11 / 23 / 15

Lecture 36 – Solving Central Potentials

1. The Radial Schrödinger Equation
2. The $\ell=0$ Case
3. Generally Solvable Potentials

1. Radial Schrödinger Equation (3.7 SAK)

We've shown that the Schrödinger wave equation is separable

radial component, spherical harmonics

$$\Psi_{\alpha\ell m}(r,\theta,\varphi) = R_{\alpha,\ell}(r)\,Y_{\ell,m}(\theta,\varphi)$$

α = unspecified Quantum Number

$R_{\alpha\ell}(r) = r\,U_{\alpha\ell}(r) \longleftrightarrow$ No m dependence! (R rotationally invariant)

$$\frac{-\hbar^2}{2m}U'' + \underbrace{V_{eff,\ell}(r)}U = E_{\alpha,\ell}U$$

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

$\mathcal{D}(R)|\ell,m\rangle \to \ell$ fixed, m changes

$$e^{-iJ_x\varphi/\hbar}\Psi_{\alpha\ell m} = \sum_{m'=-\ell}^{\ell}\mathcal{D}^{(\ell)}_{mm'}(R_x)\Psi_{\alpha\ell m'}$$

cannot change energy because $[\mathcal{H}, J_x]=0$

$$\rightarrow E_{\alpha\ell m} = E_{\alpha\ell m'} = \underbrace{E_{\alpha\ell}}_{\text{energy eigenstates m-independent}}$$

(no degeneracies in 1-Dimension)

$$\Rightarrow R_{\alpha\ell m}(r) = R_{\alpha\ell m'}(r) = R_{\alpha\ell}(r)$$

Boundary condition:

@ $r=0$, for $\ell>0$

$$\frac{-\hbar^2}{2m}U'' + \frac{\ell(\ell+1)\hbar^2}{2mr^2}U = 0$$

$$U'' = \frac{U}{r^2}\ell(\ell+1)$$

$\longrightarrow U(r) \propto r^{(\ell+1)}$; $\cancel{r^{-\ell}}$ not allowed - diverges for $\ell>0$

*Note: Sakurai's argument for $\ell>0$ is problematic because he uses the current, $\vec{j}$, but $\vec{j}=0$ if Ψ is chosen to be real

A separate argument is needed for $\ell=0$:

$$\ell=0 \rightarrow m=0 \rightarrow Y_{\ell m}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

$$\Psi(r,\theta,\varphi) = \frac{R(r)}{\sqrt{4\pi}}$$

but $\nabla\Psi$ must be well-defined @ $r=0$

$$\nabla\Psi = \frac{\hat{r}}{\sqrt{4\pi}}\partial_r R\Big|_{r=0} = 0$$

$\Rightarrow$ **The function Ψ must be symmetric in every direction!**

($\nabla\Psi \neq 0$ implies a prefered direction -- breaks rotational symmetry)

$$\partial_r(rU)\big|_{r=0} = 0 \Rightarrow \underbrace{U(r\to 0)=0}_{\text{our boundary condition as } r\to 0\ (\ell=0)}$$

$$\underbrace{r\partial_r U}_{0} + U = 0$$

* While our argument for $\ell>0$ did not work for $\ell=0$, this argument works for all ℓ

$$U(r) \propto r^{(\ell+1)},\ \ell \geq 0$$

$\rightarrow$ **These relations are applicable for <u>any</u> central potential**

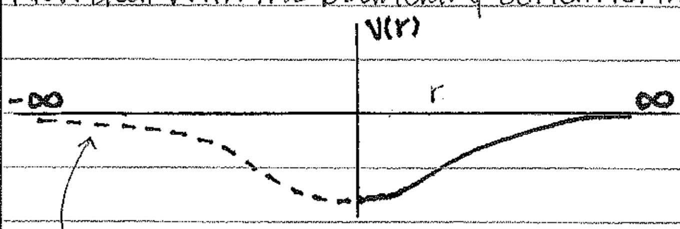
2. <u>Solving the $\ell=0$ [Central Potential] Case</u>

$$V_{eff,\ell}(r) = V(r)$$

$\Rightarrow$ **3D problem $\rightarrow$ 1D problem** (spherical symmetry simplification)

$$\frac{-\hbar^2}{2m}U''_\alpha + V(r)U_\alpha(r) = E_{\alpha,\ell=0}U(r)$$

Now deal with the boundary condition...



