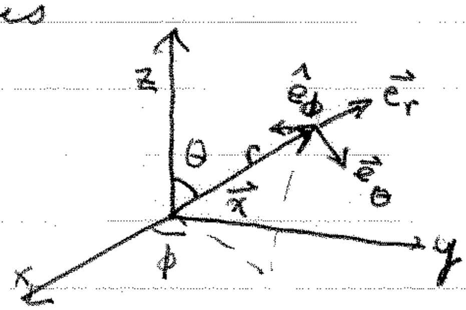
# Lecture 8 : Central Potentials and the Radial Equation

- **Review Classical Dynamics**

A central force is one that depends only on the distance from the origin. In such cases it is most convenient to use spherical coördinates to describe dynamics




$$\int d^3x = \int_0^\infty r^2 dr \int d\Omega$$

Note: $\vec{e}_r, \vec{e}_\theta, \vec{e}_\phi$ depend on the position $\vec{x}$

$$\vec{e}_r = \frac{\vec{x}}{r}$$

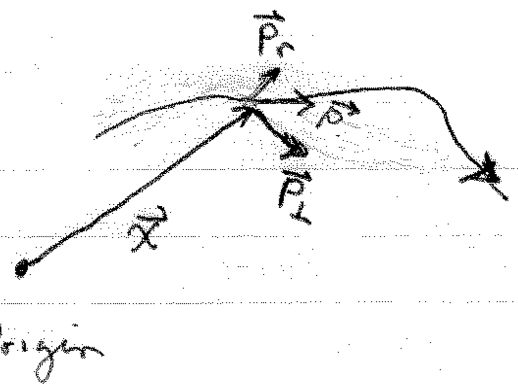
Since for a central force $\vec{F}$ is in the $\vec{e}_r$ direction, the potential energy must be a function only or $r$ and not $\theta$ and $\phi$ $\quad V(x,y,z) = V(r)$

$\Rightarrow$ Hamiltonian for a spinless particle

$$H = \frac{p^2}{2m} + V(r)$$

Classical equations of motion
$$\dot{\vec{x}} = \frac{\vec{p}}{m}$$
$$\dot{\vec{p}} = -\vec{\nabla}V = -\frac{dV}{dr}\vec{e}_r$$

In is useful to break up the trajectory into radial and angular motion




Origin

$$\vec{p} = \vec{p}_r + \vec{p}_\perp$$

radial momentum

$$p_r = |\vec{p}_r| = \vec{e}_r \cdot \vec{p}$$
$$= \frac{\vec{x}}{r}\cdot\vec{p}$$

The angular momentum $\vec{L} = \vec{x} \times \vec{p} = \vec{x} \times (\vec{p}_r + \vec{p}_\perp)$

$$\Rightarrow \vec{L} = \vec{x} \times \vec{p}_\perp \Rightarrow \frac{d\vec{L}}{dt} = \underbrace{\dot{\vec{x}}}_{\vec{p}} \times \vec{p}_\perp + \vec{x} \times \underbrace{\dot{\vec{p}}_\perp}_{0}$$

$$\Rightarrow \boxed{\frac{d\vec{L}}{dt} = 0}$$ In a central potential angular momentum is conserved

Decomposition of kinetic energy into radial and angular components:

Note: $|\vec{L}|^2 = L^2 = |\vec{x} \times \vec{p}_\perp|^2 = r^2 p_\perp^2 \Rightarrow p_\perp^2 = \frac{L^2}{r^2}$

$$\therefore |\vec{p}|^2 = p^2 = p_r^2 + p_\perp^2 = p_r^2 + \frac{L^2}{r^2}$$

$$\therefore H = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(r)$$

Since L is fixed for a given trajectory we can set is equal to a constant

$$\Rightarrow H = \frac{p_r^2}{2m} + V_{eff}^{(L)}(r)$$

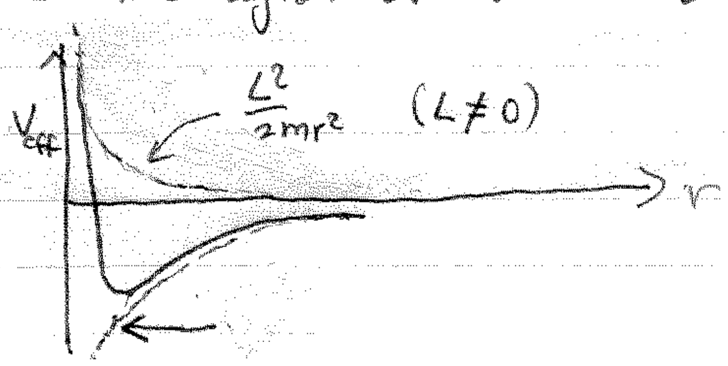
$$V_{eff}^{(L)}(r) = \frac{L^2}{2mr^2} + V(r)$$

