

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? $\mu = ?$

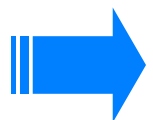
Q3: What are \vec{P} , \vec{p} in terms of \vec{p}_1 and \vec{p}_2

Just in terms of classical mechanics

Lecture 28: The Quantum Two-body Problem

Phy851 Fall 2009

Common Mistake: $\vec{P} = \frac{m_1 \vec{p}_1 + m_2 \vec{p}_2}{m_1 + m_2}$ } wrong
 $\vec{p} = \vec{p}_1 - \vec{p}_2$



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:

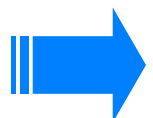
$$\vec{R}_{CM} = \frac{m_1 \vec{R}_1 + m_2 \vec{R}_2}{m_1 + m_2}$$

- 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:

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

- Answer: No, this is very wrong!

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

$$M = m_1 + m_2$$

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

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

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

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

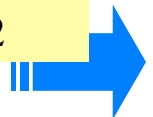
$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

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

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

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

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



Transformation to Center-of-mass coordinates

- We have defined new coordinates:

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

- 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:

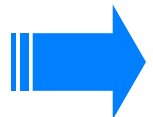
$$[X_{CM}, P_{CM,x}] = \frac{m_1}{m_1 + m_2} [X_1, P_{1,x}] + \frac{m_2}{m_1 + m_2} [X_2, P_{2,x}] = i\hbar$$

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

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

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

- So our choices for the momentum operators were correct



Inverse Transformation

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

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

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

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

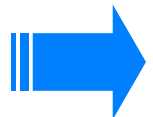
- The inverse transformations work out to:

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

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

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

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



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:

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

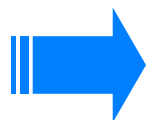
$$\vec{P}_2 \cdot \vec{P}_2 = \frac{m_2^2}{M^2} P_{CM}^2 - \frac{2m_2}{M} \vec{P} \cdot \vec{P}_{CM} + P^2$$

- 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

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

- Becomes:

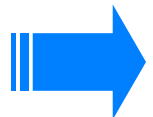
$$H = \frac{P_{CM}^2}{2M} + \frac{P^2}{2\mu} + V(R)$$

- 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

$$\left| \vec{p}_{CM} \right\rangle^{(C)} \left| \begin{array}{l} \vec{P}_{CM} \left| \vec{p}_{CM} \right\rangle^{(C)} = \vec{p}_{CM} \left| \vec{p}_{CM} \right\rangle^{(C)} \\ H_{CM} \left| \vec{p}_{CM} \right\rangle^{(C)} = \frac{p_{CM}^2}{2M} \left| \vec{p}_{CM} \right\rangle^{(C)} \end{array} \right.$$

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

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

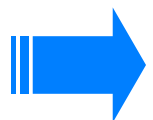
- Bound states: $H_{rel} \left| n, m \right\rangle^{(R)} = E_n \left| n, m \right\rangle^{(R)}$

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

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

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

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

- We can form tensor product states:

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

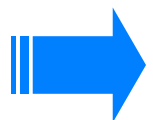
$$|\vec{p}_{CM}, n, m\rangle := |\vec{p}_{CM}\rangle^{(C)} \otimes |n, m\rangle^{(R)}$$

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

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

$$I^{(R)} = I_{bound}^{(R)} + I_{continuum}^{(R)} \quad \text{'or'}$$

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



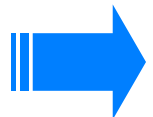
Tensor Product States are Eigenstates of the Full Hamiltonian

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

- Proof:

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

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



Example: Hydrogen Atom

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

$$H = \frac{P_e^2}{2m_e} + \frac{P_p^2}{2m_p} - \frac{e^2}{4\pi\epsilon_0 |\vec{R}_e - \vec{R}_p|}$$

- Switch to relative and COM coordinates gives:

$$H = \frac{P_{CM}^2}{2M} + \frac{P^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0 R} = H_{CM} + H_{rel}$$

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

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

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

$$H_{rel} = \frac{P^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0 R}$$