Extend the potential symmetrically to $r \in [-\infty,\infty]$ by defining $V(r) = V(-r)$

$\rightarrow$ U must be an eigenstate of parity symmetry

Changing variable $r \rightarrow -r$

$$\hookrightarrow \left[\frac{-\hbar^2}{2m}\partial_r^2 + V(r)\right]U(-r) = EU(-r)$$

and since there is no degeneracy in 1D...

$$U(r) \propto U(-r)$$

Since $U(r\to 0)\propto r$ and $U(r)$ is an $\underbrace{\text{analytic function}}_{\text{has a nice series expansion}}$

$\Rightarrow U(r) = -U(-r)$

(i.e. odd states)

More generally:

Parity operator $\hat{P}$ defined such that $\underbrace{\hat{x}\hat{P} = -\hat{P}\hat{x}}_{\hat{x}\ \&\ \hat{P}\text{ anti-commute}}$

└ a.k.a. space inversion

(unitary; expressed as $\hat{\pi}$ in Sakurai, pg. 269)

$\hat{P}^2|x'\rangle = |x'\rangle \Rightarrow \hat{P}^2 = 1,\ [\mathcal{H}, P] = 0$

$P_U = \pm U$ ~ U is the eigenstate of the parity operator

Wavefunctions under parity:

for $\psi(x') = \langle x'|\alpha\rangle$

$\langle x'|\hat{P}|\alpha\rangle = \langle -x'|\alpha\rangle = \psi(-x')$

assuming $|\alpha\rangle$ is an eigenket of $\hat{P}$

$\hat{P}|\alpha\rangle = \pm|\alpha\rangle \rightarrow \langle x'|\hat{P}|\alpha\rangle = \pm\langle x'|\alpha\rangle$

$$\langle x'|\hat{P}|\alpha\rangle = \begin{cases} \pm\langle x'|\alpha\rangle \\ \langle -x'|\alpha\rangle \end{cases}$$

$\Rightarrow$ All wavefunctions are either even or odd

$$\psi(-x') = \pm\psi(x') \begin{cases} \text{even parity} \\ \text{odd parity} \end{cases}$$

*Only odd functions satisfy the boundary condition!

for $U(r\to 0) = 0$

$\Rightarrow U(r) = -U(-r)$

3. Three Generally Solvable Cases

① The free particle & the infinite spherical well

$$V(r) = \begin{cases} V_0, & r < r_0 \\ V_1, & r > r_0 \end{cases}$$

for $\ell = 0$, solve as above.

for $\ell > 0$:

$$\frac{-\hbar^2}{2m}U'' + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r) = EU$$

~~let $E \equiv \frac{\hbar^2 k^2}{2m}$, $\rho = kr$~~

$$\frac{d^2R}{d\rho^2}+\frac{2}{\rho}\frac{dR}{d\rho}+\left[1-\frac{\ell(\ell+1)}{\rho^2}\right]R=0$$

↳ recognize solutions as the spherical bessel functions ↓

$$U_\ell(r)\propto j_\ell(\rho)=(-\rho)^\ell\left[\frac{1}{\rho}\frac{d}{d\rho}\right]^\ell\left(\frac{\sin(\rho)}{\rho}\right)$$

$$\propto n_\ell(\rho)=-(-\rho)^\ell\left[\frac{1}{\rho}\frac{d}{d\rho}\right]^\ell\left(\frac{\cos(\rho)}{\rho}\right)$$

as $r\to 0$, $j_\ell(\rho\to 0)\to\rho^\ell$, $n_\ell(\rho\to 0)\to\rho^{-\ell-1}$

choose $j_\ell(\rho)$ solutions (satisfy B.C.)

② Hydrogen Atom – The Coulomb Potential

$$V(r)=-1/r$$

In addition to Angular Momentum, Lenz's Vector is conserved

$$\vec{A}=\vec{p}\times\vec{L}-\frac{\hat{r}}{r}$$

$$[\vec{L},\mathcal{H}]=[\vec{A},\mathcal{H}]=0$$

6 generators

$\Rightarrow$ Symmetry group for the H atom is SO(4)

(p.g. 265, SAK)

...bit of group theory...

