

# Angular Momentum

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

$$\vec{\nabla} = \hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}$$

$$\hat{\theta} = \cos \theta \cos \phi \hat{x} + \cos \theta \sin \phi \hat{y} - \sin \theta \hat{z}$$

$$\hat{\phi} = -\sin \phi \hat{x} + \cos \phi \hat{y}$$

$$\begin{aligned} \vec{L} &= \frac{\hbar}{i} \left[ \vec{r} \times \hat{r} \frac{\partial}{\partial r} + \vec{r} \times \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \vec{r} \times \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right] \\ &= \frac{\hbar}{i} \left[ \hat{\phi} \frac{\partial}{\partial \theta} - \hat{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right] \\ &= \frac{\hbar}{i} \left[ (-\sin \phi \hat{x} + \cos \phi \hat{y}) \frac{\partial}{\partial \theta} \right. \\ &\quad \left. - (\cos \theta \cos \phi \hat{x} + \cos \theta \sin \phi \hat{y} - \sin \theta \hat{z}) \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right] \end{aligned}$$

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

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

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

# Angular Momentum

$$\begin{aligned}
 L_{\pm} &= L_x \pm i L_y \\
 &= \frac{\hbar}{i} \left[ (-\sin \phi \pm i \cos \phi) \frac{\partial}{\partial \theta} - (\cos \phi \pm i \sin \phi) \cot \theta \frac{\partial}{\partial \phi} \right] \\
 &= \pm \hbar e^{\pm i\phi} \left[ \frac{\partial}{\partial \theta} \pm i \cot \theta \frac{\partial}{\partial \phi} \right]
 \end{aligned}$$

$$\begin{aligned}
 L_+ L_- &= \hbar^2 e^{i\phi} \left[ \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right] (-e^{-i\phi}) \left[ \frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right] \\
 &= -\hbar^2 e^{i\phi} \left[ e^{-i\phi} \left( \frac{\partial^2}{\partial \theta^2} - i \frac{-1}{\sin^2 \theta} \frac{\partial}{\partial \phi} - i \cot \theta \frac{\partial^2}{\partial \theta \partial \phi} \right) \right. \\
 &\quad \left. i \cot \theta (-i) e^{-i\phi} \left( \frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right) \right. \\
 &\quad \left. i \cot \theta e^{-i\phi} \left( \frac{\partial^2}{\partial \theta \partial \phi} - i \cot \theta \frac{\partial^2}{\partial \phi^2} \right) \right] \\
 &= -\hbar^2 \left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \cot^2 \theta \frac{\partial^2}{\partial \phi^2} + i \frac{\partial}{\partial \phi} \right]
 \end{aligned}$$

$$\begin{aligned}
 L^2 &= L_+ L_- - i[L_y, L_x] + L_z^2 = L_+ L_- + L_z^2 - \hbar L_z \\
 &= -\hbar^2 \left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \cot^2 \theta \frac{\partial^2}{\partial \phi^2} + i \frac{\partial}{\partial \phi} + \frac{\partial^2}{\partial \phi^2} + \frac{1}{i} \frac{\partial}{\partial \phi} \right] \\
 &= -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]
 \end{aligned}$$

# Angular Momentum

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

eigenfunctions  $Y_\ell^m(\theta, \phi)$

no  $Y_\ell^m$  for half-integer  $\ell$

$$\left[ \frac{1}{2\mu r^2} \left( -\hbar^2 \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) + L^2 \right) + V(r) \right] \psi = E \psi$$

$$K_{rad} = \frac{p^2}{2\mu}, \quad K_{rot} = \frac{I^2}{2I}, \quad I = \mu r^2$$

# Diatomic Molecule

$$m_1 r_1 = m_2 r_2$$

$$(m_1 + m_2) r_1 = m_2 (r_1 + r_2), \quad (m_1 + m_2) r_2 = m_1 (r_1 + r_2)$$

$$\begin{aligned} I &= m_1 r_1^2 + m_2 r_2^2 = m_1 \frac{m_2^2 (r_1 + r_2)^2}{(m_1 + m_2)^2} + m_2 \frac{m_1^2 (r_1 + r_2)^2}{(m_1 + m_2)^2} \\ &= \frac{m_1 m_2 (r_1 + r_2)^2}{m_1 + m_2} = \mu r^2 \end{aligned}$$

$$H\psi = \frac{L^2}{2I} \psi = E\psi$$

$$\psi = Y_\ell^m(\theta, \phi)$$

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

# O<sub>2</sub> Diatomic Molecule

$$\begin{aligned} E_{rot} &= \frac{\hbar^2 2}{M_O r^2} = \frac{2\hbar^2 c^2}{16M_p c^2 r^2} \approx \frac{(6.58 \times 10^{-16} \text{ eVs})^2 (3 \times 10^8 \text{ m/s})^2}{8 \times 938 \times 10^6 \text{ eV} (10^{-10} \text{ m})^2} \\ &\approx \frac{40 \times 10^{-16} \text{ eV}^2}{8 \times 10^8 \text{ eV} 10^{-20}} \\ &\approx 5 \times 10^{-3} \text{ eV} \end{aligned}$$

$$f_{vib} = 5 \times 10^{13} \text{ Hz}$$

$$\begin{aligned} E_{vib} &= hf_{vib} = 2\pi 6.58 \times 10^{-16} \text{ eVs} \times 5 \times 10^{13} \text{ 1/s} \\ &= 0.2 \text{ eV} \end{aligned}$$

$$E_{vib} \gg E_{rot}$$

# Diatomic Molecule