Angular momentum "barrier"

For a fixed L the dynamics is reduced to one dimension

e.g. $V(r) = \frac{C}{r}$

$C > 0$



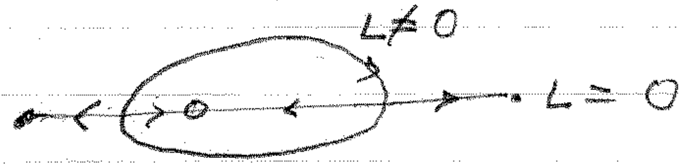

Note

$0 \leq r \leq \infty$

no negative $r$

The angular momentum term provides a "centrifugal" barrier to motion near origin

Kepler motion




Quantum problem:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r}) \quad , \quad \hat{r}^2 = \hat{x}^2 + \hat{y}^2 + \hat{z}^2$$

Angular momentum $\hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}}$

Aside: $\left.\begin{aligned} [\hat{L}_i, \hat{p}_j] &= i\hbar\, \epsilon_{ijk}\, \hat{p}_k \\ [\hat{L}_i, \hat{x}_j] &= i\hbar\, \epsilon_{ijk}\, \hat{x}_k \end{aligned}\right\}$ Vector operators

$$\Rightarrow [\hat{L}_i, \hat{p}^2] = [\hat{L}_i, \hat{r}^2] = 0$$

$\hat{p}^2$ and $\hat{r}^2$ are scalar w.r.t. rotation

$\therefore$ If $\hat{V}$ is a function only of $\hat{r}$

$[\hat{H}, \hat{L}_i] = 0$ i.e. $\hat{H}$ is rotationally invariant about any axis

$\Rightarrow [\hat{H}, \hat{L}^2] = 0$

$\Rightarrow$ L is conserved

# Separability of $\hat{H}$

Aside: $\hat{L}^2 = \hat{\vec{L}}\cdot\hat{\vec{L}} = (\hat{\vec{x}}\times\hat{\vec{p}})\cdot(\hat{\vec{x}}\times\hat{\vec{p}}) = -(\hat{\vec{x}}\times\hat{\vec{p}})\cdot(\hat{\vec{p}}\times\hat{\vec{x}}$

$$= -\hat{\vec{x}}\cdot\left[\hat{\vec{p}}\times(\hat{\vec{p}}\times\hat{\vec{x}})\right] = -\hat{\vec{x}}\cdot\left[\hat{\vec{p}}(\hat{\vec{p}}\cdot\hat{\vec{x}}) - \hat{p}^2\hat{\vec{x}}\right.$$

$$\Rightarrow \hat{L}^2 = -(\hat{\vec{x}}\cdot\hat{\vec{p}})(\hat{\vec{p}}\cdot\hat{\vec{x}}) + \hat{\vec{x}}\cdot(\hat{p}^2\hat{\vec{x}})$$

Aside: $\hat{p}^2\hat{\vec{x}} = \hat{\vec{x}}\,\hat{p}^2 - 2i\hbar\,\hat{\vec{p}}$

$$\Rightarrow \hat{L}^2 = \hat{r}^2\,\hat{p}^2 - (\hat{\vec{x}}\cdot\hat{\vec{p}})(\hat{\vec{p}}\cdot\hat{\vec{x}}) - 2i\hbar\,\hat{\vec{x}}\cdot\hat{\vec{p}}$$

$$\Rightarrow \hat{p}^2 = \left\{\frac{1}{\hat{r}^2}(\hat{\vec{x}}\cdot\hat{\vec{p}})(\hat{\vec{p}}\cdot\hat{\vec{x}}) + \frac{2i\hbar}{\hat{r}^2}\hat{\vec{x}}\cdot\hat{\vec{p}}\right\} + \frac{\hat{L}^2}{r^2}$$