In SO(4): $RR^T=\mathbb{1}$ – R unitary

↳ $\underbrace{R(\epsilon)}=e^{i\epsilon Q/\hbar}$

small/infinitesimal rotations in SO(4) algebra can be expressed as an exponential

R unitary $\to$ Q is Hermitian

If R is also real

$e^{i\epsilon Q/\hbar}=e^{i\epsilon Q^*/\hbar}\Rightarrow$ Q is imaginary & anti-symmetric

$$Q=i\begin{pmatrix}0 & Q_{12} & \cdot & \cdot\\ & 0 & \cdot & \cdot\\ & & 0 & \cdot\\ & & & 0\end{pmatrix}$$

6 parameters

$\to$ 6 generators

Degeneracies of Hydrogen Atom states:

$E_n\equiv n^2$ degeneracies

Orbital configurations

1s $-\ \ell=0$

2s 2p $-\ \ell=1$ (3 states)

3s 3p 3d $-\ \ell=2$ (5)

4s 4p 4d 4f $-\ \ell=3$ (7)

In SO(3):

All 3 states of 2p must be degenerate and all 5 states of 3d must be degenerate, but there is no reason why the states of 3p & 3d must be degenerate.

In SO(4):

The states of 3p & 3d must now be degenerate, yielding the n^2 degeneracies in the Hydrogen atom

③ 3D Harmonic Oscillator

let $k=m=\hbar=1$

$$\mathcal{H}=\frac{1}{2}(p_x^2+p_y^2+p_z^2+x^2+y^2+z^2)$$
$$=\mathcal{H}_x+\mathcal{H}_y+\mathcal{H}_z$$
$$\mathcal{H}_\alpha=\left(\frac{p_\alpha^2+X_\alpha^2}{2}\right)\ ;\ X_{\alpha=x,y,z}=x,y,z$$

$[\mathcal{H}_\alpha,\mathcal{H}_\beta]=0$ as usual

→ We can diagonalize $\mathcal{H}_x, \mathcal{H}_y, \mathcal{H}_z$ simultaneously

└ now three separate oscillator Hamiltonians, allowing us to use the creation and number operators to simultaneously diagonalize them

$$a_\alpha^\dagger=\frac{(x_\alpha-ip_\alpha)}{\sqrt{2}}\ ;\ \hat{n}_\alpha=a_\alpha^\dagger a_\alpha \quad (\mathrm{I})$$

└ $[n_\alpha, n_\beta]=0$

$$\mathcal{H}_\alpha=\hat{n}_\alpha+\frac{1}{2}$$
$$\mathcal{H}=\sum_\alpha\left(\hat{n}_\alpha+\frac{1}{2}\right)\quad(\mathrm{II})$$
$$=\underbrace{N_{tot}}_{N_{tot}=n_x+n_y+n_z}+3/2$$

E	n_x	n_y	n_z
3/2	0	0	0
5/2	1	0	0
5/2	0	1	0
5/2	0	0	1
⋮			etc.

→

for N_{tot} $(E = N_{tot} + 3/2)$

degeneracies: $\frac{1}{2}(N_{tot}+1)(N_{tot}+2)$

$[a^\dagger_\alpha, a_\beta] = \delta_{\alpha\beta}$

$[a_\alpha, a_\beta] = 0$ (III)

Combinatorics partition problem:

- Define problem by equations (I), (II), and (III)

$N_{tot} = n_x + n_y + n_z;\ n_\alpha \geq 0$

Check $\tilde{a}^\dagger_\alpha = \sum_{\beta = x,y,z} U_{\alpha\beta} a_\beta$, with $UU^\dagger = \mathbb{1}$ and $\det\{U\} = 1$

$\rightarrow$ **The creation operators leave $\mathcal{H}$ invariant**

$\rightarrow$ **SU(3) is a good symmetry for the 3D H.O.** (explains degeneracy)

* **Since L & $\mathcal{H}$ commute, how do we construct simultaneous eigenstates of both L & $\mathcal{H}$?** (our current eigen-problem solutions are only eigenstates of $\mathcal{H}$)