QM Lecture 17

RADIAL PART OF CENT. POT.

DID Y_{lm}, NEED RADIAL PART $R(r)$

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)+\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}+V(r)\right]R(r)=ER(r)$$

* FIX $V(r)$. $R(r)=R_{E,\ell}(r)$ $\quad$ E,ℓ- DEP.

ANSATZ: $R_{E,\ell}(r)=\frac{u_{E,\ell}(r)}{r}$ $\quad$ (chain rule cancels $\frac{d}{dr}$ term)

$$\Rightarrow\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}+V(r)\right]u_{E,\ell}(r)=E\,u_{E,\ell}(r)$$

Q: LOOKS 1D. HOW IS IT DIFFERENT?

A: $\int_0^\infty dr$. - "CUT OFF" 1D @ 0 if $V(x)=\infty$ $x<0$
- BUT THEN $\psi=0$ @ 0

ORIGIN BEHAVIOR

- CAN'T HAVE $r^{p<0}$ NEAR ORIGIN!
- NOTE:
  1) 2^{ND} TERM $\sim\frac{1}{r^2}$
  2) 3^{RD} " V-DEP
  3) 1^{ST} very $u(R)$ DEP

- IF $V(r)$ NOT MORE SING THAN $\frac{1}{r^2}$, $\exists$ POWER SER SOLN

(regular singularity)

TRY: $u(r) = r^s$ Q: WHAT S-VALUE MAKES SOL'S EASY?

$$-\frac{\hbar^2}{2\mu} s(s-1) r^{s-2} + \frac{\ell(\ell+1)\hbar^2}{2\mu} r^{s-2} + V(r) r^s = E r^s \quad *$$

HOW TO SATISFY?

- EXISTENCE OF u POWER SERIES SOL'N $\Rightarrow r^2 V(r) \to 0 \Rightarrow$ FIRST TWO TERMS DOM.
- SO HAVE THEM SELF-CANCEL

$$-s(s-1) + \ell(\ell+1) = 0$$

$$\Rightarrow s = \ell + 1 \quad \underline{\text{OR}} \quad s = -\ell$$

SUPPOSE $s = -\ell$ $\Rightarrow u \sim r^{-\ell}$ $R \sim r^{-\ell-1}$

$\ell \geq 0 \Rightarrow$ SINGULAR R @ $r=0$!   X

SO TAKE $s = \ell + 1$ $\Rightarrow R \sim r^{\ell}$ ✓

POINT   GUARANTEED EXISTENCE OF POWER SERIES $R(r)$ SOLUTIONS

SUMMARY $\psi(r,\theta,\phi) \sim R(r)\, Y_{\ell m}(\theta,\phi)$

$\hat{H}_{rel} \neq f(\theta,\phi)$

$= V(r) \Rightarrow$ AFFECTS $R(r)$. HAVE $Y_{\ell m}$ SO NOW NEED $V(r)$.

EXAMPLE 1: COULOMB POTENTIAL

Hydrogen: 1 PROTON 1 ELECTRON

"Hydrogenic" Z PROTONS 1 ELECTRON

$$V(r) = -\frac{q_1 q_2}{r} = \frac{Ze^2}{r}$$

$$\Rightarrow \left[\frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} - \frac{Ze^2}{r}\right] u_{E,\ell}(r) = E\, u_{E,\ell}(r)$$

SIMPLIFY $\rho = \sqrt{\frac{8\mu|E|}{\hbar^2}}\, r$ $\left(E<0 \Rightarrow E = -|E|\right)$ BOUND STATE

$$\lambda = \frac{Ze^2}{\hbar}\sqrt{\frac{\mu}{2|E|}}$$

$$\Rightarrow \frac{d^2u}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2}u + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)u = 0$$

GOAL POWER SERIES & REC. REL

LIM $\rho \to \infty$ $\frac{d^2u}{d\rho^2} - \frac{1}{4}u = 0$

$$\Rightarrow u = Ae^{-\rho/2}$$

so $\rho \to 0$ $u(\rho) \to \rho^{\ell+1}$

$\rho \to \infty$ $u \to e^{-\rho/2}$

TRIAL SOL'N $u(\rho) = \rho^{\ell+1} e^{-\rho/2} F(\rho)$ (**) E-DEP FROM $F(\rho)$

POWER SERIES $F(\rho) = \sum_{k=0}^{\infty} C_k \rho^k$ w/ $C_0 \neq 0$ (WHY?)

