Reduction of two-particle into center of mass plus a one-body problem in the case of central potential

We start with a two-particle Hamiltonian:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(|\vec{r}_2 - \vec{r}_1|) = -\frac{\hbar^2}{2m_1}\nabla_{\vec{r}_1}^2 - \frac{\hbar^2}{2m_2}\nabla_{\vec{r}_2}^2 + V(|\vec{r}_2 - \vec{r}_1|)$$

If we define the position of the center of mass as

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{M} \quad \text{where} \quad M = m_1 + m_2$$

and the relative position

$$\vec{r} = \vec{r}_2 - \vec{r}_1$$

then

$$\nabla_{\vec{r}_1} = \frac{\partial}{\partial\vec{R}}\frac{\partial\vec{R}}{\partial\vec{r}_1} + \frac{\partial}{\partial\vec{r}}\frac{\partial\vec{r}}{\partial\vec{r}_1} = \frac{m_1}{M}\nabla_{\vec{R}} - \nabla_{\vec{r}}$$

$$\nabla_{\vec{r}_2} = \frac{\partial}{\partial\vec{R}}\frac{\partial\vec{R}}{\partial\vec{r}_2} + \frac{\partial}{\partial\vec{r}}\frac{\partial\vec{r}}{\partial\vec{r}_2} = \frac{m_2}{M}\nabla_{\vec{R}} + \nabla_{\vec{r}}$$

The Hamiltonian can be written then as

$$H = -\frac{\hbar^2}{2m_1}\left(\frac{m_1}{M}\nabla_{\vec{R}} - \nabla_{\vec{r}}\right)^2 - \frac{\hbar^2}{2m_2}\left(\frac{m_2}{M}\nabla_{\vec{R}} + \nabla_{\vec{r}}\right)^2 + V(r) =$$

$$= -\frac{\hbar^2}{2M}\nabla_{\vec{R}}^2 - \frac{\hbar^2}{2m_1}\nabla_{\vec{r}}^2 - \frac{\hbar^2}{2m_2}\nabla_{\vec{r}}^2 + V(r) =$$

$$= \underbrace{-\frac{\hbar^2}{2M}\nabla_{\vec{R}}^2}_{H_{CM}} \underbrace{- \frac{\hbar^2}{2\mu}\nabla_{\vec{r}}^2 + V(r)}_{H_{relative}}$$

H_{cm} describes free motion of the center of mass while $H_{relative}$ describes the relative motion of particle 2 with respect to particle 1.

Since H_{CM} depends only on $\vec{R}$ and $H_{relative}$ depends only on $\vec{r}$ the eigenfunction of H is a product of the eigenfunctions of H_{CM} and $H_{relative}$:

$$\Psi(\vec{R},\vec{r}) = \psi_{CM}(\vec{R})\,\psi_{relative}(\vec{r})$$

$$H_{CM}\psi_{CM} = E_{CM}\psi_{CM} \qquad H_{relative}\psi_{relative} = E_{relative}\psi_{relative}$$

and

$$E = E_{CM} + E_{relative}$$

In a similar way we can show that the operator of the angular momentum of a two-particle system can be decomposed into a sum of two operators corresponding to the angular momentum of the center of mass and the angular momentum of the relative motion :

$$\vec{L} = \vec{L}_1 + \vec{L}_2 = \vec{r}_1 \times \vec{p}_1 + \vec{r}_2 \times \vec{p}_2 = -i\hbar(\vec{r}_1 \times \nabla_{\vec{r}_1}) - i\hbar(\vec{r}_2 \times \nabla_{\vec{r}_2})$$

$$= -i\hbar\left(\vec{r}_1 \times \left(\frac{m_1}{M}\nabla_{\vec{R}} - \nabla_{\vec{r}}\right)\right) - i\hbar\left(\vec{r}_2 \times \left(\frac{m_2}{M}\nabla_{\vec{R}} + \nabla_{\vec{r}}\right)\right) =$$

$$= -i\hbar\left[\left(\frac{m_1}{M}\vec{r}_1 + \frac{m_2}{M}\vec{r}_2\right) \times \nabla_{\vec{R}} + (\vec{r}_2 - \vec{r}_1) \times \nabla_{\vec{r}}\right] =$$

$$= -i\hbar\left[\vec{R} \times \nabla_{\vec{R}} + \vec{r} \times \nabla_{\vec{r}}\right] = \vec{L}_{CM} + \vec{L}_{relative}$$

Quantum rigid rotor

Motion of a rigid diatomic molecule serves as an application of the quantum-mechanical treatment of angular momentum to a physical system

Suppose we have two point particles of mass m_1 and m_2, which can rotate about their center of mass while the distance between the two masses is kept fixed. Let us denote this distance R

The time τ for a classical particle to make a complete revolution on its circular path is equal to the distance traveled divided by its linear velocity

$$\tau = \frac{2\pi r_i}{v_i}$$

where v_i can be expressed as $v_i = \frac{2\pi r_i}{\tau} = \omega r_i$

The angular momentum $\vec{L}_i$ of particle i is

$$\vec{L}_i = \vec{r}_i \times \vec{p}_i = m_i(\vec{r}_i \times \vec{v}_i)$$

Since we deal with a rigid rotor, $\vec{v}_i$ is perpendicular to $\vec{r}_i$. Hence

$$|\vec{L}_i| = m_i r_i v_i = \omega m_i r_i^2$$

The potential energy can be treated as zero (because the distance between particles, R, cannot change anyway)

The classical Hamiltonian function is given by

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} = \frac{m_1 v_1^2}{2} + \frac{m_2 v_2^2}{2} = \frac{1}{2}\omega^2(m_1 r_1^2 + m_2 r_2^2) =$$

$$= \frac{1}{2} I \omega^2 \qquad \text{where} \qquad I = m_1 r_1^2 + m_2 r_2^2$$

Let us now determine the moment of inertia relative to the axis of rotation :

$r_1 + r_2 = R \qquad m_1 r_1 = m_2 r_2$

$$\therefore r_1 = \frac{m_2}{m_1+m_2} R \qquad r_2 = \frac{m_1}{m_1+m_2} R$$

Now if we plug these expressions into the formula for I we obtain

$$I = \mu R^2 \quad \text{where} \quad \mu = \frac{m_1 m_2}{m_1+m_2}$$

The total angular momentum L for the two-particle system is given by

$$L = L_1 + L_2 = \omega (m_1 r_1^2 + m_2 r_2^2) = I\omega$$

then

$$H = \frac{L^2}{2I}$$

Accordingly, the quantum-mechanical Hamiltonian for this system is

$$\hat{H} = \frac{1}{2I} \hat{L}^2$$

The eigenvalues of $\hat{H}$ are obtained by noting that

$$\hat{H} Y_J^M(\theta, \varphi) = \frac{1}{2I} \hat{L}^2 Y_J^M(\theta, \varphi) = \frac{J(J+1)\hbar^2}{2I} Y_J^M(\theta, \varphi)$$

The energy levels E_J for the rigid rotor are given by

$$E_J = J(J+1)\frac{\hbar^2}{2I} = J(J+1) B \qquad J = 0, 1, 2, \ldots$$

where $B = \frac{\hbar^2}{2I}$ is the rotational constant