Note Title 04-11-2016

Quick recap

$$\Phi(\phi) = \cancel{\frac{1}{\sqrt{2\pi}}}\, a_{m_l} e^{i m_l \phi}$$

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{i m_l \phi} \quad ; \quad m_l = 0, \pm 1, \pm 2, \ldots$$

$$\underbrace{Y_{l,m_l}(\theta,\phi)}_{\text{spherical harmonics}} = \Theta(\theta)\, \Phi(\phi)$$

$$\hat{L}^2 Y_{l,m_l}(\theta,\phi) = \hbar^2 l(l+1) Y_{l m_l}(\theta,\phi)$$

$$\hat{L}_z Y_{l,m_l}(\theta,\phi) = m_l \hbar\, Y_{l,m_l}(\theta,\phi)$$

$$\int_0^{2\pi} \Phi^*_{m_l'}(\phi)\, \Phi_{m_l}(\phi)\, d\phi = \delta_{m_l' m_l}$$

$$\delta_{m_l' m_l} = 1 \quad \text{if } m_l' = m_l$$

(normalization cond.)

$$= 0 \quad \text{if } m_l' \neq m_l$$

(orthogonality)

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\; Y^*_{l',m_l'}(\theta,\phi)\, Y_{l,m_l}(\theta,\phi)$$

$$= \delta_{l' l}\, \delta_{m_l' m_l}$$

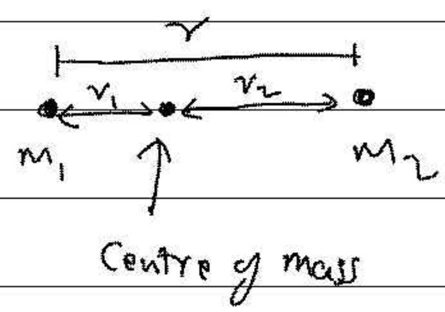
$$\delta_{l'l}\,\delta_{m_l' m_l} = 1 \quad \text{if } l' = l \text{ and } m_l' = m_l$$

$$= 0 \quad \text{if } l' \neq l \text{ or } m_l' \neq m_l$$

$$\int_0^a \int_0^b \int_0^c \Psi^* \Psi \underbrace{dx\,dy\,dz}_{d\tau \,\equiv\, dV}$$

$$dV = r^2\,dr\,\sin\theta\,d\theta\,d\phi = d\tau$$

Rotational Motion



$$m_1 r_1 = m_2 r_2$$

$$r = r_1 + r_2$$

$$I = m_1 r_1^2 + m_2 r_2^2$$

$$= \mu r^2$$

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

$$E_J = \frac{\hbar^2}{2I} J(J+1) \quad \cdots \quad (1)$$

$J \Rightarrow$ rotational quantum number

$= 0, 1, 2, 3 \cdots$

$$\Delta E_J = E_{J+1} - E_J$$

$$= \frac{\hbar^2}{2I}(J+1)(J+2) - \frac{\hbar^2}{2I} J(J+1)$$

$$\Delta E_J = \frac{\hbar^2}{2I} 2(J+1) \quad \ldots\ldots (2)$$

$$\Delta E_J = \frac{\hbar^2}{I}(J+1) \quad \ldots\ldots (3)$$

$$\Delta E = \frac{h^2}{4\pi^2 I}(J+1)$$

$$= 2 \cdot \frac{h^2}{8\pi^2 I}(J+1)$$

$$\cancel{\Delta E = 2B(J+1) \quad \ldots\ldots (4)}$$

$$\cancel{B = h}$$

$$\Delta E = h\nu = 2 \cdot \frac{h^2}{8\pi^2 I}(J+1)$$

$$\nu = 2\frac{h}{8\pi^2 I}(J+1)$$

$$\nu = 2B(J+1) \quad \ldots\ldots (4)$$

rotational constant $\longrightarrow$ $B = \dfrac{h}{8\pi^2 I}$ (Hz)

$$\Delta E = hc\tilde{\nu} = 2\frac{h^2}{8\pi^2 I}(J+1)$$

$$\tilde{\nu} = 2\frac{h}{8\pi^2 I c}(J+1)$$

$$\tilde{\nu} = 2\tilde{B}(J+1)$$

with $\tilde{B} = \dfrac{h}{8\pi^2 I c}$ (wavenumber)

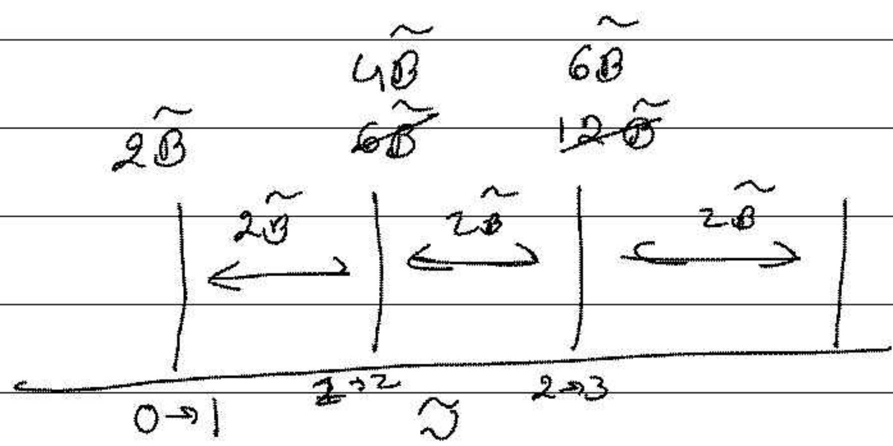
$$I = \mu r^2$$

$\frac{12\hbar^2}{2I} = 12\frac{h^2}{8\pi^2 I} = 12\tilde{B}hc$

$J=2$ — $\frac{6\hbar^2}{2I} = 6\tilde{B}hc$

$J=1$ — $\frac{2\hbar^2}{2I} = 2\frac{h^2}{8\pi^2 I} = 2\tilde{B}hc$

$J=0$ — $0 = 0$



rotational lines for a rigid rotor are always equally spaced.

Hydrogen atom

$$\Psi(r, \theta, \phi)$$

$\uparrow$ radial dependence

$$\hat{H} = \hat{H}_{cm} + \hat{H}_{u} \qquad (\text{K.E.})$$

$$= \frac{\hat{p}_M^2}{2M} + \frac{\hat{p}_u^2}{2u}$$

$$\frac{p_M^2}{2M} \Psi_{CM} = E_M \Psi_{CM}$$

$$\underbrace{\frac{\hat{p}_u^2}{2u} \Psi_u = E_u \Psi_u}_{} \rightarrow \underline{\underline{\text{H-atom}}}$$

internal or relative motion

that we discuss!

Hydrogen-like (Hydrogenic) atom

$$\hat{H}\,\Psi(r, \theta, \phi) = E\,\Psi(r, \theta, \phi) \quad \cdots (1)$$

$$\hat{H} = -\frac{\hbar^2}{2u} \nabla_e^2 + -\frac{\hbar^2}{2m_N} \nabla_N^2 + V(r)$$

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla_e^2 + V(r)$$

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$\underbrace{\left[-\frac{\hbar^2}{2\mu}\nabla_e^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}\right]}_{\hat{H}}\Psi(r,\theta,\phi) = E\,\Psi(r,\theta,\phi)$$

$$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi)$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$