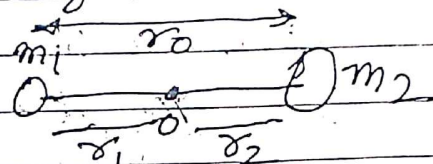


PHYSICS B.Sc Part-III (H) Paper-V Gr-C
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Rigid Rotator

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



* Kinetic energy of rigid rotator

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

Where $I = m_1 r_1^2 + m_2 r_2^2 =$ moment of inertia of the system about fixed axis: $\frac{1}{2} I \omega^2$

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 inertia $I = m_1 r_1^2 + m_2 r_2^2$ and potential energy $V = 0$. The distance $r = 1$, the wave equation:

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

Eigen function:-

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

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

$$\text{So } \frac{\partial^2 \psi}{\partial \theta^2} = Z \frac{\partial^2 Y}{\partial \theta^2} \quad \& \quad \frac{\partial^2 \psi}{\partial \phi^2} = Y \frac{\partial^2 Z}{\partial \phi^2}$$

From equⁿ B:

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

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

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

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

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

$$\text{or } \frac{d^2 Z}{d\phi^2} + m^2 Z = 0$$

The solution of equⁿ (E) is given by

$$Z = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

where $m = 0, \pm 1, \pm 2, \dots$

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

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

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

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

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

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

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

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

The solⁿ of equⁿ(G) in this form.

$\frac{d}{dx} \left[(1-x^2) \frac{dY}{dx} \right] + \left(\beta - \frac{m^2}{1-x^2} \right) Y = 0$ — (A1)

This equⁿ known as Legendre equⁿ.

$(1-x^2) \frac{d^2Y}{dx^2} + 2x \frac{dY}{dx} + \left[l(l+1) - \frac{m^2}{(1-x^2)} \right] Y = 0$ — A2

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

$P_l^m(x) = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x)$, — A3

The General solution of equⁿ(G) is given by.

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

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

$\beta = \frac{1}{\sqrt{2\pi}} \frac{(l-m)!}{(l+m)!} =$ Normalisation constant given by.

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

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

The total Eigen function can be expressed as

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

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

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

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

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

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

The solⁿ of equⁿ(G) in this form.

$$\frac{d}{dx} \left[(1-x^2) \frac{dY}{dx} \right] + \left(\beta - \frac{m^2}{1-x^2} \right) Y = 0 \quad \text{--- (A1)}$$

This equⁿ known as Legendre equⁿ.

$$(1-x^2) \frac{d^2 Y}{dx^2} + 2x \frac{dY}{dx} + \left[l(l+1) - \frac{m^2}{(1-x^2)} \right] Y = 0 \quad \text{--- A2}$$

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

$$P_l^m(x) = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x), \quad \text{--- A3}$$

The General solution of equⁿ(G) is given by.

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

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

So $\beta = \text{Normalisation constant}$ given by.

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

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

The total Eigen function can be expressed as

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

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

$$B = l(l+1)$$

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

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

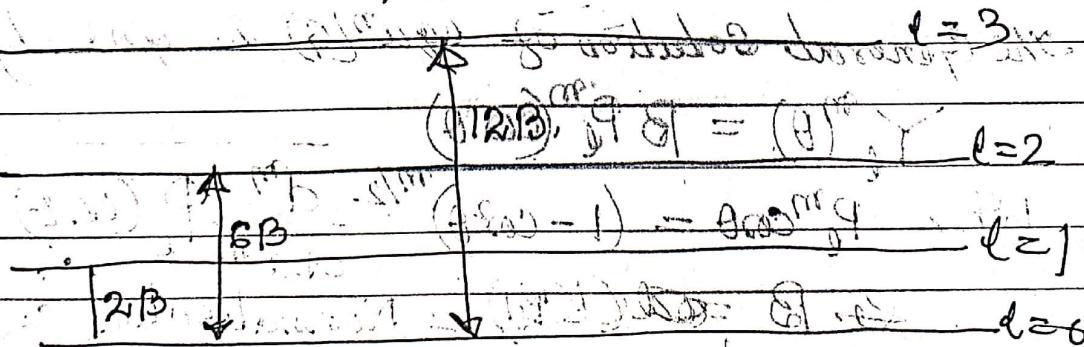
Thus we conclude that the S.E for the rigid rotator can have physically acceptable solⁿ only for certain discrete value of energy called energy eigen value (E_l)

When $l=0$, $E_0 = 0$

When $l=1$, $E_1 = \frac{\hbar^2}{2I} \cdot 2 = 2B$

When $l=2$, $E_2 = \frac{\hbar^2}{2I} \cdot 6 = 6B$

When $l=3$, $E_3 = \frac{\hbar^2}{2I} \cdot 12 = 12B$ (say)



The Energy level diagram is shown above