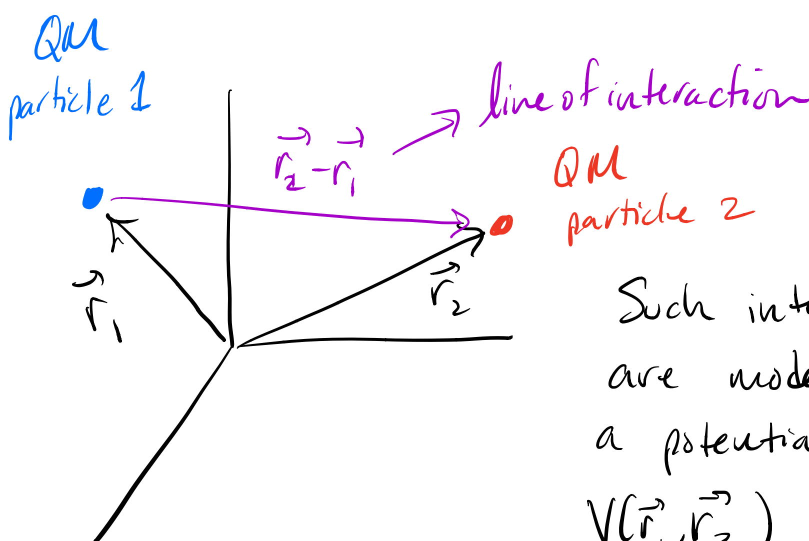
Central Potentials & the Energy Eigenvalue Problem

- Up to now we have focused on abstract 1D models of reality $\Rightarrow$ square well potentials.
- But now, we begin to build the architecture to tackle more refined models of quantum systems.
- these models will highlight the pairwise interaction between two particles. This pairwise interaction occurs along the line directly connecting the two particles, the relative position vector



Such interactions are modeled with a potential function $V(\vec{r}_1, \vec{r}_2)$

In our case we focus on central potentials, where only the absolute distance between the particles matter, $V(|\vec{r}_2 - \vec{r}_1|)$

Our Hamiltonian for this two particle system is thus,

$$H_{sys} = \frac{|\vec{p}_1|^2}{2m_1} + \frac{|\vec{p}_2|^2}{2m_2} + V(\vec{r}_1, \vec{r}_2)$$

$$H_{sys} = \frac{|\vec{p}_1|^2}{2m_1} + \frac{|\vec{p}_2|^2}{2m_2} + V(|\vec{r}_2 - \vec{r}_1|)$$

central potential

Now this Hamiltonian is significantly more complex than what we have dealt with previously.

(1) There's two particles!

(2) In 3D!

(3) with an interaction!

We can separate the center of mass from relative motion about the center of mass to simplify things.

Center of Mass & Relative Motion

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We first define $\vec{R}_{cm}$ the center of mass coordinate,

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

and the relative position coordinate, $\vec{r}$,

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

The momentum of the center of mass is just the total momentum of the system,

$$\vec{P} = \vec{p}_1 + \vec{p}_2$$

and the relative momentum is,

$$\vec{p}_{rel} = \frac{m_1\vec{p}_2 - m_2\vec{p}_1}{m_1+m_2}$$

⇐ note m_2 & m_1 are swapped from R_{cm} def.

⇒ comes from relative $\vec{v}$ def.

If we let $\frac{1}{\mu} \equiv \frac{1}{m_1} + \frac{1}{m_2}$ or $\mu \equiv \frac{m_1 m_2}{m_1 + m_2}$ (4)

↑ reduced mass

then,

$$\frac{\vec{P}_{rel}}{\mu} = \frac{\vec{p}_2}{m_2} - \frac{\vec{p}_1}{m_1}$$

and we can show,

$$H_{sys} = \frac{|\vec{p}_1|^2}{2m_1} + \frac{|\vec{p}_2|^2}{2m_2} + V(|\vec{r}_2 - \vec{r}_1|)$$

$$H_{sys} = \underbrace{\frac{|\vec{P}|^2}{2M}}_{H_{cm}} + \underbrace{\frac{|\vec{P}_{rel}|^2}{2\mu} + V(r)}_{H_{rel}}$$ where $M = m_1 + m_2$

we have separated the CM & rel parts of the Hamiltonian

How does this change the energy eigenvalue eqn?

$$H_{sys} \psi(\vec{R}_{cm}, \vec{r}) = E_{sys} \psi(\vec{R}_{cm}, \vec{r})$$

$$(H_{cm} + H_{rel}) \underbrace{\psi_{cm}(\vec{R}_{cm}) \psi_{rel}(\vec{r})}_{} = E_{sys} \psi_{cm}(\vec{R}_{cm}) \psi_{rel}(\vec{r})$$

proposed separated wave function $\Leftarrow$ $\psi(\vec{R}_{cm}, \vec{r}) = \psi_{cm}(\vec{R}_{cm}) \psi_{rel}(\vec{r})$

