

QM Lecture 17

RADIAL PART OF CENT. POT.

DID Ψ_{lm} , NEED RADIAL PART $R(r)$

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

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

ANSATZ: $R_{E,\ell}(r) = \frac{U_{E,\ell}(r)}{r}$ (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 $V(x)=\infty$ $x \leq 0$
 - BUT THEN $\psi=0 @ 0$

ORIGIN BEHAVIOR

- CAN'T HAVE $r^{p<0}$ NEAR ORIGIN!

- NOTE:

1) 2nd TERM $\sim \frac{1}{r^2}$

2) 3rd " V-DEP

3) 1st very $U(r)$ DEP

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

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

$$\frac{-t^2}{2\mu} s(s-1) r^{s-2} + \frac{\ell(\ell+1)t^2}{2\mu} r^{s-2} + v(r) r^s = Er^s \quad \text{⊗}$$

HOW TO SATISFY?

- EXISTENCE OF u POWER SERIES

SOL'N $\Rightarrow r^2 v(r) \rightarrow 0 \Rightarrow$ FIRST
TWO TERMS DOM.

- SO HAVE THEM SELF-CANCEL

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

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

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

$\ell > 0 \Rightarrow$ 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 $\psi(r, \theta, \phi) \sim R(r) Y_{\ell m}(\theta, \phi)$

$\hat{F}_{\ell m} \neq f(\theta, \phi)$

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

EXAMPLE 1: COULOMB POTENTIAL

Hydrogen: 1 PROTON 1 ELECTRON

"Hydrogenic" 2 PROTONS 1 ELECTRON

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

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

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

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

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

GOAL POWER SERIES \vdash REC. REL

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

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

so $\rho \rightarrow 0 \quad u(\rho) \rightarrow \rho^{\ell+1}$
 $\rho \rightarrow \infty \quad u \rightarrow e^{-\rho/2}$

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

POWER SERIES $F(p) = \sum_{k=0}^{\infty} c_k p^k$ w/ $c_0 \neq 0$ (why?)

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

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

\hookrightarrow why? (k=0, 1 TERMS 0)

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

MAKE SAME SUM

TERM 1 $k' = k-1$ THEN RENAME $k' \rightarrow k$

$$\sum_{k=0}^{\infty} \{ [(k+1)k + (2\ell+2)(k+1)] c_{k+1} + [-k+\lambda-(\ell+1)] c_k \} p^{k-1} = 0$$

HOLD TERM BY TERM:

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

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

ASYMPTOTICS

$$\frac{c_{k+1}}{c_k} \xrightarrow{k \rightarrow \infty} \frac{1}{k}$$

\sim asymptotic behavior of e^ℓ

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

TO SOLVE
MUST TRUNCATE

NEED $NUM=0$

FOR SOME k_{trunc}

$$\text{TAKE } \lambda = l + \ell + n_r \quad n_r \in \mathbb{Z}_{>0}$$

*need
for num=0*

$$n_r \text{ DET } k_{\text{true}}$$

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

$$\text{THIS } \lambda \Rightarrow E = \frac{-\mu z^2 e^4}{2\hbar^2 (1+l+n_r)^2} =: \frac{-\mu z^2 e^4}{2\hbar^2 n^2}$$

WHERE $n = l + \ell + n_r$ IS THE PRINCIPAL QUANTUM NUMBER

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

Coulomb Pot. Sol'n's

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

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

$$\rho = \sqrt{\frac{8\mu|E|}{\hbar^2}} r \xrightarrow{\text{E-SUB}} \frac{2z}{n} \left(\frac{r}{a_0} \right) \quad a_0 = \frac{\hbar^2}{me^2} = .529 \text{ \AA} = \frac{\text{BOHR RAD.}}{\text{RAD.}}$$

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

Review after T-giving 2018

TRACE!