SUBSTITUTE $$\frac{d^2 F(\rho)}{d\rho^2} + \left(\frac{2\ell+2}{\rho} - 1\right)\frac{dF(\rho)}{d\rho} + \left(\frac{\lambda}{\rho} - \frac{\ell+1}{\rho}\right)F(\rho) = 0$$

$$\Rightarrow \sum_{k=2}^{\infty} k(k-1)\, C_k \rho^{k-2} + \sum_{k=1}^{\infty} (2\ell+2)\, k C_k \rho^{k-2} + \sum_{k=0}^{\infty} [-k+\lambda-(\ell+1)]\, C_k \rho^{k-1} = 0$$

↳ WHY 2?
($k = 0, 1$ TERMS 0)

WHAT NOW? (what did we do for S.H.O.?)

MAKE SAME SUM

TERM 1 & 2 $k' = k-1$ THEN RENAME $k' \to k$

$$\sum_{k=0}^{\infty} \left\{ [(k+1)k + (2\ell+2)(k+1)]\, C_{k+1} + [-k+\lambda-(\ell+1)]\, C_k \right\} \rho^{k-1} = 0$$

HOLD TERM BY TERM:

$$\frac{C_{k+1}}{C_k} = \frac{k+\ell+1-\lambda}{(k+1)(k+2\ell+2)}$$

$\lambda \sim E^{-1/2}$

SO ENERGY IN REC REL, LIKE S.H.O.!

ASYMPTOTICS $\frac{C_{k+1}}{C_k} \xrightarrow{k\to\infty} \frac{1}{k}$ ~ asymptotic behavior of e^{ρ}

RECALL THIS $\Rightarrow u(\rho) \to e^{\rho/2}$ AS $\rho \to \infty$!

TO SOLVE MUST TRUNCATE NEED NUM = 0 FOR SOME k_{trunc}

TAKE $\lambda = 1 + \ell + n_r$ $\quad n_r \in \mathbb{Z}_{\geq 0}$

need for num = 0

n_r DET k_{trunc}

$$\Rightarrow \frac{C_{k+1}}{C_k} = \frac{k - n_r}{(k+1)(k+2\ell+2)}$$

THIS $\lambda \Rightarrow$

$$E = \frac{-\mu Z^2 e^4}{2\hbar^2 (1+\ell+n_r)^2} =: \frac{-\mu Z^2 e^4}{2\hbar^2 n^2}$$

WHERE $n \equiv 1 + \ell + n_r$ IS THE PRINCIPAL QUANTUM NUMBER

* $F(\rho)$ DEG n_r POLY IN ρ, A LAGUERRE POLY.

COULOMB POT. SOL'NS

$$\langle \vec{r} | n, \ell, m \rangle = R_{n,\ell}(r) Y_{\ell m}(\theta, \phi) = \frac{u_{n,\ell}(r)}{r} Y_{\ell m}(\theta, \phi)$$

WHERE $u_{n,\ell}(r) = \rho^{\ell+1} e^{-\rho/2} F(\rho)$

$$\rho = \sqrt{\frac{8\mu |E|}{\hbar^2}}\, r \xrightarrow{\text{E-SUB}} \frac{2Z}{n}\left(\frac{r}{a_0}\right)$$

$a_0 = \frac{\hbar^2}{\mu e^2} = .529\,\text{Å} =$ BOHR RAD.

