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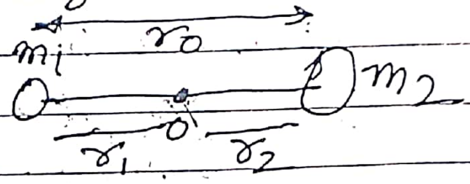
Rigid Rotatar

The rigid rotator is a system of two particle situated at a fixed distance from one another capable of rotating about an axis passing through the centre of mass.



* Kinetic energy of rigid rotator

$$T = \frac{1}{2} I\left[\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right]$$

Where $I = m_1 r_1^2 + m_2 r_2^2$ = moment of Inertia of the system about fixed axis.

$\frac{1}{2} I\omega^2$ $\dot{\theta}$

Q. 6/ SCHRÖDINGER EQUATION FOR RIGID ROTATOR

The Schrödinger equation in spherical polar co-ordinate (r, θ, ϕ) is given by

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial\psi}{\partial r}\right] + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta \frac{\partial\psi}{\partial\theta}\right] + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{2m}{\hbar^2}[E-V]\psi = 0 \quad (A)$$

For rigid rotator, the mass m is replaced by moment of ~~inter~~ inertia $I = m_1 r_1^2 + m_2 r_2^2$ and potential energy $V = 0$. The distance $r = 1$, the wave equation

$$\frac{1}{\cancel{r^2}\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial\psi}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{2I}{\hbar^2}E\psi = 0 \quad (B)$$

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Eigen function :-

Let $\psi(\theta,\phi) = Y(\theta)\,Z(\phi)$

$$\frac{\partial\psi}{\partial\theta} = Z\cdot\frac{\partial Y}{\partial\theta}, \quad \frac{\partial\psi}{\partial\phi} = Y\cdot\frac{\partial Z}{\partial\phi}$$

$$\&\ \frac{\partial^2\psi}{\partial\theta^2} = Z\frac{\partial^2 Y}{\partial\theta^2} \ \&\ \frac{\partial^2\psi}{\partial\phi^2} = Y\cdot\frac{\partial^2 Z}{\partial\phi^2}$$

— (C)

From equ^n B:

$$\frac{Z}{\sin\theta}\cdot\frac{d}{d\theta}\left[\sin\theta\cdot\frac{dY}{d\theta}\right] + \frac{Y}{\sin^2\theta}\cdot\frac{d^2 Z}{d\phi^2} + \frac{2I}{\hbar^2}EYZ = 0$$

Multiplying by $\frac{\sin^2\theta}{YZ}$ and putting $B = \frac{2I}{\hbar^2}E$

$$\frac{\sin\theta}{Y}\cdot\frac{d}{d\theta}\left[\sin\theta\cdot\frac{dY}{d\theta}\right] + \frac{1}{Z}\frac{d^2 Z}{d\phi^2} + B\sin^2\theta = 0$$

$$\text{or, } \frac{\sin\theta}{Y}\cdot\frac{d}{d\theta}\left[\sin\theta\frac{dY}{d\theta}\right] + B\sin^2\theta = -\frac{1}{Z}\frac{d^2 Z}{d\phi^2}$$

— (D)

Let $-\frac{1}{Z}\frac{d^2 Z}{d\phi^2} = m^2$

$$\text{or, } \frac{d^2 Z}{d\phi^2} + m^2 Z = 0 \quad \text{— (E)}$$

The solution of equ^n (E) is given by

$$Z = \frac{1}{\sqrt{2\pi}}e^{im\phi} \quad \text{— (F)}$$

where $m = 0, \pm1, \pm2 \ldots$

Multiplying equ^n D by $Y/\sin^2\theta$ we get

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left[\sin\theta\frac{dY}{d\theta}\right] + \left(B - \frac{m^2}{\sin^2\theta}\right)Y = 0 \quad \text{— (G)}$$

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Using method of substitution: $\cos\theta = x$

or, $-\sin\theta\, d\theta = dx$ and $\beta = l(l+1)$

or, $\dfrac{dx}{d\theta} = -\sin\theta$

$\therefore \dfrac{dY}{d\theta} = \dfrac{dY}{dx}\cdot\dfrac{dx}{d\theta} = -\sin\theta\cdot\dfrac{dY}{dx}$

$\Rightarrow \dfrac{d}{d\theta} = -\sin\theta\cdot\dfrac{d}{dx}$ [operator].

and $\sin\theta\cdot\dfrac{dY}{d\theta} = -\sin^2\theta\cdot\dfrac{dY}{dx} = -(1-x^2)\dfrac{dY}{dx}$

The sol^n of equ^n(G) in this form.

$$\frac{d}{dx}\left[(1-x^2)\frac{dY}{dx}\right] + \left(\beta - \frac{m^2}{1-x^2}\right)Y = 0 \quad \text{—— } (A_1)$$