Classically $p^2 = p_r^2 + \frac{L^2}{\hat{r}^2}$

$$\Rightarrow \boxed{\begin{aligned}\hat{p}^2 &= \hat{p}_r^2 + \frac{\hat{L}^2}{\hat{r}^2}\\ \hat{p}_r^2 &= \frac{1}{\hat{r}^2}(\hat{\vec{x}}\cdot\hat{\vec{p}})(\hat{\vec{p}}\cdot\hat{\vec{x}}) + \frac{2i\hbar}{\hat{r}^2}\hat{\vec{x}}\cdot\hat{\vec{p}}\end{aligned}}$$

Careful at origin

Does this make sense?

Classically $p_r = \vec{e}_r\cdot\vec{p} = \frac{\vec{x}}{r}\cdot\vec{p}$

Quantum $\hat{p}_r = \frac{1}{2}\left(\frac{\hat{\vec{X}}}{r}\cdot\hat{\vec{p}} + \hat{\vec{p}}\cdot\frac{\hat{\vec{X}}}{r}\right)$

Check $\hat{p}_r^2$ gives result above

Thus, $$\hat{H} = \frac{\hat{P}_r^2}{2m} + \frac{\hat{L}^2}{2m\hat{r}^2} + V(\hat{r})$$

3 degrees of freedom requires three mutually commuting operators to specify state

$$[\hat{H}, \hat{L}^2] = 0 \quad \text{and} \quad [\hat{H}, \hat{L}_i] = 0$$

$$[\hat{L}^2, \hat{L}_i] = 0 \quad \text{but} \quad [\hat{L}_i, \hat{L}_j] \neq 0$$

$\Rightarrow$ Pick <u>one</u> component of $\hat{L}$ (say z)

$\Rightarrow$ Mutually commuting set $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$

Decompose Hilbert space as tensor product in spherical coordinates:

$$\mathcal{H} = h_r \otimes h_\theta \otimes h_\phi$$

~~Eign~~ Energy eigenstates:

$$|\psi_{n_r, l, m}\rangle = \underbrace{|n_r\rangle}_{\substack{\text{radial state} \\ \text{acts on } h_r}} \otimes \underbrace{|l, m\rangle}_{\substack{\text{eigenstates of } \hat{L}^2 \text{ and } \hat{L}_z \\ \text{acts on } h_\theta \otimes h_\phi}}$$

$$\hat{H}|\psi_{n_r, l, m}\rangle = E_{n_r, l}|\psi_{n_r, l, m}\rangle$$

Note: $\hat{H}$ independent of $\hat{L}_z$ $\Rightarrow$ E independent of m $\Rightarrow$ <u>essential degeneracy</u>

$$\hat{H}\,|\psi_{n_r,\ell,m}\rangle = \left(\frac{\hat{P}_r^2}{2m} + \frac{\hbar^2}{2mr^2}\ell(\ell+1) + V(\hat{r})\right)|n_r\rangle \otimes |\ell,m\rangle$$

$$= E_{n_r,\ell}\;|n_r\rangle \otimes |\ell,m\rangle$$

Project out $|\ell,m\rangle$ component

radial equation:

$$\Rightarrow \boxed{\left[\frac{\hat{P}_r^2}{2m} + \underbrace{\frac{\hbar^2}{2mr^2}\ell(\ell+1) + V(\hat{r})}_{V_{eff}^{(\ell)}(\hat{r})}\right]|n_r\rangle = E_{n_r,\ell}\,|n_r\rangle}$$

Position representation:

$$\psi(\vec{x}) = \psi(r,\theta,\phi) = \langle \vec{x}|\psi\rangle$$

$$\langle\psi|\psi\rangle = \int_0^\infty r^2 dr \int d\Omega\; |\psi(r,\theta,\phi)|^2$$

