❖ Energy of Rigid Rotator

The energy of a rigid rotator can be understood only after considering its classical and quantum mechanical aspects. In the previous section of this chapter, we discussed the classical and quantum mechanical nature of the rigid rotator. consider a system two masses m_1 and m_2 joined by a rigid rod of length "*r*". Now assume that this dumbbell type geometry rotates about an axis that is perpendicular to *r* and passes through the center of mass.

➢ *The energy of Classical Rigid Rotator*

If v_1 and v_2 are the velocities of the mass m_1 and m_2 revolving about the axis of rotation, the total kinetic energy (*T*) of the rotator can be given by the following relation.

$$T = \frac{1}{2}m_1v_1^2 + \frac{1}{2}m_2v_2^2 \tag{215}$$

Since we know that linear velocity v is simply equal to the angular velocity ω multiplied by the radius of rotation *r* i.e. $v = \omega r$, the equation (215) takes the form

$$T = \frac{1}{2}m_1(r_1\omega)^2 + \frac{1}{2}m_2(r_2\omega)^2 \tag{216}$$

$$T = \frac{1}{2}(m_1r_1^2 + m_2r_2^2)\omega^2 \tag{217}$$

$$T = \frac{1}{2}I\omega^2 \tag{218}$$

Where *I* is the moment of inertia equal with definition $I = \sum m_ir_i^2$. Furthermore, the value of I can also be written as

$$I = \left(\frac{m_1m_2}{m_1 + m_2}\right)r^2 \tag{219}$$

$$I = \mu r^2 \tag{220}$$

Where $\mu = m_1m_2/m_1 + m_2$ is the reduced mass of the rigid diatomic system. After multiplying and dividing the rotational kinetic energy by *I* i.e. equation (218), we have

$$T = \frac{I^2\omega^2}{2I} = \frac{(I\omega)^2}{2I} = \frac{L^2}{2I} \tag{221}$$

Where *L* is the angular momentum of the rotator. It is clear from the above equation that the kinetic energy of a classical rotator can have any value because the value-domain of angular velocity is continuous. Moreover, as now the external force is working on the rotator, the potential can be set to zero. Therefore, we can conclude that the total energy of a classical diatomic rigid rotator is given by equation (221).

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- ***The energy of Quantum Mechanical Rigid Rotator***

In order to understand the energy of a quantum mechanical rigid rotator, recall the Schrodinger wave equation for the same first i.e.

$$\frac{1}{Sin\,\theta}\frac{\partial}{\partial\theta}\left(Sin\,\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{Sin^2\,\theta}\frac{\partial\psi}{\partial\phi}+\frac{8\pi^2 IE\psi}{h^2}=0 \tag{222}$$

Where ψ is the mathematical expression defining various quantum mechanical states depending upon two variables θ and ϕ. During the course of the solution of the above equation, a constant β is defined for simplicity as given below.

$$\beta=\frac{8\pi^2 IE}{h^2} \tag{223}$$

However, the boundary conditions that keep the function single-valued, continuous and finite; also proved that the constant β must satisfy the following condition also.

$$\beta=l(l+1) \tag{224}$$

Where $l=0,1,2,3,4$ etc. After equating the value of β from equation (223) and equation (224), we get

$$\frac{8\pi^2 IE}{h^2}=l(l+1) \tag{225}$$

$$E_l=\frac{h^2}{8\pi^2 I}\,l(l+1) \tag{226}$$

Hence, unlike the classical counterpart, the energy levels of quantum mechanical rigid rotators are discontinuous.

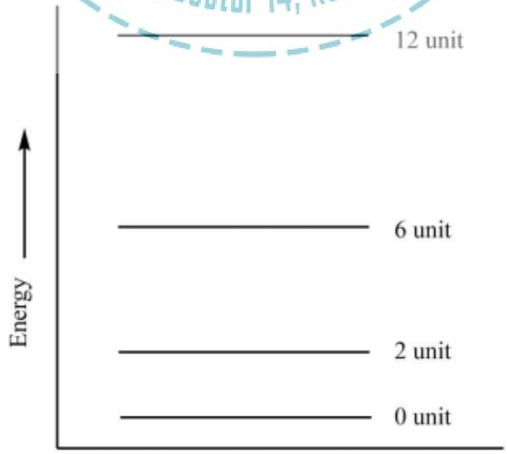

Figure 8. The energy level diagram of the diatomic rigid rotator in units of $h^2/8\pi^2 I$.

