Quantum Mechanics: Rotation of Diatomics: Reducing the Problem

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Consider two masses, m_1 and m_2, separated by a constant distance r_0. You can think of the masses as being "connected" or "bonded", but this is in some loose sense. Mass m_1 is a distance r_1 from the center of mass of the system; mass m_2 is a distance r_2 from the center of masss. The system is now taken to be rotating in three dimensions about some axis of rotation. The angular frequency (in $\frac{radians}{sec}$) of rotation is ω. The kinetic energy of the system is:

$$\begin{aligned} KE &= \frac{1}{2}\, m_1\, v_1^2 \,+\, \frac{1}{2}\, m_2\, v_2^2 \\ &= \frac{1}{2}\, m_1\, r_1^2\, \omega^2 \,+\, \frac{1}{2}\, m_2\, r_2^2\, \omega^2 \\ &= \frac{1}{2}\left(m_1\, r_1^2 \,+\, m_2\, r_2^2 \right)\omega^2 \\ &= \frac{1}{2}\, I\, \omega^2 \end{aligned}$$

where I is defined as the moment of inertia. If we consider the sum of r_1 and r_2 (considering only their **magnitues**) as $r_0 \;=\; r_1 + r_2$, we can write the moment of inertia in terms of the reduced mass as follows:

$$I \;=\; m_1\, r_1^2 \,+\, m_2\, r_2^2 \;=\; \mu\, r_0^2$$

where the reduced mass is defined as:

$$\mu \;=\; \frac{m_1\, m_2}{m_1 \,+\, m_2}$$

Thus, the kinetic energy in terms of the reduced mass becomes:

$$KE \;=\; \frac{1}{2}\,\mu\, r_0^2\, \omega^2 \;=\; \frac{1}{2}\,\mu\, v_0^2$$

The last equation shows us that in terms of the reduce mass, the dynamics of a rigid, "diatomic" rotor is equivalent to that of a particle of reduced mass μ (effectively, we have reduced a two-body problem to a one-body problem).