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Rigid Rotator with Free Axis.

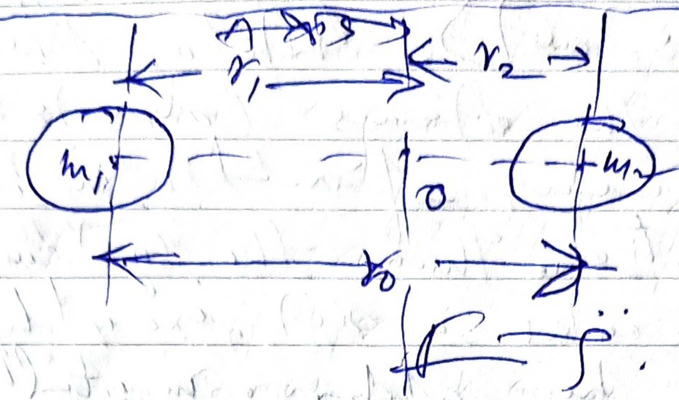

Fig.

The system having two spherical particles attached together separated by finite fixed distance and capable of rotating about an axis passing through the centre of mass and normal to the plane containing the two particles, constitutes a rigid rotator. If two particles are remaining in one plane & the direction of the axis of rotation is fixed then this particular system is known as the rigid rotator with fixed axis. Against if the plane containing these two separated particles are about to move freely, then the axis of rotation is free to take any position in space and hence this system is called the rigid rotator with free-axis.

In a diatomic molecule the atoms vibrate w.r.t. to each other and so the distance bet^n atoms will not be always remains fixed (constant); while the distance bet^n the atoms (diatomic molecule) remains fixed in equilibrium position. Thus the system of diatomic molecules is not exactly rigid but may be approximated as a rigid rotator with free axis.

Energy for the rotator:

The K.E. of a mass (m) is given by;

$$T = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2 + \dot{z}^2) \quad \text{--- (1)}$$

where $\dot{x}, \dot{y}, \dot{z}$ are the components of the velocity of a particle along X, Y and Z axes respectively.

The transformations between cartesian coordinates (x, y, z) and spherical co-ordinates (r, θ, ϕ) are given by;

$$\left.\begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned}\right\} \longrightarrow (2)$$

so that the kinetic energy in spherical coordinates is expressed as

$$T = \frac{1}{2} m (\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta \, \dot{\phi}^2) \longrightarrow (3)$$

If the distance r is fixed then $\dot{r} = 0$;
Hence;
$$T = \frac{1}{2} m r^2 \left(\dot{\theta}^2 + \sin^2\theta \, \dot{\phi}^2\right) \rightarrow (4)$$

Taking O, the centre of mass, as origin, the K.E. of the particle of mass m_1 is given by

$$T_1 = \frac{1}{2} m_1 r_1^2 \left(\dot{\theta}^2 + \sin^2\theta \, \dot{\phi}^2\right)$$

Similarly the K.E. of the particle of mass m_2 is

$$T_2 = \frac{1}{2} m_2 r_2^2 \left(\dot{\theta}^2 + \sin^2\theta \, \dot{\phi}^2\right)$$

Hence the total K.E. of the rotator is

$$T = T_1 + T_2 = \frac{1}{2} m_1 r_1^2 \left(\dot{\theta}^2 + \sin^2\theta \, \dot{\phi}^2\right) + \frac{1}{2} m_2 r_2^2 \left(\dot{\theta}^2 + \sin^2\theta \, \dot{\phi}^2\right)$$

$$= \left(\frac{1}{2} m_1 r_1^2 + \frac{1}{2} m_2 r_2^2\right)\left(\dot{\theta}^2 + \sin^2\theta \, \dot{\phi}^2\right) \rightarrow (5)$$

Since the total energy is of the form of K.E. only and NO P.E. is involved i.e., P.E. = 0 & hence the total energy is given by;

$$E = T + V = T \quad [\because V = 0]$$

$$= \left(\frac{1}{2} m_1 r_1^2 + \frac{1}{2} m_2 r_2^2\right)\left(\dot{\theta}^2 + \sin^2\theta \, \dot{\phi}^2\right) \rightarrow (6)$$

But $m_1 r_1^2 + m_2 r_2^2 = I$ the M.I. of the system about the axis passing through the C.M. and ⊥r to the line joining the two masses.

