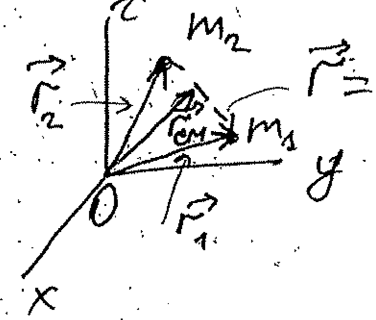
Lecture #1

Motion in central potential. Two-body problem.

Consider a system of two particles with masses m_1 and m_2 and positions $\vec{r}_1$ and $\vec{r}_2$ exerting equal and opposite forces on each other.



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

In classical mechanics the Lagrangian (L) that describes such a system is:

$$L = \underset{\substack{\uparrow \\ \text{kinetic} \\ \text{energy}}}{T} - \underset{\substack{\uparrow \\ \text{potential} \\ \text{energy}}}{V} = \frac{m_1}{2}|\dot{\vec{r}}_1|^2 + \frac{m_2}{2}|\dot{\vec{r}}_2|^2 - V(\vec{r}_1, \vec{r}_2) \tag{1.1}$$

Central potential is a potential that depends only on $|\vec{r}| = |\vec{r}_1 - \vec{r}_2|$, i.e. $V(\vec{r}_1, \vec{r}_2) = V(|\vec{r}_1 - \vec{r}_2|)$

Since V is a function of $|\vec{r}|$ (only), it's more convenient to use variables $\vec{r}$, & $\vec{r}_{CM}$ instead of $\vec{r}_1, \vec{r}_2$ $\Longrightarrow$

center of mass

Center of mass $\Rightarrow$ $\vec{r}_{CM} = \dfrac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}$

In $\vec{r}_{CM}$, $\vec{r}$ - coordinates, the Lagrangian is

$$L = \frac{1}{2} M |\dot{\vec{r}}_{CM}|^2 + \frac{1}{2}\mu |\dot{\vec{r}}|^2 - U(|\vec{r}|), \qquad (1.2)$$

where $M = m_1 + m_2$ - total mass

$\mu = \dfrac{m_1 m_2}{m_1 + m_2}$ - reduced mass

So, instead of considering the motion of two particles separately ($\vec{r}_1, \vec{r}_2$) we use $\vec{r}_{CM}$ that describes a position of the center of mass with respect to some origin O and $\vec{r}$ that describes a <u>relative</u> position of one particle with respect to another one.

<u>How is (1.2) better than (1.1)?</u>

1) The problem of two <u>mutually interacting</u> particles is reduced to that of the two <u>fictitious</u> particles that do <u>not</u> interact with each other, i.e. $U(|\vec{r}|)$, <u>not</u> $U(\vec{r}_{CM}, \vec{r})$!

2) One of the two fictitious particles is the center-of with a mass $M = m_1 + m_2$

From classical mechanics, recall the Lagrangian equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0$$

valid for central forces

q — generalized coordinate

If $\frac{\partial L}{\partial q} = 0 \Rightarrow q$ is a <u>cyclic</u> variable $\Rightarrow$

$$\underline{\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0}$$

If we define $p = \frac{\partial L}{\partial \dot{q}} \Rightarrow$

p — generalized momentum

$$\boxed{\frac{dp}{dt} = 0}$$

, i.e. the momentum corresponding to a cyclic variable is <u>conserved</u>

From (1.2) $\Rightarrow$ $\vec{r}_{CM}$ is a cyclic variable $\left(\frac{\partial L}{\partial \vec{r}_{CM}} = 0 !\right)$

$\Downarrow$

$\vec{P}_{CM} = M\dot{\vec{r}}_{CM}$ – total momentum is conserved

3) Another fictitious particle has mass μ, momentum $\vec{p} = \mu\dot{\vec{r}}$ and moves under potential $v(|\vec{r}|)$.

$\Downarrow$

two-body problem is reduced to one-body problem!

