Lecture 11

Rotationally-invariant problems

1 $$\left(\frac{\hat{p}^2}{2m} + V(|\vec{r}|)\right)\psi_E(\vec{r}) = E\,\psi_E(\vec{r})$$

scalars! i.e. $V(x,y,z) = V(r)$

$\Rightarrow [H, L_z] = [H, L^2] = 0$

$\Rightarrow$ go to spherical coordinates:

$$\Big[-\frac{\hbar^2}{2m}\underbrace{\left(\partial_r^2 + \frac{2}{r}\partial_r\right)}_{\frac{1}{r^2}\partial_r r^2 \partial_r = \frac{1}{r}\partial_r^2 r} + \frac{L^2}{2mr^2} + V(r)\Big]\psi_{Elm}(r,\theta,\varphi) = E\psi_{Elm}$$

$$= \left(\partial_r + \frac{1}{r}\right)\left(\partial_r + \frac{1}{r}\right) \equiv p_r^2$$

$$\frac{L^2}{\hbar^2} = -\frac{1}{\sin\theta}\partial_\theta \sin\theta\,\partial_\theta - \frac{1}{\sin^2\theta}\partial_\varphi^2$$

separable $\Rightarrow \psi_{Elm}(r,\theta,\varphi) = R_{Elm}(r)\,Y_{lm}(\theta,\varphi)$

$$-\frac{\hbar^2}{2m}\frac{1}{r}\partial_r^2(rR_{Elm}) + \left(V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right)R_{Elm} = E\,R_{Elm}(r)$$

centrifugal barrier for $l>0$!

nothing depends on m

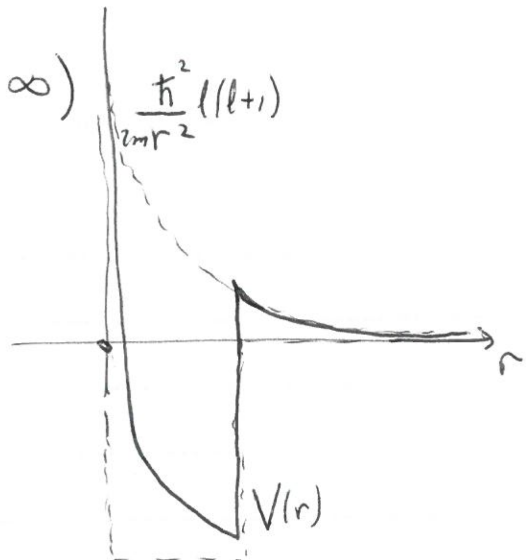
$\Rightarrow 2l+1$ - fold degeneracy.
as expected.

Take: $R_{El}(r) = \dfrac{u_{El}(r)}{r}$

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m}\partial_r^2 u_{El} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right)u_{El} = E\,u_{El}(r)}$$

1d radial eqn with $u_{El}(r=0) = 0$.

- <u>Differences from 1d</u>:



→ $0 < r < \infty$ (<u>not</u> $-\infty < x < \infty$)

→ repulsive centrifugal barrier for $l \neq 0$

→ $u_{El}(r \to 0) \to 0$

otherwise $\psi_{0,0}(r) = \frac{c}{r}$

although square-integrable does not satisfy Schrodinger's Eqn.

due to $\nabla^2(1/r) = -4\pi\delta^{(3)}(\vec{r})$.

Since $V(r) \not\propto \delta^{(3)}(r) \Rightarrow c = 0$.

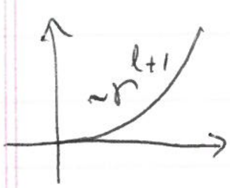
- <u>General props of soln $u_{El}(r)$</u>:

→ $r \to 0$, for $V(r) \ll \frac{1}{r^2}$ for $r \to 0$

$\Rightarrow$ drop $V(r)$ & E

$\Rightarrow -\partial_r^2 u + \frac{l(l+1)}{r^2} u = 0$; ok only for $l \neq 0$

$\boxed{u(r) \sim r^{l+1}}$ or r^{-l} ← irregular



increasing l, particle avoids origin for $l \neq 0$

$l = 0$: $u_{l=0} \simeq r$

$\Rightarrow R_{l=0} \simeq \frac{r}{r} = \text{const}$.