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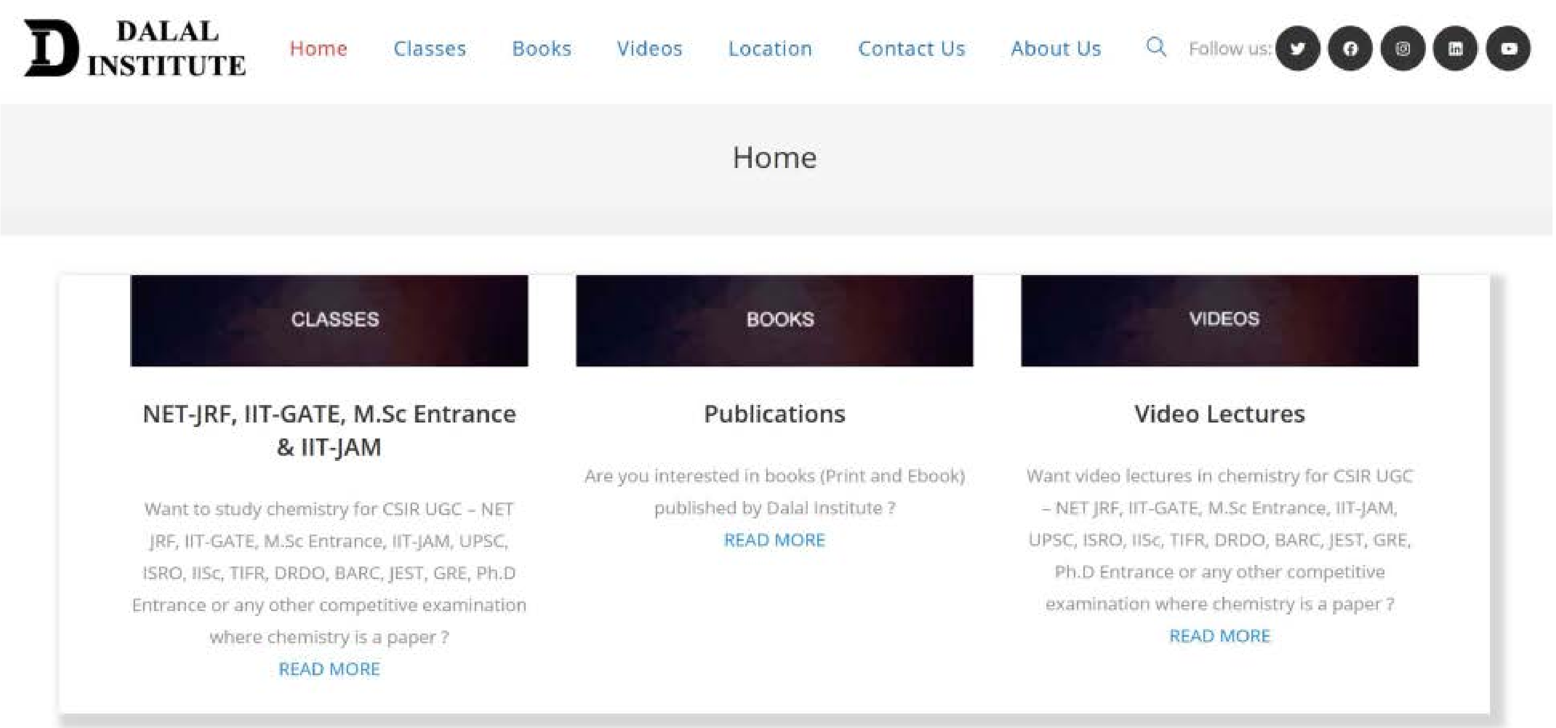

