· given two particles
masses: m_1 and m_2
positions: $\vec{r}_1$ and $\vec{r}_2$

Q1: what are the C.O.M and relative coordinates? $\vec{R}$, $\vec{r}$ = ?

Q2: What is the reduced mass? μ = ?

Q3: What are $\vec{P}$, $\vec{p}$ in terms of $\vec{p}_1$ and $\vec{p}_2$

Just in terms of classical mechanics

Lecture 28:
The Quantum Two-body Problem

Phy851 Fall 2009

Common Mistake: $$\left.\begin{aligned}\vec{P} &= \frac{m_1\vec{p}_1 + m_2\vec{p}_2}{m_1+m_2} \\ \vec{p} &= \vec{p}_1 - \vec{p}_2\end{aligned}\right\}\text{wrong}$$

Two interacting particles

- Consider a system of two particles with no external fields

- By symmetry, the interaction energy can only depend on the separation distance:

$$H = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V\left(\left|\vec{R}_1 - \vec{R}_2\right|\right)$$

- From our experience with Classical Mechanics, we might want to treat separately the Center-of-mass and relative motion:
  - Center-of-mass coordinate:

$$\vec{R}_{CM} = \frac{m_1\vec{R}_1 + m_2\vec{R}_2}{m_1 + m_2}$$

  - Relative coordinate:

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

  - This is recommended because the potential depends only on the relative coordinate:

$$V\left(\left|\vec{R}_1 - \vec{R}_2\right|\right) = V(R)$$

Center-of-mass and relative momentum

- How do we go about finding the center-of-mass and relative-motion momentum operators:
  - Can we use:

$$\vec{P}_{CM} = \frac{m_1\vec{P}_1 + m_2\vec{P}_2}{m_1 + m_2} \qquad \vec{P} = \vec{P}_1 - \vec{P}_2 \quad ?$$

- Answer: No, this is very wrong!

- Lets *try* instead to use what we know from classical mechanics:

$$M = m_1 + m_2$$

$$\vec{V}_{CM} = \frac{d}{dt}\vec{R}_{CM} = \frac{m_1\vec{V}_1 + m_2\vec{V}_2}{m_1 + m_2}$$

$$\vec{P}_{CM} = M\,\vec{V}_{CM}$$

$$= m_1\vec{V}_1 + m_2\vec{V}_2$$

$$\vec{P}_{CM} = \vec{P}_1 + \vec{P}_2$$

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

$$\vec{V} = \frac{d}{dt}\vec{R} = \vec{V}_1 - \vec{V}_2$$

$$\vec{P} = \mu\,\vec{V}$$

$$= \frac{m_1 m_2}{m_1 + m_2}\left(\vec{V}_1 - \vec{V}_2\right)$$

$$\vec{P} = \frac{m_2 P_1 - m_1 P_2}{m_1 + m_2}$$

Transformation to Center-of-mass coordinates

- We have defined new coordinates:

$$\vec{R}_{CM} = \frac{m_1\vec{R}_1 + m_2\vec{R}_2}{m_1 + m_2} \qquad \vec{R} = \vec{R}_1 - \vec{R}_2$$

- We have guessed that the corresponding momentum operators are:

$$\vec{P}_{CM} = \vec{P}_1 + \vec{P}_2 \qquad \vec{P} = \frac{m_2 P_1 - m_1 P_2}{m_1 + m_2}$$

- To verify, we need to check the commutation relations:

$$[X_{CM}, P_{CM,x}] = \frac{m_1}{m_1 + m_2}[X_1, P_{1x}] + \frac{m_2}{m_1 + m_2}[X_2, P_{2x}] = i\hbar$$

$$[X, P_x] = \frac{m_2}{m_1 + m_2}[X_1, P_{1,x}] + \frac{m_1}{m_1 + m_2}[X_2, P_{2,x}] = i\hbar$$

$$[X_{CM}, P_x] = \frac{m_1 m_2}{(m_1 + m_2)^2}[X_1, P_{1,x}] - \frac{m_2 m_1}{(m_1 + m_2)^2}[X_2, P_{2,x}] = 0$$

$$[X, P_{CM,x}] = [X_1, P_{1,x}] - [X_2, P_{2,x}] = 0$$

- So our choices for the momentum operators were correct

Inverse Transformation

$$\vec{R}_{CM} = \frac{m_1\vec{R}_1 + m_2\vec{R}_2}{m_1 + m_2}$$

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

$$\vec{P}_{CM} = \vec{P}_1 + \vec{P}_2$$

$$\vec{P} = \frac{m_2 P_1 - m_1 P_2}{m_1 + m_2}$$

- The inverse transformations work out to:

