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 coordinates to describe dynamics.

\[
\int_0^\infty \int_0^{2\pi} \int_0^\pi \rho^2 \sin \theta \, d\rho \, d\theta \, d\phi = \int_0^\infty \int_0^{2\pi} \int_0^\pi \rho^2 \sin \theta \, d\rho \, d\theta \, d\phi
\]

Since for a central force \( \vec{F} \) is in the \( \vec{e}_r \) direction, the potential energy must be a function only of \( r \) and not \( \theta \) and \( \phi \)

\[
V(x, y, z) = V(r)
\]

\( \Rightarrow \) Hamiltonian for a spinless particle

\[
H = \frac{\vec{p}_r^2}{2m} + V(r)
\]

Classical equations of motion:

\[
\dot{r} = \frac{\vec{p}_r}{m}, \quad \dot{\theta} = \frac{\vec{p}_\theta}{r}, \quad \dot{\phi} = \frac{\vec{p}_\phi}{r^2}
\]

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

\[
\vec{p} = \vec{p}_r + \vec{p}_\perp
\]

Radial momentum:

\[
P_r = |\vec{p}_r| = \frac{\vec{e}_r \cdot \vec{p}}{r}
\]
The angular momentum \( \vec{L} = \vec{r} \times \vec{p} = \vec{r} \times (\vec{p}_r + \vec{p}_\perp) \)

\[ \Rightarrow \vec{L} = \vec{r} \times \vec{p}_\perp \quad \Rightarrow \frac{dL^2}{dt} = \frac{d\vec{L}}{dt} = \vec{r} \times \vec{p}_\perp + \vec{\dot{r}} \times \vec{p}_\perp \]

\[ \Rightarrow \frac{dL^2}{dt} = 0 \quad \text{In a central potential angular momentum is conserved} \]

**Decomposition of kinetic energy into radial and angular components:**

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

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

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

Since \( L \) is fixed for a given trajectory we can set it equal to a constant

\[ \Rightarrow H = \frac{p_r^2}{2m} + V_{\text{eff}}^{(L)}(r) \quad \text{Angular momentum barrier} \]

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

For a fixed \( L \) the dynamics is reduced to one dimension

\[ V(r) = \frac{C}{r} \quad \text{for } C > 0 \]

\[ \text{Note } \quad 0 \leq r \leq \infty \quad \text{no negative } \]

\[ \text{e.g. } V(r) = \frac{C}{r} \quad \frac{L^2}{2mr^2} \quad (L \neq 0) \]
The angular momentum term provides a "centrifugal" barrier to motion near origin

\[ L \neq 0 \quad \text{ Kepler motion } \quad \Rightarrow \quad L = 0 \]

**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 \( \hat{L} = \hat{\mathbf{x}} \times \hat{\mathbf{p}} \)

Aside: \[
[\hat{L}_i, \hat{p}_j] = ik \epsilon_{ijk} \hat{p}_k \quad \text{ } \quad [\hat{L}_i, \hat{x}_j] = ik \epsilon_{ijk} \hat{x}_k \]

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

\( \hat{r}^2 \) and \( \hat{r}^2 \) are scalar w.r.t. rotation

\[ \therefore \text{ If } \hat{V} \text{ is a function only of } \hat{r} \]

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

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

\[ \Rightarrow L \text{ is conserved} \]
Separability of $\hat{A}$

Aside: \[ \hat{L}^2 = \hat{L} \cdot \hat{L} = (\hat{\mathbf{x}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{x}} \times \hat{\mathbf{p}}) = -(\hat{\mathbf{x}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{p}} \times \hat{\mathbf{x}}) = -\hat{\mathbf{x}} \cdot [\hat{\mathbf{p}} \times (\hat{\mathbf{p}} \times \hat{\mathbf{x}})] = -\hat{\mathbf{x}} \cdot \left[ \hat{\mathbf{p}} (\hat{\mathbf{p}} \cdot \hat{\mathbf{x}}) - \hat{\mathbf{p}}^2 \hat{\mathbf{x}} \right] \]

\[ \Rightarrow \hat{L}^2 = - (\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}) (\hat{\mathbf{p}} \cdot \hat{\mathbf{x}}) + \hat{\mathbf{x}} \cdot (\hat{\mathbf{p}}^2 \hat{\mathbf{x}}) \]