H_{cm} & H_{rel} only act on $\vec{R}_{cm}$ & $\vec{r}$ respectively so that,

$$\psi_{rel}(\vec{r})\,H_{cm}\,\psi_{cm}(\vec{R}_{cm}) + \psi_{cm}(\vec{R}_{cm})\,H_{rel}\,\psi_{rel}(\vec{r})$$

$$= E_{sys}\,\psi_{cm}(\vec{R}_{cm})\,\psi_{rel}(\vec{r})$$

Leap of faith: we assert that each Hamiltonian has it's own eigenvalue eqn.

$$H_{cm}\,\psi_{cm}(\vec{R}_{cm}) = E_{cm}\,\psi_{cm}(\vec{R}_{cm})$$

$$H_{rel}\,\psi_{rel}(\vec{r}) = E_{rel}\,\psi_{rel}(\vec{r})$$

So that,

$$H_{sys}\,\psi_{cm}(\vec{R}_{cm})\,\psi_{rel}(\vec{r}) = (E_{cm}+E_{rel})\,\psi_{cm}(\vec{R}_{cm})\,\psi_{rel}(\vec{r})$$

or

$$E_{sys} = E_{cm} + E_{rel}$$

Given this approach we can show that H_{cm} just gives rise to free particle solutions with $\vec{P}_{tot} = \vec{p}_1 + \vec{p}_2$

$$H_{cm}\psi_{cm}(\vec{R}) = E_{cm}\psi_{cm}(\vec{R})$$

$$\frac{|\vec{P}|^2}{2M}\psi_{cm}(\vec{R}) = E_{cm}\psi_{cm}(\vec{R})$$

if $\vec{R} = \langle X, Y, Z \rangle$ ← all caps, then the operator is simply,

$$\vec{P} \doteq -i\hbar\left(\frac{\partial}{\partial X}\hat{i} + \frac{\partial}{\partial Y}\hat{j} + \frac{\partial}{\partial Z}\hat{k}\right) = -i\hbar\nabla_R$$

gradient operator for R.

$$\frac{-\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right)\psi_{cm}(X, Y, Z) = E_{cm}\psi_{cm}$$

the solution is the 3D version of the free particle,

$$\psi_{cm}(X, Y, Z) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i(P_x X + P_y Y + P_z Z)/\hbar}$$

with

$$E_{cm} = \frac{1}{2M}\left(P_x^2 + P_y^2 + P_z^2\right)$$

Now this is all we get from H_{cm}. It's not quite as interesting as H_{rel} as we will see.

H_{rel} & Spherical Coordinates

Now, the bulk of the interesting physics is in how the two particles interact relative to the center of mass,

$$H = \frac{|P_{rel}|^2}{2\mu} + V(r)$$

the momentum operator here is given by,

$$\vec{P}_{rel} \doteq -i\hbar\underbrace{\left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right)}_{\text{lower case}} = -i\hbar\nabla_{\underset{\sim}{r}}$$

lower case

we will drop the subscripts as we know we are focused on the relative Hamiltonian,

$$H \doteq -\frac{\hbar^2}{2\mu}\nabla^2 + V(r)$$

all relative H_{rel}, E_{rel}, etc.

So,

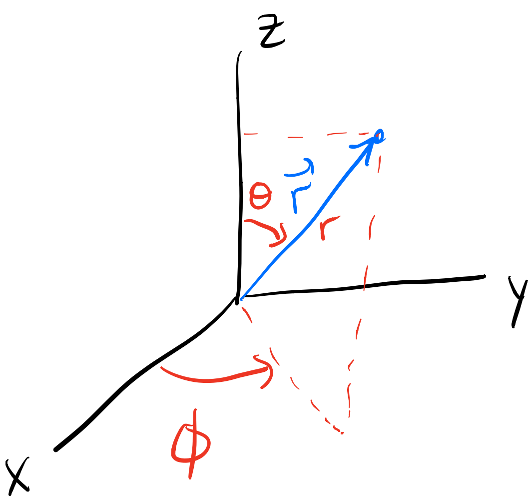
$$H\psi(\vec{r}) = E\psi(\vec{r})$$

$$\boxed{\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\psi(\vec{r}) = E\psi(\vec{r})}$$

energy eigenvalue eqn. for central potential

Because the potential is central (only r dependent) it makes sense to solve this problem in spherical coordinates. So we need ∇^2 in spherical coords. 8

Reminder: Spherical Coords



$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$

From this, volume element.

$dV = r^2 \sin\theta \, dr \, d\theta \, d\phi$

For us it's useful to introduce $d\Omega$, the solid angle,

$$dV = (r^2 dr)(\sin\theta \, d\theta \, d\phi) = (r^2 dr)\, d\Omega$$

$$d\Omega \equiv \sin\theta \, d\theta \, d\phi$$

these definitions also give us,

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}$$

and finally (yikes)

$$\nabla^2 = \nabla \cdot \nabla$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}$$

We are seeking $H|E\rangle = E|E\rangle$ just for a central potential with relative coordinates. We get the following,

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi + V(r)\psi = E\psi$$

where $\psi = \psi(r,\theta,\phi)$

and our game is to find energy eigenstates,

$$|E\rangle \doteq \psi_E(r,\theta,\phi)$$

This will be helped alot by using orthogonal & complete functions (soon).