Since in QM we deal with Hamiltonians (4)
rather than Lagrangians $\Rightarrow$ write down Hamiltonian
for such a system using $\vec{P}_{cm} = M\dot{\vec{r}}_{cm}$ and $\vec{p} = \mu\dot{\vec{r}}$.

$$H = \frac{\vec{P}_{cm}^{\,2}}{2M} + \frac{\vec{p}^{\,2}}{2\mu} + V(|\vec{r}|)$$ – classical-mechanics Hamiltonian

In QM – the same, but $\vec{P}, \vec{r}$ are replaced with the momentum and position operators.

$$H = \underbrace{\frac{\vec{\underline{P}}_{cm}^{\,2}}{2M}}_{H_{cm}} + \underbrace{\frac{\vec{\underline{p}}^{\,2}}{2\mu} + V(|\vec{r}|)}_{H_r}$$

Obviously, $[H_{cm}, H_r] = 0 \Rightarrow$ share a basis of eigenvectors

$$H_{cm}|\psi\rangle = E_{cm}|\psi\rangle$$
$$H_r|\psi\rangle = E_r|\psi\rangle$$
$$\Rightarrow \underbrace{(H_{cm} + H_r)}_{H}|\psi\rangle = \underbrace{(E_{cm}+E_r)}_{E}|\psi\rangle$$

How can we use the fact that the total Hamiltonian is the sum of H_{cm} and H_r? $\Rightarrow$

In coordinate representation (for convenience) $\Rightarrow \underbrace{\psi(\vec{r}_{cm}, \vec{r}) = \psi_{cm}(\vec{r}_{cm})\psi_r(\vec{r})}_{\Downarrow}$

can separate variables!

To describe the motion of the system $\Rightarrow$ consider Schrödinger equation (let's forget about time evolution for now) $\Rightarrow$

$$H\Psi = E\Psi \Rightarrow$$

$$-\frac{\hbar^2}{2M}\underbrace{\Delta_{CM}}_{\frac{\partial^2}{\partial x_{CM}^2}+\frac{\partial^2}{\partial y_{CM}^2}+\frac{\partial^2}{\partial z_{CM}^2}}\Psi_{CM}(\vec{r}_{CM})\Psi_r(\vec{r}) - \frac{\hbar^2}{2\mu}\underbrace{\Delta_r}_{\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}}\Psi_r(\vec{r})\Psi_{CM}(\vec{r}_{CM}) +$$

$$+ U(|\vec{r}|)\Psi_{CM}(\vec{r}_{CM})\Psi_r(\vec{r}) = E\,\Psi_{CM}(\vec{r}_{CM})\Psi_r(\vec{r})$$

Divide by $\Psi_{CM}(\vec{r}_{CM})\Psi_r(\vec{r}) \Rightarrow$

$$\underbrace{-\frac{\hbar^2}{2M}\frac{\Delta_{CM}\Psi_{CM}(\vec{r}_{CM})}{\Psi_{CM}(\vec{r}_{CM})}}_{\text{depends only on } \vec{r}_{CM}} \underbrace{- \frac{\hbar^2}{2\mu}\frac{\Delta_r\Psi_r(\vec{r})}{\Psi_r(\vec{r})} + U(|\vec{r}|)}_{\text{depends only on } \vec{r}} = \underbrace{E}_{\text{const}} \qquad (1.3)$$

$$\Downarrow$$

$$\underbrace{E_{CM}}_{\text{const}} + \underbrace{E_r}_{\text{const}} = E$$

So, (1.3) breaks into two independent equations:

$$-\frac{\hbar^2}{2M}\frac{\Delta_{CM}\Psi_{CM}(\vec{r}_{CM})}{\Psi_{CM}(\vec{r}_{CM})} = E_{CM} \qquad (1.4a)$$

$$-\frac{\hbar^2}{2\mu}\frac{\Delta_r \Psi_r(\vec{r})}{\Psi_r(\vec{r})} + V(|\vec{r}|) = E_r, \qquad (1.4b)$$ ⑥

where $E_{cm} + E_r = E$

<u>HW</u>: show that the center-of-mass whose motion is described by (1.4a) moves as a free particle.