Aside: \[ \hat{p}^2 \hat{x} = \hat{x} \hat{p}^2 \equiv 2 i \hbar \hat{p} \]

\[ \Rightarrow \hat{L}^2 = \hat{p}^2 \hat{p}^2 - (\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}) (\hat{\mathbf{p}} \cdot \hat{\mathbf{x}}) = 2 i \hbar \hat{x} \cdot \hat{p} \]

\[ \Rightarrow \hat{p}^2 = \left\{ \frac{1}{\hbar^2} (\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}) (\hat{\mathbf{p}} \cdot \hat{\mathbf{x}}) + \frac{2 i \hbar}{\hbar^2} \hat{x} \cdot \hat{p} \right\} + \frac{\hat{L}^2}{\hbar^2} \]

Classically \[ p^2 = p^2_r + \frac{L^2}{\hbar^2} \]

\[
\begin{align*}
\hat{p}^2 &= \hat{p}^2_r + \frac{\hat{L}^2}{\hbar^2} \\
\hat{p}^2_r &= \frac{1}{\hbar^2} (\hat{x} \cdot \hat{p}) (\hat{p} \cdot \hat{x}) + \frac{2 i \hbar}{\hbar^2} \hat{x} \cdot \hat{p} \\
\end{align*}
\]

Does this make sense?

Classically \[ p_r = \mathbf{\hat{e}}_r \cdot \hat{p} = \frac{\hat{x}}{\hat{r}} \cdot \hat{p} \]

Quantum \[ \hat{p}_r = \frac{1}{2} \left( \hat{x} \cdot \frac{\hat{p}}{\hat{r}} + \frac{\hat{p}}{\hat{r}} \cdot \hat{x} \right) \]

Check \[ \hat{p}^2_r \] gives result above
Thus, \[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{\hat{L}^2}{2m} + V(\hat{r}) \]

3 degrees of freedom requires three mutually commuting operators to specify state \[ [\hat{L}_z, \hat{L}_i] = 0 \quad \text{and} \quad [\hat{L}_z, \hat{L}_j] = 0 \]
\[ [\hat{L}_i, \hat{L}_j] \neq 0 \]

\[ \Rightarrow \text{Pick one component of } \hat{L}_z \text{ (say } z) \]
\[ \Rightarrow \text{ Mutually commuting set } \{ \hat{A}, \hat{L}_i, \hat{L}_z \} \]

Decompose Hilbert space as tensor product in spherical coordinates:
\[ \mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_\theta \otimes \mathcal{H}_\phi \]

Energy eigenstates:
\[ |\psi_{n_r, l, m}\rangle = |n_r\rangle \otimes |l, m\rangle \]
\[ \hat{A} |\psi_{n_r, l, m}\rangle = E_{n_r, l} |\psi_{n_r, l, m}\rangle \]

Note: \( \hat{A} \) independent of \( \hat{L}_z \) \( \Rightarrow \) \( E \) independent of \( m \) \( \Rightarrow \) essential degeneracy
\[ \hat{H} |\psi_{n, l, m}\rangle = \left( \frac{\hat{p}_r^2}{2m} + \frac{\hbar^2}{2mr^2} l(l+1) + V(r) \right) |\psi_{n, l, m}\rangle = E_{n, l, m} |\psi_{n, l, m}\rangle \]

Project out \( |l, m\rangle \) component

\[ \Rightarrow \left[ \frac{\hat{p}_r^2}{2m} + \frac{\hbar^2}{2mr^2} l(l+1) + V(r) \right] |n, \ell\rangle = E_{n, \ell, m} |n, \ell\rangle \]

Radial equation:

\[ V_{\text{eff}}^{(\ell)}(\hat{r}) \]