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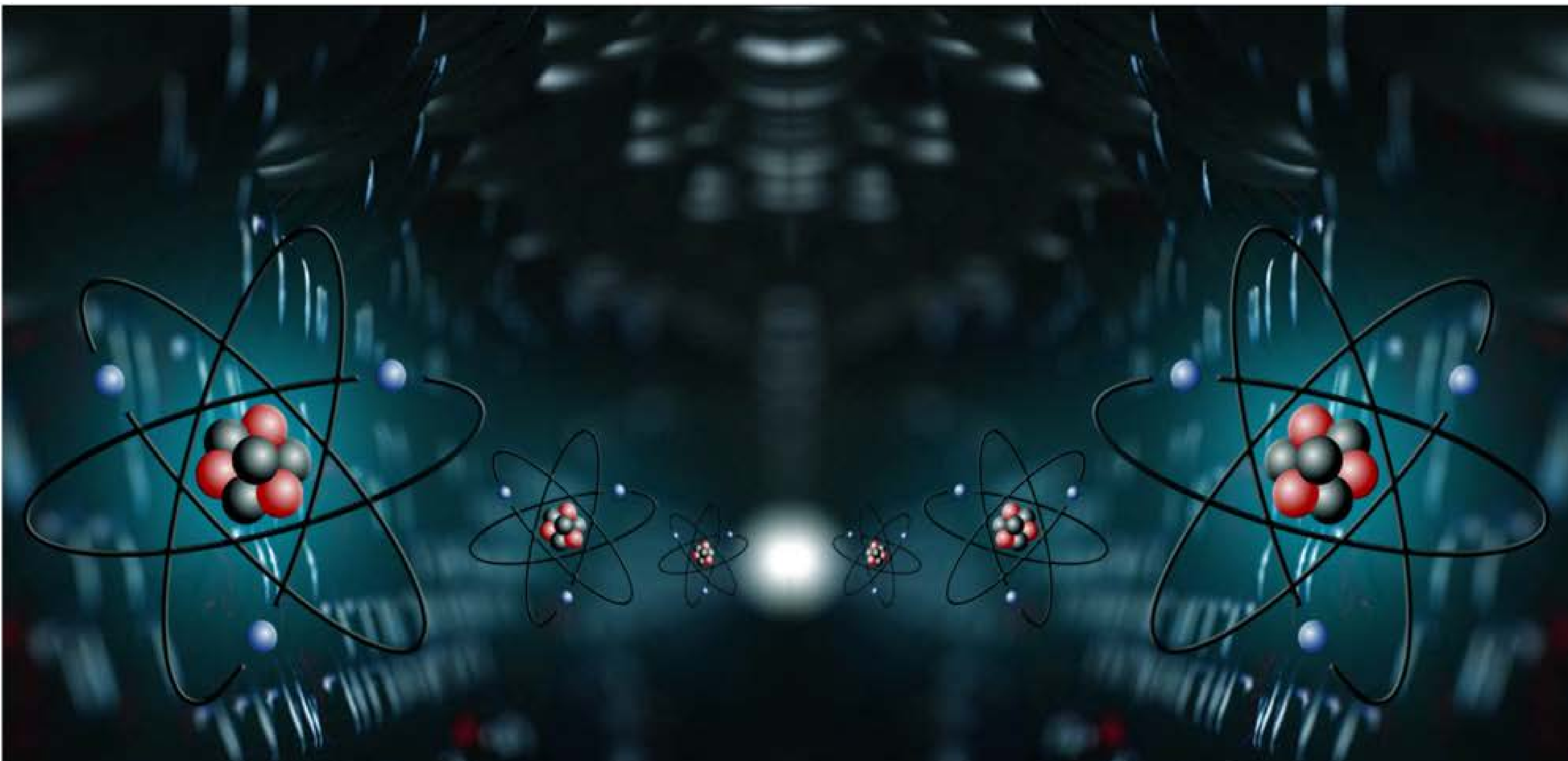

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