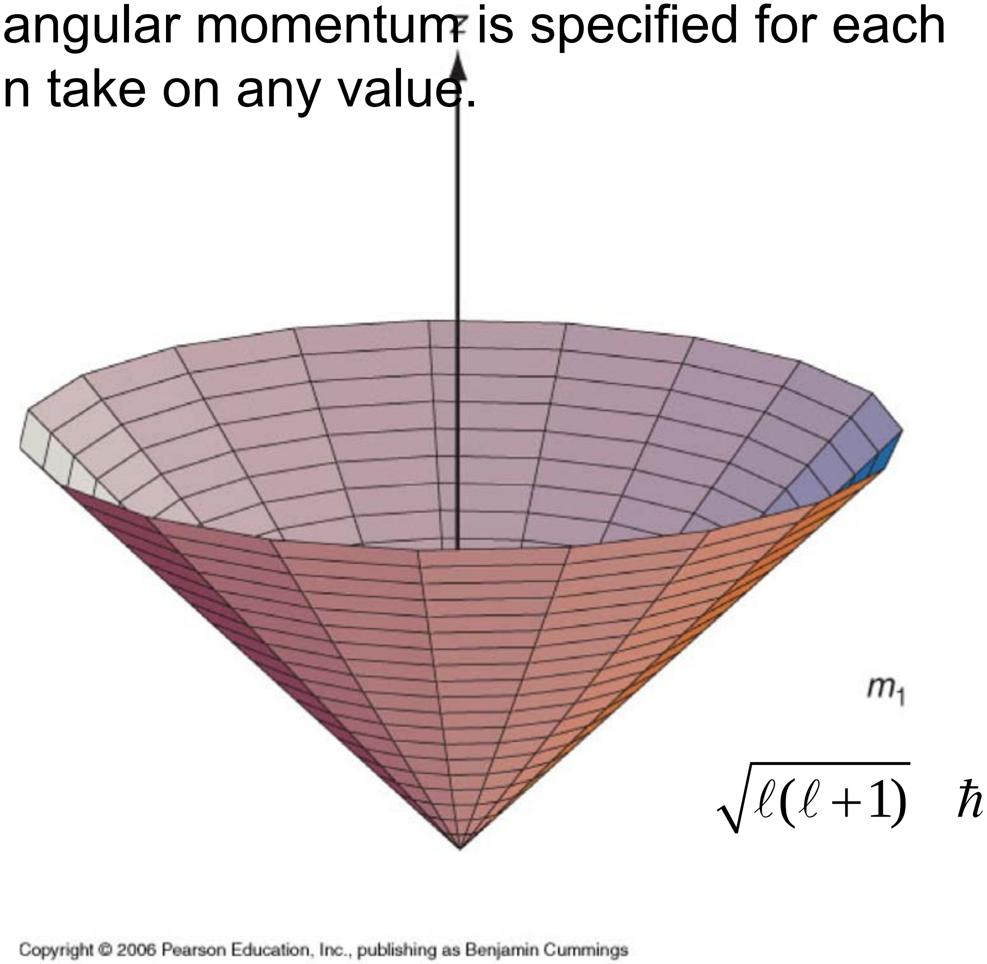
$$\left\{\begin{array}{ll} \sqrt{\frac{15}{16\pi}}\sin^2\theta\cos 2\phi & \longrightarrow d_{x^2-y^2} \\ \sqrt{\frac{15}{16\pi}}\sin^2\theta\sin 2\phi & \longrightarrow d_{xy} \end{array}\right.$$

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

For ℓ=2, the allowed solutions can be represented as 4 cones and 1 disk.

Although the z component of the angular momentum is specified for each cone, the x and y components can take on any value.





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