$E_n =$ above $= \frac{-13.6\,eV}{n^2}$ for hydrogen

RADIAL WVFNS

$\boxed{n=1}$ GROUND STATE

$* \; n = 1 + \ell + n_r \Rightarrow \ell = 0$ & $n_r = 0 \Rightarrow \lambda = 1$

$\therefore$ POWER SERIES TERM @ $k = 0$

$\therefore \; u_{1,0}(\rho) = C_0 \rho^1 e^{-\rho/2} \qquad F(\rho) = C_0$

$\therefore \; R_{1,0}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$ (WHY NO $\rho^{\text{POW?}}$ $u/\rho \to \rho^0$)

$\boxed{n=2}$ FIRST EXCITED STATES

$* \; n = 1 + \ell + n_r \Rightarrow \underbrace{\ell = 0 / n_r = 1}_{C_0 \,\&\, C_1}$ OR $\underbrace{\ell = 1 / n_r = 0}_{C_0}$

$*$ $\underline{\ell = 1 \quad n_r = 0}$ $\quad U_{2,1}(\rho) = C_0 \rho^2 e^{-\rho/2} \Rightarrow R_{2,1}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0}$

$*$ $\underline{\ell = 0 \; n_r = 1}$ $\quad F(\rho) = C_0 + C_0\left(-\frac{1}{2}\right)\rho \Rightarrow u_{2,0} = C_0\left(1 - \frac{\rho}{2}\right)\rho e^{-\rho/2}$

$$\Rightarrow R_{2,0}(r) = 2\left(\frac{Z}{2a_0}\right)^{3/2}\left(1 - \frac{Zr}{2a_0}\right)e^{-\frac{Zr}{2a_0}}$$

$\boxed{n=3}$ SECOND EXCITED STATES... (HW?)

EXAMPLE 2: 3D ISO. HARM. OSC.

- ISOTROPIC: SAME IN ALL DIRS (FRW SPACET.)

$V(r) = ?$ (GUESS?)

$$V(r) = \frac{1}{2}\mu w^2 r^2 = \frac{1}{2}\mu \omega^2 (x^2+y^2+z^2)$$

SOLVE

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2}u + \frac{1}{2}\mu \cdot u = Eu$$

FOLLOW STANDARD STEPS

1) WRITE AS DIM-LESS QUANTS

$$\rho = \sqrt{\frac{\mu\omega}{\hbar}}\, r \qquad \lambda = \frac{2E}{\hbar\omega}$$

$$\Rightarrow \frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2}u - \rho^2 u = -\lambda u \qquad *$$

2) CONSIDER ASYMPS

$\rho \to \infty \Rightarrow$ SE $\to \frac{d^2u}{d\rho^2} = \rho^2 u$

FROM $\rho \to \infty$

SUGGESTS $u(\rho) = \rho^{l+1} e^{-\rho^2/2} f(\rho)$

ANY CENT. POT

3) POWER SERIES $\quad f(\rho) = \sum_{k=0}^{\infty} c_k \rho^k$

$$\Rightarrow \frac{d^2 f}{d\rho^2} + \left[\frac{2(\ell+1)}{\rho} - 2\rho\right]\frac{df}{d\rho} + (\lambda - 3 - 2\ell) f = 0$$

$$\Rightarrow \sum_{k=0}^{\infty} c_k k(k-1)\rho^{k-2} + \sum_{k=0}^{\infty} c_k 2(\ell+1)k\rho^{k-2} - 2\sum_{k=0}^{\infty} c_k k\rho^k$$

$$+(\lambda-3-2\ell)\sum_{k=0}^{\infty} c_k \rho^k = 0$$

* SEC. TERM. PROB FOR $k=1 \Rightarrow c_1 = 0$

* RENAME

$$\sum_{k'=0}^{\infty} c'_{k+2}(k'+2)(k'+1)\rho^{k'} + \sum_{k'=0}^{\infty} c'_{k+2}\, 2(\ell+1)(k'+2)\rho^{k'} + \sum_{k=0}^{\infty}(\lambda-3-2\ell-2k) \times c_k \rho^k = 0$$

4) REC. REL. TO SOLVE

$$\frac{c_{k+2}}{c_k} = \frac{3+2\ell+2k-\lambda}{(k+2)(k+1+2\ell+2)}$$

($c_1 = 0 \Rightarrow$ ALL ODD VANISH!)