$$\vec{R}_1 = \vec{R}_{CM} + \frac{\mu}{m_1}\vec{R}$$

$$\vec{R}_2 = \vec{R}_{CM} - \frac{\mu}{m_2}\vec{R}$$

$$\vec{P}_1 = \frac{m_1}{M}\vec{P}_{CM} + \vec{P}$$

$$\vec{P}_2 = \frac{m_2}{M}\vec{P}_{CM} - \vec{P}$$

Transforming the Kinetic Energy Operator

- Using the inverse transformations:

$$\vec{R}_1 = \vec{R}_{CM} + \frac{\mu}{m_1}\vec{R}$$

$$\vec{P}_1 = \frac{m_1}{M}\vec{P}_{CM} + \vec{P}$$

$$\vec{R}_2 = \vec{R}_{CM} - \frac{\mu}{m_2}\vec{R}$$

$$\vec{P}_2 = \frac{m_2}{M}\vec{P}_{CM} - \vec{P}$$

- We find:

$$\vec{P}_1 \cdot \vec{P}_1 = \frac{m_1^2}{M^2}P_{CM}^2 + \frac{2m_1}{M}\vec{P}\cdot\vec{P}_{CM} + P^2$$

$$\vec{P}_2 \cdot \vec{P}_2 = \frac{m_2^2}{M^2}P_{CM}^2 - \frac{2m_2}{M}\vec{P}\cdot\vec{P}_{CM} + P^2$$

- So that:

$$\frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} = \frac{m_1 + m_2}{2M^2}P_{CM}^2 + \frac{1}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)P^2$$

$$\frac{1}{\mu} = \frac{m_1 + m_2}{m_1 m_2} = \frac{1}{m_2} + \frac{1}{m_1}$$

$$\frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} = \frac{P_{CM}^2}{2M} + \frac{P^2}{2\mu}$$

The New Hamiltonian

$$H = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V\left(\vec{R}_1 - \vec{R}_2\right)$$

- Becomes:

$$H = \frac{P_{CM}^2}{2M} + \frac{P^2}{2\mu} + V(R)$$

- Note that:

$$H = H_{CM} + H_{rel}$$

$$H_{CM} = \frac{P_{CM}^2}{2M} \qquad H_{rel} = \frac{P^2}{2\mu} + V(R)$$

- We call this ‘separability’
  - System is ‘separable’ in COM and relative coordinates

- When a system is separable, it means we can solve each problem separately, and use the tensor product to construct the full eigenstates of the complete system

Eigenstates of the Separated Systems

$$H_{CM} = \frac{P_{CM}^2}{2M} \in \mathcal{H}^{(C)}$$

- The eigenstates of this Hamiltonian are free-particle eigenstates

$$\left|\vec{p}_{CM}\right\rangle^{(C)} \quad \Bigg| \quad \begin{aligned} \vec{P}_{CM}\left|\vec{p}_{CM}\right\rangle^{(C)} &= \vec{p}_{CM}\left|\vec{p}_{CM}\right\rangle^{(C)} \\ H_{CM}\left|\vec{p}_{CM}\right\rangle^{(C)} &= \frac{p_{CM}^2}{2M}\left|\vec{p}_{CM}\right\rangle^{(C)} \end{aligned}$$

$$I^{(C)} = \int_{-\infty}^{+\infty} d^3 p_{CM} \left|\vec{p}_{CM}\right\rangle\left\langle\vec{p}_{CM}\right|^{(C)}$$

$$H_{rel} = \frac{P^2}{2\mu} + V(R) \in \mathcal{H}^{(R)}$$

- Bound states: $H_{rel}\left|n,m\right\rangle^{(R)} = E_n\left|n,m\right\rangle^{(R)}$

n is the 'principle quantum number'

→ labels energy levels

- Continuum states: $H_{rel}\left|\vec{k}\right\rangle^{(R)} = E(\vec{k})\left|\vec{k}\right\rangle^{(R)}$

$$I^{(R)} = \sum_{n=1}^{n_{\max}} \sum_{m=1}^{d(n)} \left|n,m\right\rangle\left\langle n,m\right|^{(R)} + \int_{-\infty}^{+\infty} d^3 k \left|\vec{k}\right\rangle\left\langle\vec{k}\right|^{(R)}$$