This equ^n known as Legendre equ^n.

$$(1-x^2)\frac{d^2Y}{dx^2} - 2x\frac{dY}{dx} + \left[l(l+1) - \frac{m^2}{(1-x^2)}\right]Y = 0 \text{ — } A_2$$

This is an associated Legendre's equation which solution is $P_l^m x$ where:

$$P_l^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x), \text{ ——— } A_3$$

The General Solution of equ^n(G) is given by.

$$Y_l^m(\theta) = \beta P_l^m(\cos\theta) \text{ ——————— } (H)$$

Where $P_l^m\cos\theta = (1-\cos^2\theta)^{m/2}\dfrac{d^m}{dx^m}P_l(\cos\theta)$ $|m| \leq l$

& β = Normalisation constant given by,

$$\beta = \left\{\frac{2l+1}{2}\cdot\frac{(l-|m|)}{(l+|m|)}\right\}^{1/2},$$

$$\therefore Y_l^m(\theta) = \left\{\frac{2l+1}{2}\cdot\frac{(l-|m|)}{(l+|m|)}\right\}^{1/2} P_l^m\cos\theta \text{ —— } I$$

The total Eigen function can be expressed as classmate Date 27

Using method of substitution:- $\cos\theta = x$ (19)

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or, $\frac{dx}{d\theta} = -\sin\theta$

$$\therefore \frac{dY}{d\theta} = \frac{dY}{dx}\cdot\frac{dx}{d\theta} = -\sin\theta\cdot\frac{dY}{dx}$$

$$\Rightarrow \frac{d}{d\theta} = -\sin\theta\cdot\frac{d}{dx} \quad [\text{operator}]$$

and $\sin\theta\cdot\frac{dY}{d\theta} = -\sin^2\theta\cdot\frac{dY}{dx} = -(1-x^2)\frac{dY}{dx}$

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$$\therefore Y_l^m(\theta) = \left[\frac{2l+1}{2}\frac{(l-|m|)}{(l+|m|)}\right]^{1/2} P_l^m\cos\theta \quad \text{—— I}$$

The total Eigen function can be expressed as

$$\Psi_{lm}(\theta,\phi) = \left\{\frac{2l+1}{2}\,\frac{(l-|m|)!}{(l+|m|)!}\right\}^{1/2} P_l^m \cos\theta \, \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad \text{—— (J)}$$

Energy Eigen Value :- The eigen value of wave function Ψ_{lm} is given by

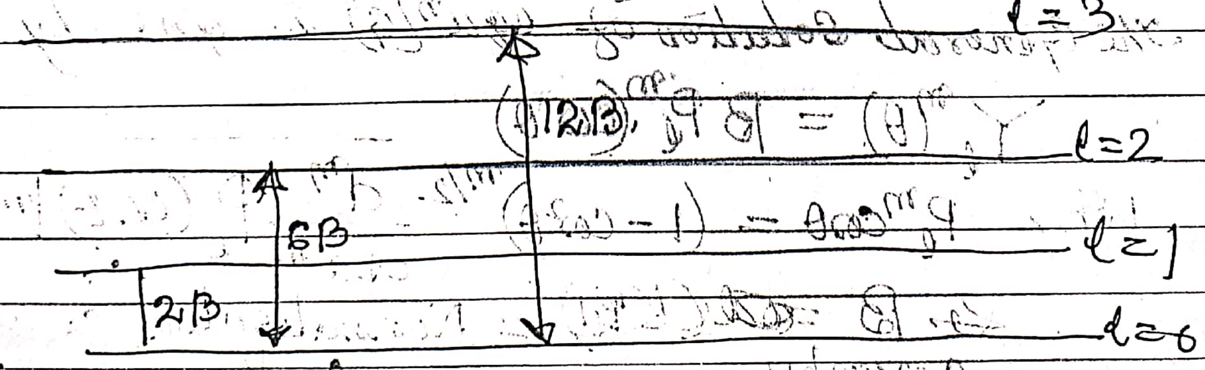
$$\beta = l(l+1)$$

$$\frac{2IE_l}{\hbar^2} = l(l+1)$$

$$\text{or,}\quad E_l = l(l+1)\frac{\hbar^2}{2I} \quad \text{—— (K)}$$

Thus we conclude the the S.E for the rigid rotator can have physically acceptable solⁿ only for certain discrete value of energy called energy eigen value (E_l)

When $l=0$, $E_0 = 0$
When $l=1$ $\quad E_1 = \frac{\hbar^2}{2I}2 = 2B$
When $l=2$, $\quad E_2 = \frac{\hbar^2}{2I}6 = 6B$
When $l=3$ $\quad E_3 = \frac{\hbar^2}{2I}12 = 12B$ (say)



The Energy level diagram is shown above