5) ASYMP.

$$k \to \infty \quad \frac{c_{k+2}}{c_k} \longrightarrow \frac{2}{k} \Rightarrow \text{like } f(\rho) \sim e^{\rho^2}$$

6) TRUNCATE DEFINE $n_r = \frac{k}{2}$

TAKE $\lambda = 3 + 2\ell + 4n_r$ TRUNCS

7) STUDY ENERGY

$$\lambda = \frac{2E}{\hbar\omega} = 3 + 2\ell + 4n_r \Rightarrow \boxed{\begin{aligned} E_n &= \left(2n_r + \ell + \tfrac{3}{2}\right)\hbar\omega \\ &=: \left(n + \tfrac{3}{2}\right)\hbar\omega \end{aligned}}$$

$$\boxed{n = 2n_r + \ell}$$

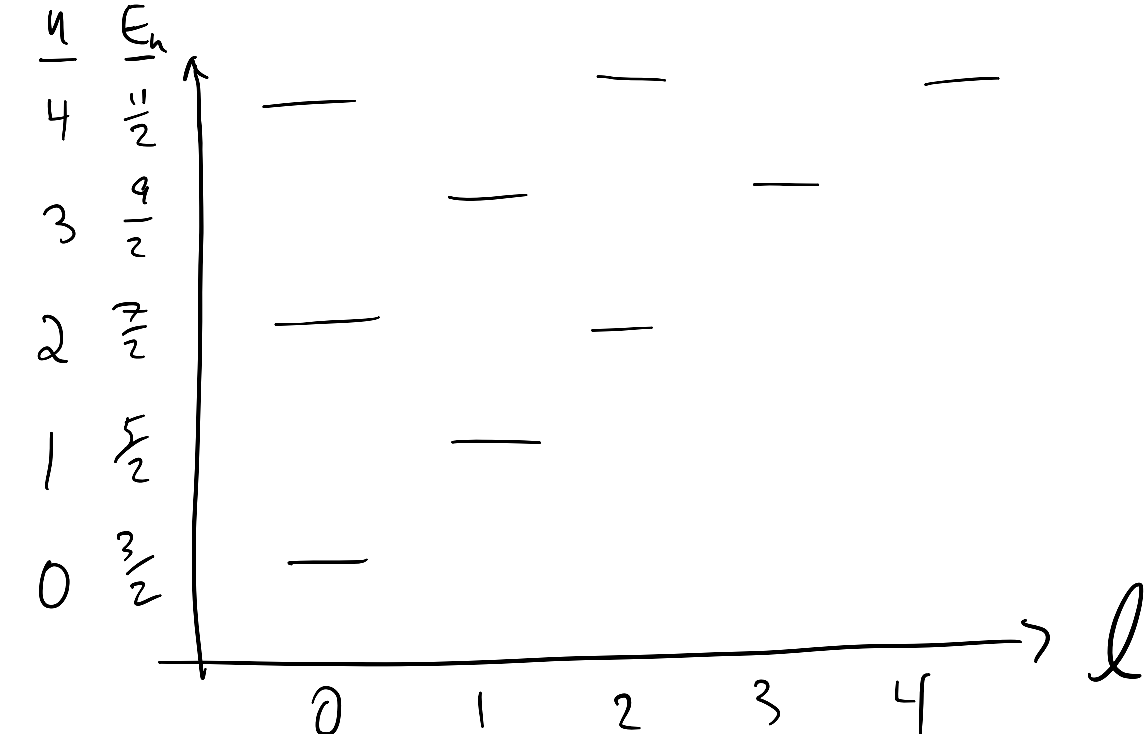
DEGEN. OF STATES

$\underline{n=0} \Rightarrow n_r = 0, \ \ell = 0$

$\underline{n=1} \Rightarrow n_r = 0 \ \ \ell = 1 \ \ \ m_\ell \in \{1, 0, -1\}$

$\underline{n=2} \Rightarrow$ i) $n_r = 1 \ \ \ell = 0 \Rightarrow m_\ell = 0$ ONE STATE

ii) $n_r = 0 \ \ \ell = 2 \Rightarrow m_\ell \in \{2, 1, 0, -1, -2\} \Rightarrow$ FIVE STATES



$\boxed{2\ell + 1 \text{ STATES FOR } (n, \ell) \text{ FIXED}}$