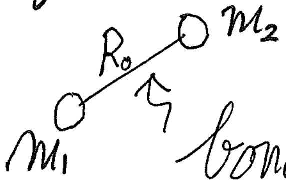
## L. Buy one get (at least) one free: 3D Rigid Rotor

Context: diatomic molecule




bond $\approx$ rigid rod
(i.e. ignore vibrations)

**Simple thought**

- One end fixed at origin + another end moves freely (on surface of sphere)
- freely $\Rightarrow$ $V=0$

**Careful thought**

- Center of Mass Motion [not our business] + relative motion
- one end fixed at origin + another end (mass $\mu$) moves freely

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

Either way $\Rightarrow$ Same problem

- $R_0$ fixed $\Rightarrow$ Only $\theta$ and $\phi$ angles

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 + \cancel{V}^{\to 0} \text{ freely moving}$$

TISE: $$-\frac{\hbar^2}{2\mu}\left[\frac{1}{R_0^2 \sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{R_0^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(\theta,\phi) = E\,\psi(\theta,\phi)$$

$$\Rightarrow \left[\frac{1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(\theta,\phi) = \frac{-2\mu R_0^2 E}{\hbar^2}\psi(\theta,\phi) \qquad (24)$$

3D Rigid Rotor [Schrödinger called it rotator] problem

<u>Solutions</u>? No need to do anything!

$$\because \left[\frac{1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] Y_{\ell m_\ell}(\theta,\phi) = -\ell(\ell+1)\,Y_{\ell m_\ell}(\theta,\phi)$$

(Same equation)

$\therefore$ Eigenstates are $Y_{\ell m_\ell}(\theta, \phi)$ with energy eigenvalues $\frac{2\mu R_0^2 E}{\hbar^2} = \ell(\ell+1)$

$$\Rightarrow \boxed{E_\ell^{(rotor)} = \frac{\ell(\ell+1)\hbar^2}{2\mu R_0^2}}$$

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

Given $\ell$, $(2\ell+1)$ values of $m_\ell$

We need these <u>rotational levels</u> next term.

<u>Short Cut</u>

- Classical Physics $E^{rotation} = \frac{L^2}{2I} = \frac{L^2}{2\mu R_0^2}$  $I$ = Moment of Inertia $= \mu R_0^2$
- QM $L^2 \to \ell(\ell+1)\hbar^2$

Done!

## Summary

- $U(r) \Rightarrow$ Eigenstates $\psi_{n\ell m_\ell}(r,\theta,\phi) = R_{n\ell}(r) \cdot Y_{\ell m_\ell}(\theta,\phi)$
  Eigenvalues $E_{n\ell}$ [degeneracy $(2\ell+1)$ at least]
- Series Solutions + Well-behaved $\psi$
- $\ell = 0, 1, 2, \cdots$ ; Given $\ell$: $m = -\ell, -\ell+1, \cdots, 0, \cdots, \ell-1, \ell$
- $\hat{L}^2 Y_{\ell m_\ell} = \ell(\ell+1)\hbar^2 Y_{\ell m_\ell}$ ; $\hat{L}_z Y_{\ell m_\ell} = m_\ell \hbar Y_{\ell m_\ell}$
- $\hat{L}^2, \hat{L}_x, \hat{L}_y, \hat{L}_z$ commutators $\Rightarrow$ can find simultaneous eigenstates of $\hat{L}^2$ and $\hat{L}_z$ (one component)
- $\vec{L}$ can't point at any specific direction
- Vector model is a way to depict the QM results
- 3D rigid rotor model is useful for rotational motion of molecules