Now Eq. (6) may be written as

$$E = T = \frac{1}{2} I \left(\dot{\theta}^2 + \sin^2\theta\, \dot{\phi}^2\right) \quad (7)$$

M.I. of Rigid Rotator

From C-M; $r_{cm} = \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2}$

$$0 = \frac{-m_1 r_1 + m_2 r_2}{m_1 + m_2}$$

$$\text{or } m_1 r_1 = m_2 r_2 \quad (8)$$

as $r_0 = r_1 + r_2$

$\Rightarrow r_2 = r_0 - r_1 \rightarrow$ put this in (8)

$$m_1 r_1 = m_2 (r_0 - r_1)$$

$$\Rightarrow r_1 = \frac{m_2}{m_1 + m_2} r_0$$

$$\& \quad r_2 = \frac{m_1}{m_1 + m_2} r_0 \quad (9)$$

Then M.I. of Rigid Rotator will be;

$$I = m_1 r_1^2 + m_2 r_2^2 = m_1 \left(\frac{m_2}{m_1 + m_2} r_0\right)^2 + m_2 \left(\frac{m_1}{m_1 + m_2} r_0\right)^2$$

$$\text{or } I = \frac{m_1 m_2}{m_1 + m_2} r_0^2$$

$$\Rightarrow I = \mu r_0^2 \quad (10)$$

where $\mu = \frac{m_1 m_2}{m_1 + m_2} \quad (11)$

μ is known as the reduced mass of the system.

Thus it is evident that the rigid rotator behaves like a single particle of mass μ; placed at a fixed distance; equal to unity (since $r=1$) from the origin; which in this case is the centre of mass of the system.

[4] Wave Eqn. for the R. Rotator

The S. Eqn in (r, θ, ϕ) in 3-D is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2m}{\hbar^2}(E-V)\psi=0 \quad (12)$$

As $V=0$ for a Rotator, $r=1$ and $m=I$. Therefore S. Eqn. becomes

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2I}{\hbar^2}E\psi=0 \quad (13)$$

Eqn. (13) consists of two variables θ as well as Φ ; that represents the precessional motion of the rotator's free axis & the rotation of the system respectively.

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PG Sem II

Rigid Rotator In A Fixed Plane.

Say the rotator be only confined in XY-plane, then $\theta = 90^\circ$ ($\pi/2$) and the S. Eqn becomes

$$\frac{\partial^2 \psi}{\partial \phi^2} + \frac{2IE}{\hbar^2}\psi = 0 \quad (1)$$

Here we choose $\psi = \Phi_m(\phi)$; so that

$$\frac{1}{\Phi}\frac{\partial^2 \Phi}{\partial \phi^2} = -\frac{2IE}{\hbar^2} = \text{constant} = -m^2 \text{ (say)}$$

Then we will have;

$$\frac{1}{\Phi}\frac{\partial^2 \Phi}{\partial \phi^2} = -\frac{2IE}{\hbar^2} = -m^2$$

Or $$\frac{1}{\Phi}\frac{\partial^2 \Phi}{\partial \phi^2} + m^2 = 0 \quad (2)$$

$$\Rightarrow \frac{\partial^2 \Phi}{\partial \phi^2} + m^2 \Phi = 0$$

Where

$$\frac{2IE}{\hbar^2} = m^2 \quad (3)$$

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Eigen-fns: The soln. of eqn (2) is given by

$$\Phi_m = A e^{im\phi} \quad (4)$$

A is any arbitrary const. & $m = 0, \pm 1, \pm 2, \ldots$

From the normalisation condition;

$$\int_0^{2\pi} \Phi_m \Phi_m^* \, d\phi = 1$$

or $$\int_0^{2\pi} A e^{im\phi} A e^{-im\phi} \, d\phi = 1$$

or $$A^2 \cdot 2\pi = 1$$

or $$A = \frac{1}{\sqrt{2\pi}}$$

Then the eigen-fns. are given by

$$\psi = \Phi_m(\phi) = A e^{im\phi}$$

or $$\psi = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad (5)$$

Eigen-values: From (3) one will have

$$E = E_m = \frac{m^2 \hbar^2}{2I} \quad (6)$$

This is the reqd. expression of the energy eigenvalue.

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