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? \( \mu = ? \)

Q3: what are \( \vec{P}, \vec{p} \) in terms of \( \vec{P}_1, \vec{P}_2 \) and \( \vec{p}_1, \vec{p}_2 \)

Just in terms of classical mechanics

**Lecture 28:**
The Quantum Two-body Problem

**Phy851 Fall 2009**

Common Mistake:
\[
\vec{P} = \frac{m_1 \vec{p}_1 + m_2 \vec{p}_2}{m_1 + m_2} \]
\[
\vec{p} = \vec{p}_1 - \vec{p}_2 \]
\[\text{Wrong} \]
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:

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

• 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:
    $$V\left(\vec{R}_1 - \vec{R}_2\right) = V(R)$$
Center-of-mass and relative momentum

- How do we go about finding the center-of-mass and relative-motion momentum operators:
  - Can we use:
    \[ \vec{P}_{CM} = \frac{m_1 \vec{P}_1 + m_2 \vec{P}_2}{m_1 + m_2} \]
    \[ \vec{P} = \vec{P}_1 - \vec{P}_2 \]

- Answer: No, this is very wrong!

- Let's try instead to use what we know from classical mechanics:

\[ M = m_1 + m_2 \]

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

\[ \vec{P}_{CM} = M \vec{V}_{CM} = m_1 \vec{V}_1 + m_2 \vec{V}_2 \]

\[ \vec{P}_{CM} = \vec{P}_1 + \vec{P}_2 \]

\[ \mu = \frac{m_1 m_2}{m_1 + m_2} \]

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

\[ \vec{P} = \mu \vec{V} = \frac{m_1 m_2}{m_1 + m_2} \left( \vec{V}_1 - \vec{V}_2 \right) \]

\[ \vec{P} = \frac{m_2 \vec{P}_1 - m_1 \vec{P}_2}{m_1 + m_2} \]
Transformation to Center-of-mass coordinates

- We have defined new coordinates:
  \[ \vec{R}_{CM} = \frac{m_1 \vec{R}_1 + m_2 \vec{R}_2}{m_1 + m_2} \quad \vec{R} = \vec{R}_1 - \vec{R}_2 \]

- We have guessed that the corresponding momentum operators are:
  \[ \vec{P}_{CM} = \vec{P}_1 + \vec{P}_2 \quad \vec{P} = \frac{m_2 P_1 - m_1 P_2}{m_1 + m_2} \]

- To verify, we need to check the commutation relations:
  \[ [X_{CM}, P_{CM,x}] = \frac{m_1}{m_1 + m_2} [X_1, P_{1,x}] + \frac{m_2}{m_1 + m_2} [X_2, P_{2,x}] = i\hbar \]
  \[ [X, P_x] = \frac{m_2}{m_1 + m_2} [X_1, P_{1,x}] + \frac{m_1}{m_1 + m_2} [X_2, P_{2,x}] = i\hbar \]
  \[ [X_{CM}, P_x] = \frac{m_1 m_2}{(m_1 + m_2)^2} [X_1, P_{1,x}] - \frac{m_2 m_1}{(m_1 + m_2)^2} [X_2, P_{2,x}] = 0 \]
  \[ [X, P_{CM,x}] = [X_1, P_{1,x}] - [X_2, P_{2,x}] = 0 \]

- So our choices for the momentum operators were correct
Inverse Transformation

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

\[
\vec{P}_{CM} = \vec{P}_1 + \vec{P}_2
\]

\[
\vec{R} = \vec{R}_1 - \vec{R}_2
\]

\[
\vec{P} = \frac{m_2 \vec{P}_1 - m_1 \vec{P}_2}{m_1 + m_2}
\]

- 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

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

- Becomes:

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

- Note that:

\[ H = H_{CM} + H_{rel} \]

\[ H_{CM} = \frac{P_{CM}^2}{2M} \quad H_{rel} = \frac{P^2}{2\mu} + V(R) \]

- 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

\[
\left| \vec{p}_{CM} \right>^{(C)} \quad \begin{align*}
\vec{P}_{CM} \left| \vec{p}_{CM} \right>^{(C)} &= \vec{p}_{CM} \left| \vec{p}_{CM} \right>^{(C)} \\
H_{CM} \left| \vec{p}_{CM} \right>^{(C)} &= \frac{p_{CM}^2}{2M} \left| \vec{p}_{CM} \right>^{(C)}
\end{align*}
\]

\[
I^{(C)} = \int_{-\infty}^{+\infty} d^3 p_{CM} \left| \vec{p}_{CM} \right> \left< \vec{p}_{CM} \right|^{(C)}
\]

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

- Bound states:

\[
H_{rel} \left| n, m \right>^{(R)} = E_n \left| n, m \right>^{(R)}
\]

\( n \) is the 'principle quantum number' → labels energy levels

- Continuum states:

\[
H_{rel} \left| \vec{k} \right>^{(R)} = E(\vec{k}) \left| \vec{k} \right>^{(R)}
\]

\[
I^{(R)} = \sum_{n=1}^{n_{\text{max}}} \sum_{m=1}^{d(n)} \left| n, m \right> \left< n, m \right|^{(R)} + \int_{-\infty}^{+\infty} d^3 k \left| \vec{k} \right> \left< \vec{k} \right|^{(R)}
\]
Full Eigenstates

\[ H_{CM} \left| \vec{p}_{CM} \right>^{(C)} = \frac{p_{CM}^2}{2M} \left| \vec{p}_{CM} \right>^{(C)} \]
\[ H_{rel} \left| n, m \right>^{(R)} = E_n \left| n, m \right>^{(R)} \]
\[ H_{rel} \left| \vec{k} \right>^{(R)} = E(\vec{k}) \left| \vec{k} \right>^{(R)} \]

- We can form tensor product states:

\[ \mathcal{H} = \mathcal{H}_{rel} \otimes \mathcal{H}_{CM} \]

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

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

\[ I = I^{(C)} \otimes I^{(R)} \quad \text{‘and’} \]
\[ I^{(R)} = I_{\text{bound}}^{(R)} + I_{\text{continuum}}^{(R)} \quad \text{‘or’} \]

\[ I = I^{(C)} \otimes I_{\text{bound}}^{(R)} + I^{(C)} \otimes I_{\text{continuum}}^{(R)} \]
Tensor Product States are Eigenstates of the Full Hamiltonian

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

- **Proof:**

\[ H \left| \tilde{p}_{CM}, n, m \right\rangle \]

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

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

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

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

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

\[ H \left| \tilde{p}_{CM}, n, m \right\rangle = \left( \frac{p_{CM}^2}{2M} + E_n \right) \left| \tilde{p}_{CM}, n, m \right\rangle \]
Example: Hydrogen Atom

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

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

- 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:

\[
\left\{ \left| \vec{p}_{CM} \right>^{(C)} \right\} : H_{CM} \left| \vec{p}_{CM} \right>^{(C)} = \frac{P_{CM}^2}{2M} \left| \vec{p}_{CM} \right>^{(C)}
\]

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

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