Eigenstates for central potential:

$$\psi_{n_r,\ell,m}(r,\theta,\phi) = \underbrace{\langle r|n_r\rangle}\;\langle\theta,\phi|\ell,m\rangle$$

$$\equiv R_{n_r}(r)\;\;Y_{\ell,m}(\theta,\phi)$$

$\Uparrow$

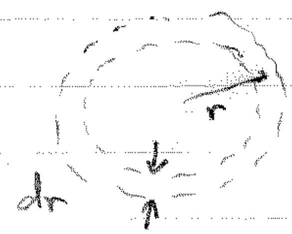
radial wave function

$$\langle\psi|\psi\rangle = \int_0^\infty r^2\,|R_{n_r}(r)|^2\,dr\;\;\underbrace{\int d\Omega\,|Y_{\ell,m}(\theta,\phi)|^2}_{=1}$$

Normalization of radial wave function

$$\int_0^\infty r^2 |R_{n_r}(r)|^2 dr = 1$$

Probability density to find particle between radius $r$ and $r+dr$ $\quad P(r) = r^2 |R_{n_r}(r)|^2 dr$





Probability depends on volume of shell $\sim r^2 dr$

Reduced radial wave function $\quad u_{n_r}(r) \equiv r R_{n_r}(r)$

Normalization $\int_0^\infty |u_{n_r}(r)|^2 = 1$

Representation of $\hat{p}_r$ in position

$$\hat{\vec{p}} \doteq -i\hbar \vec{\nabla} \qquad \hat{\vec{x}} \doteq \vec{x} = r\,\vec{e}_r$$

$$\hat{p}_r \doteq \frac{1}{2}\left(\frac{\vec{x}}{r}\cdot(-i\hbar\vec{\nabla}) + (-i\hbar\vec{\nabla})\cdot\left(\frac{\vec{x}}{r}\right)\right)$$

$$\langle \vec{x}|\hat{p}_r|\psi\rangle = -\frac{i\hbar}{2}\left(\frac{\partial\psi}{\partial r} + \vec{\nabla}\cdot(\vec{e}_r\psi)\right)$$

$$= -\frac{i\hbar}{2}\left(\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\psi)\right) = -\frac{i\hbar}{2}\left(2\frac{\partial\psi}{\partial r} + \frac{2\psi}{r}\right)$$

$$= -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\psi = -\frac{i\hbar}{r}\frac{\partial}{\partial r}(r\psi)$$

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Thus: In position representation

$$\hat{p}_r \doteq \frac{-i\hbar}{r}\frac{\partial}{\partial r}(r\ \ )$$

$$\hat{p}_r^2 = -\frac{\hbar^2}{r}\frac{\partial^2}{\partial r^2}(r\ \ )$$

Thus, the differential form of the radial eqn.

$$-\frac{\hbar^2}{2mr}\frac{d^2}{dr^2}\left(r R_{n_r}(r)\right) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} R_{n_r}(r) + V(r) R_{n_r}(r)$$

$$= E_{n_r,\ell} R_{n_r}(r)$$

Multiply through by r ; use reduced radial fnct

$$\Rightarrow \boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2 u_{n_r}}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r)\right] u_{n_r}(r)\Big) = E_{n_r,\ell} u}$$

radial equation

Looks like T.I.S.E. in 1D with potential

$$V_{eff}(r) = V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$

<u>However</u>: Only on ½-line $0 < r < \infty$

$\Rightarrow$ Need boundary condition at $r = 0$

## Boundary condition at origin

Suppose $V(r)$ is not horribly singular at $r=0$, and does not blow up faster than $\frac{1}{r^2}$

$\Rightarrow$ Near origin the radial equation looks like

$$\frac{\hbar^2}{2m}\left(\frac{-d^2}{dr^2} + \frac{l(l+1)}{2mr^2}\right) u = E\, u$$

Asymptotically near origin $u(r) \sim C r^s$

$$\Rightarrow -s(s-1) + l(l+1) = 0$$

$$\Rightarrow \text{ either } s = l+1 \text{ or } s = -(l+2)$$

$\Rightarrow$ Solution near origin $u \sim \begin{cases} C r^{l+1} \\ \text{or} \\ C \frac{1}{r^{l+2}} \end{cases}$

Physical solution does not blow up. thus if potential includes origin we must reject the $\frac{1}{r^{l+2}}$ solution

$\Rightarrow$ $u(r) \sim r^{l+1}$ near origin

$\Rightarrow$ Extra boundary condition $u(r=0) = 0$ like wall at $\infty$

Note: $R = r\, u(r) \sim r^l$ so for $l = 0$ $R$ does not vanish at origin