Full Eigenstates

$$H_{CM}\left|\vec{p}_{CM}\right\rangle^{(C)} = \frac{p_{CM}^2}{2M}\left|\vec{p}_{CM}\right\rangle^{(C)}$$

$$H_{rel}\left|n,m\right\rangle^{(R)} = E_n\left|n,m\right\rangle^{(R)}$$

$$H_{rel}\left|\vec{k}\right\rangle^{(R)} = E(\vec{k})\left|\vec{k}\right\rangle^{(R)}$$

- We can form tensor product states:

$$\mathcal{H} = \mathcal{H}_{rel} \otimes \mathcal{H}_{CM}$$

$$\left|\vec{p}_{CM}, n, m\right\rangle := \left|\vec{p}_{CM}\right\rangle^{(C)} \otimes \left|n,m\right\rangle^{(R)}$$

$$\left|\vec{p}_{CM}, \vec{k}\right\rangle := \left|\vec{p}_{CM}\right\rangle^{(C)} \otimes \left|\vec{k}\right\rangle^{(R)}$$

$$I = I^{(C)} \otimes I^{(R)}$$ 'and'

$$I^{(R)} = I^{(R)}_{bound} + I^{(R)}_{continuum}$$ 'or'

$$I = I^{(C)} \otimes I^{(R)}_{bound} + I^{(C)} \otimes I^{(R)}_{continuum}$$

Tensor Product States are Eigenstates of the Full Hamiltonian

$$H\left|\vec{p}_{CM},n,m\right\rangle = \left(\frac{p_{CM}^2}{2M}+E_n\right)\left|\vec{p}_{CM},n,m\right\rangle$$

- Proof:

$$H\left|\vec{p}_{CM},n,m\right\rangle$$

$$=\left(H_{CM}^{(C)}+H_{rel}^{(R)}\right)\left|\vec{p}_{CM}\right\rangle^{(C)}\otimes\left|n,m\right\rangle^{(R)}$$

$$=H_{CM}^{(C)}\left|\vec{p}_{CM}\right\rangle^{(C)}\otimes\left|n,m\right\rangle^{(R)}+H_{rel}^{(R)}\left|\vec{p}_{CM}\right\rangle^{(C)}\otimes\left|n,m\right\rangle^{(R)}$$

$$=\left(H_{CM}^{(C)}\left|\vec{p}_{CM}\right\rangle^{(C)}\right)\otimes\left|n,m\right\rangle^{(R)}+\left|\vec{p}_{CM}\right\rangle^{(C)}\otimes\left(H_{rel}^{(R)}\left|n,m\right\rangle^{(R)}\right)$$

$$=\frac{p_{CM}^2}{2M}\left|\vec{p}_{CM}\right\rangle^{(C)}\otimes\left|n,m\right\rangle^{(R)}+\left|\vec{p}_{CM}\right\rangle^{(C)}\otimes E_n\left|n,m\right\rangle^{(R)}$$

$$=\left(\frac{p_{CM}^2}{2M}+E_n\right)\left|\vec{p}_{CM}\right\rangle^{(R)}\otimes\left|n,m\right\rangle^{(C)}$$

$$H\left|\vec{p}_{CM},n,m\right\rangle = \left(\frac{p_{CM}^2}{2M}+E_n\right)\left|\vec{p}_{CM},n,m\right\rangle$$

Example: Hydrogen Atom

- For the hydrogen system (e + p) we have:

$$H = \frac{P_e^2}{2m_e} + \frac{P_p^2}{2m_p} - \frac{e^2}{4\pi\varepsilon_0 \left|\vec{R}_e - \vec{R}_p\right|}$$

- Switch to relative and COM coordinates gives:

$$H = \frac{P_{CM}^2}{2M} + \frac{P^2}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 R} = H_{CM} + H_{rel}$$

- The eigenstates of H_{CM} in $\mathcal{H}^{(C)}$ are free-particle eigenstates:

$$\left\{ \left| \vec{p}_{CM} \right\rangle^{(C)} \right\} : \; H_{CM} \left| \vec{p}_{CM} \right\rangle^{(C)} = \frac{p_{CM}^2}{2M} \left| \vec{p}_{CM} \right\rangle^{(C)}$$

- The non-trivial task is to find the eigenstates of H_{rel} in $\mathcal{H}^{(R)}$:

$$H_{rel} = \frac{P^2}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 R}$$