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.

\[
T = \frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2
\]

(215)

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

\[
T = \frac{1}{2} m_1 (r_1 \omega)^2 + \frac{1}{2} m_2 (r_2 \omega)^2
\]

(216)

\[
T = \frac{1}{2} (m_1 r_1^2 + m_2 r_2^2) \omega^2
\]

(217)

\[
T = \frac{1}{2} I \omega^2
\]

(218)

Where \( I \) is the moment of inertia equal with definition \( I = \sum m_i r_i^2 \). Furthermore, the value of \( I \) can also be written as

\[
I = \left( \frac{m_1 m_2}{m_1 + m_2} \right) r^2
\]

(219)

\[
I = \mu r^2
\]

(220)

Where \( \mu = m_1 m_2 / (m_1 + m_2) \) 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

\[
T = \frac{I^2 \omega^2}{2I} = \frac{(I \omega)^2}{2I} = \frac{L^2}{2I}
\]

(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).
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.

\[
\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial \psi}{\partial \phi} + \frac{8\pi^2 I E \psi}{\hbar^2} = 0
\]  
(222)

Where \( \psi \) is the mathematical expression defining various quantum mechanical states depending upon two variables \( \theta \) and \( \phi \). During the course of the solution of the above equation, a constant \( \beta \) is defined for simplicity as given below.

\[
\beta = \frac{8\pi^2 I E}{\hbar^2}
\]  
(223)

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

\[
\beta = l(l + 1)
\]  
(224)

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

\[
\frac{8\pi^2 I E}{\hbar^2} = l(l + 1)
\]  
(225)

\[
E_l = \frac{\hbar^2}{8\pi^2 l} l(l + 1)
\]  
(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 \( \hbar^2/8\pi^2 l \).
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Mandeep Dalal is an Indian research scholar who is primarily working in the field of Science and Philosophy. He received his Ph.D in Chemistry from Maharshi Dayanand University, Rohtak, in 2018. He is also the Founder and Director of "Dalal Institute", an India-based educational organization which is trying to revolutionize the mode of higher education in Chemistry across the globe. He has published more than 40 research papers in various international scientific journals, including mostly from Elsevier (USA), IOP (UK) and Springer (Netherlands).

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