Position representation:

\[ \Psi(x) = \Psi(r, \theta, \phi) = \langle x | \Phi \rangle \]

\[ \langle \Phi | \Phi \rangle = \int_0^\infty r^2 dr \int d\Omega \ |\Psi(r, \theta, \phi)\|^2 \]

Eigenstates for central potential:

\[ \Psi_{n, \ell, m} = \langle r|n, \ell\rangle \langle \theta, \phi | l, m \rangle \]

\[ \equiv R_n(r) \ Y_{\ell m}(\theta, \phi) \]

Radial wave function

\[ \langle \Phi | \Phi \rangle = \int_0^\infty r^2 |R_n(r)|^2 dr \int d\Omega \ |Y_{\ell m}(\theta, \phi)|^2 = 1 \]
Normalization of radial wave function
\[ \int_0^\infty r^2 |R_n(r)|^2 \, dr = 1 \]

Probability density to find particle between radius \( r \) and \( r + dr \):
\[ P(r) = r^2 |R_n(r)|^2 \, dr \]

Reduced radial wave function \( \mathcal{U}_n(r) = r R_n(r) \)
Normalization \( \int_0^\infty |\mathcal{U}_n(r)|^2 \, dr = 1 \)

Representation of \( \hat{p}_r \) in position:
\[ \hat{\mathbf{p}} = -i\hbar \hat{\nabla} \]
\[ \hat{\mathbf{x}} = \hat{\mathbf{x}} = r \hat{\mathbf{e}}_r \]
\[ \hat{p}_r = \frac{1}{i} \left( \frac{\hat{\mathbf{x}} \cdot (-i\hbar \hat{\nabla})}{r} + (-i\hbar \hat{\nabla}) \cdot \left( \frac{\hat{\mathbf{x}}}{r} \right) \right) \]
\[ \langle \mathbf{x} | \hat{p}_r | \psi \rangle = -i\hbar \left( \frac{2\psi}{\partial r} + \hat{\nabla} \cdot (\hat{\mathbf{e}}_r \psi) \right) \]
\[ = -i\hbar \left( \frac{2\psi}{\partial r} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \psi) \right) = -i\hbar \left( \frac{2}{\partial r} + \frac{2}{r} \right) \]
\[ = -i\hbar \left( \frac{2}{\partial r} + \frac{1}{r} \right) \psi = -i\hbar \frac{2}{r} \left( r \psi \right) \]

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Thus: In position representation
\[ \hat{p}_r = -\frac{i\hbar}{r} \frac{\partial}{\partial r} (r) \]
\[ \hat{p}_r^2 = -\frac{\hbar^2}{r} \frac{\partial^2}{\partial r^2} (r) \]
Thus, the differential form of the radial eqn.
\[ -\frac{\hbar^2}{2mr^2} \frac{d^2}{dr^2} (r R_n(r)) + \frac{\hbar^2}{2mr^2} \frac{l(l+1)}{2} R_n(r) + V(r) R_n(r) = E \frac{n}{r} R_n(r) \]
Multiply through by \( r \); use reduced radial ansat
\[ \Rightarrow \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2}{2mr^2} \frac{l(l+1)}{2} + V(r) \right] R_n(r) = E_n R_n(r) \]
radial equation
Looks like T.I.S.E. in 1D with potential
\[ V_{\text{eff}}(r) = V(r) + \frac{\hbar^2}{2mr^2} \frac{l(l+1)}{2} \]
However: Only on \( 1/2 \)-line \( 0 < r < \infty \)
\[ \Rightarrow \text{Need boundary condition at } r = 0 \]
Boundary condition at origin

Suppose $V(r)$ is not horribly singualr at $r=0$, and does not blow up faster than $1/r^2$

$\Rightarrow$ 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 $u(r) \sim Cr^n$

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

$\Rightarrow$ Either $s = l+1$ or $s = -(l+2)$

$\Rightarrow$ Solution near origin $u \sim \begin{cases} Cr^{l+1} & \text{on } r \leq 1 \\ C \frac{1}{r^{l+2}} & \text{on } r \geq 1 \end{cases}$

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

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

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

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