① Central Pot: $H = \frac{\vec{p}^2}{2M} + \frac{\vec{p}^2}{2\mu} + V(r)$

② Solve for $\Psi(\vec{r})$ w/ sep of vars

$$\Psi(\vec{r}) = R(r) \Theta(\theta) \Phi(\phi)$$

$$=: R(r) Y_{lm}(\theta, \phi)$$

$$Y_{lm}(\theta, \phi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} e^{im\phi} \frac{1}{\sin^m \theta} \frac{d^l}{d(\cos)^{l-m}} \sin^{2l} \theta$$

③ NEED $V(r)$ TO DET $R(r)$

④ Outline: $V(r) \sim \frac{1}{r}$ (eg Hydrogen atom)

* \exists Power series

* $\Psi(\vec{r})$ not blowing up $\Rightarrow C_k = 0$ for some k

$$\Rightarrow E_n = \frac{-\mu e^2 e^4}{2\hbar^2 (1+l+n_r)^2} =: -\frac{\mu e^2 e^4}{2\hbar^2 n^2}$$

⑤ $R(r)$ DET By $U(p)$

$$U(p) = p^{l+1} e^{-p/2} F(p) \quad F(p) = \sum_{k=0}^{\infty} C_k p^k$$

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

n	l	n_r
1	0	0
2	1	0
2	0	1
3	2	0
1	1	1

RADIAL WFN'S

$n=1$ GROUND STATE

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

\therefore POWER SERIES TERM @ $k = 0$

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

$$\therefore R_{1,0}(r) = 2 \left(\frac{z}{a_0} \right)^{\frac{3}{2}} e^{-\frac{zr}{a_0}} \quad (\text{why } \underbrace{u}_{\text{no }} / \rho \xrightarrow{\rho^{\text{pow?}}} \rho^0)$$

$n=2$ FIRST EXCITED STATES

$$* n = l + \ell + n_r \Rightarrow \underbrace{\ell = 0 / n_r = 1}_{C_0 \neq C_1} \quad \text{OR} \quad \underbrace{\ell = 1 / n_r = 0}_{C_0}$$

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

$$* \underline{\ell = 0 \quad n_r = 1} \quad F(\rho) = C_0 + C_1 \left(-\frac{1}{2} \right) \rho \Rightarrow U_{2,0} = C_0 \left(1 - \frac{\rho}{2} \right) \rho e^{-\rho/2}$$

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

$n=3$ SECOND EXCITED STATES... - ($H\omega?$)

EXAMPLE 2: 3D ISO. HARM. OSC.

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

$$V(r) = ? \quad (\text{GUESS?})$$

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

SOLVE

$$-\frac{\hbar^2}{2\mu} \frac{d^2 u}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} u + \frac{1}{2}\mu E u = 0$$

FOLLOW STANDARD STEPS

1) WRITE AS DIM-LESS QUANTS

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

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

2) CONSIDER ASYMPs

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

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

L_ANY CENT. POT

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

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

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

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

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

* RENAME

$$\sum_{k'=0}^{\infty} c'_{k+2} (k'+2)(k'+1)p^{k'} + \sum_{k'=0}^{\infty} c'_{k+2} 2(\ell+1)(k'+2)p^{k'} + \sum_{k=0}^{\infty} (\lambda - 3 - 2\ell - 4k) \times c_k p^k = 0$$

4) REC. REC. 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.

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

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

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

7) STUDY ENERGY

$$\lambda = \frac{2E}{\hbar\omega} = 3 + 2l + 4n_r \Rightarrow \begin{cases} E_n = \left(2n_r + l + \frac{3}{2} \right) \hbar\omega \\ = \left(n + \frac{3}{2} \right) \hbar\omega \end{cases}$$

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

DEGEN. OF STATES

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

$$\underline{n=1} \Rightarrow n_r=0, l=1 \quad m_l \in \{1, 0, -1\}$$

$$\underline{n=2} \Rightarrow i) n_r=1, l=0 \Rightarrow m_l=0 \quad \text{ONE STATE}$$

$$ii) n_r=0, l=2 \Rightarrow m_l \in \{2, 1, 0, -1, -2\} \Rightarrow \text{FIVE STATES}$$