Eq. (1.4b) describes the behavior of the fictitious "relative" particle, i.e. that of the system of two interacting particles in the center-of-mass frame.

For the next 2 weeks, we'll be dealing with (1.4b), specify $V(|\vec{r}|)$ and look for $\Psi_r(\vec{r})$ and allowed energies E_r

<u>How to approach Eq. (1.4b)</u>? $\Rightarrow$ depends on the potential $V(\vec{r})$!

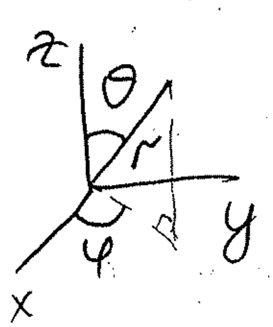
For many physical problems (such as particles in gravitational fields, Coulomb fields, etc.), the potential $V(|\vec{r}|)$ is spherically-symmetric, i.e.

$V(\vec{r}) = V(|\vec{r}|)$ In such cases, it is convenient to use <u>spherical</u> coordinates (r, θ, φ) instead of Cartesian coordinates (x, y, z). Why? $\Rightarrow$

$$V\left(\sqrt{x^2+y^2+z^2}\right) = V(r)$$

[illegible]! $\qquad$ simple!

Spherical coordinates



$$\left.\begin{aligned} x &= r\sin\theta\cos\varphi \\ y &= r\sin\theta\sin\varphi \\ z &= r\cos\theta \end{aligned}\right\} \Rightarrow x^2+y^2+z^2=r^2$$

$$r \geq 0$$
$$0 \leq \theta \leq \pi$$
$$0 \leq \varphi \leq 2\pi$$

Since for the Schrödinger equation we need

Laplacian $\underset{\text{Cartesian}}{\Delta} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \Rightarrow$ write it down in spherical coordinates

(Bonus HW)

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

Let's rewrite Eq. (1.4b) as

$$\Delta\Psi(r,\theta,\varphi) + \frac{2\mu}{\hbar^2}\left[E - V(r)\right]\Psi(r,\theta,\varphi) = 0 \qquad (1.5)$$

where $\Delta \equiv \Delta_r$, $\Psi \equiv \Psi_r$, $E \equiv E_r$

Note that $V \neq f(\theta,\varphi) \Rightarrow$ promising for the separation of variables!

$\Psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi) \Rightarrow$ substitute in (1.5)

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)Y + \frac{R}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \right.$$

$$\left. + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right] + \frac{2\mu}{\hbar^2}\left[E - U(r)\right]RY = 0$$

Divide by $R(r)Y(\theta,\varphi)$ and multiply by $r^2 \Rightarrow$

$$\underbrace{\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\cdot\frac{1}{R} + \frac{2\mu r^2}{\hbar^2}\left[E - U(r)\right]}_{= f_1(r)} +$$

$$+ \underbrace{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right]\cdot\frac{1}{Y}}_{= f_2(\theta,\varphi)} = 0 \qquad (1.6)$$

$$\underbrace{f_1(r)}_{=\lambda} + \underbrace{f_2(\theta,\varphi)}_{=-\lambda} = 0$$

$\lambda \leftarrow$ const

$\Rightarrow$ when does that happen for arbitrary (r,θ,φ)? $\Rightarrow$
$f_1(r) = -f_2(\theta,\varphi) = \text{const}$

So, solve (1.6) separately for radial and angular variables:

1) Radial part $f_1(r) = \lambda$

2) Angular part $f_2(\theta,\varphi) = -\lambda$

<u>Note</u>: (1.6) does <u>not</u> specify $U(r)$ and is valid for <u>any</u> spherically symmetric potential