→ $r \to \infty$, if $V(r \to \infty) \to 0$ (otherwise cannot ignore (1))
e.g. Coulomb's potential.

$$\Rightarrow \partial_r^2 U_E = -\frac{2mE}{\hbar^2} U_E(r)$$

(a) $E > 0$: free particle, able to escape → ∞
→ oscillates $e^{\pm ikr}$

(b) $E < 0$: classically forbidden at large r
⇒ bound state. $e^{-\kappa r}$.

(a) $\underline{E > 0}$:

$$U_E(r) = A e^{ikr} + B e^{-ikr}$$ ← spherical waves

$$\left(R(r) = \frac{1}{r}\left(e^{ikr} + \frac{B}{A} e^{-ikr}\right) \right)$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

(b) $\underline{E < 0}$: $U_E(r) = A e^{-\kappa r} + B e^{+\kappa r}$ → 0, $\kappa = \sqrt{\frac{2m|E|}{\hbar^2}}$

$E>0$ → B/A is fixed by demanding $U_E(r \to 0) \to 0$

→ A fixed by normalization

$E<0$ ⇒ only for discrete values of E (κ) will

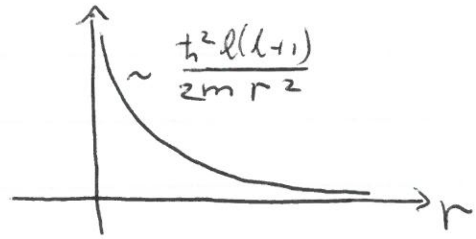
$\underline{B = 0}$, required to satisfy $\psi(r \to \infty) \to 0$.

Notice: $$\int \frac{d^3r}{4\pi} \psi_E^*(r) \psi_E(r) = \underbrace{\int_0^\infty dr}_{1d} |U_E(r)|^2 = 1$$

② Free particle in spherical coordinates:

(nontrivial due to centrifugal barrier)

- $V_{eff}(r) > 0$ everywhere
  $\Rightarrow$ no bound state.



$$\Psi_{E\ell m}(r,\theta,\varphi) = \frac{1}{r} u_{E\ell}(r) Y_{\ell m}(\theta,\varphi)$$

$$\Rightarrow \left(\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right) u_{E\ell}(r) = 0 \,, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

scale out k, i.e. $r = \rho/k$

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

spherical B. eqn.

$x^2 R'' + 2x R' + (x^2 - n(n+1))R = 0$

$\Rightarrow R = a\, j_n + b\, n_n$.

- solns:

$R_{k\ell}(r)$ spherical Bessel fncs

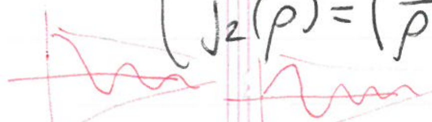
$$\frac{u}{r} = \begin{cases} j_\ell(\rho) = (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \left(\frac{\sin\rho}{\rho}\right), & \text{regular} \\ n_\ell(\rho) = -(-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \left(\frac{\cos\rho}{\rho}\right), & \text{irregular} \end{cases}$$

$\sin x$ & $\cos x$

ρ^ℓ

$$\begin{cases} j_0(\rho) = \frac{\sin\rho}{\rho}, & n_0(\rho) = -\frac{\cos\rho}{\rho} \\ j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}, & n_1(\rho) = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho} \\ j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3}{\rho^2}\cos\rho, & n_2(\rho) = -\left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\cos\rho - \frac{3}{\rho^2}\sin\rho. \end{cases}$$

$\rho^{-(\ell+1)}$



$\vdots$

spherical Hankel fncs:

$$\begin{cases} e^{ix} & h_\ell^{(1)}(\rho) = j_\ell(\rho) + i\, n_\ell(\rho) \\ e^{-ix} & h_\ell^{(2)}(\rho) = j_\ell(\rho) - i\, n_\ell(\rho) = \left(h_\ell^{(1)}(\rho)\right)^* \end{cases}$$

- limits:

→ $\rho \ll l$:

$$\left.\begin{aligned} j_l(\rho) &\simeq \frac{1}{(2l+1)!!}\,\rho^l \\ n_l(\rho) &\simeq -(2l-1)!!\,\frac{1}{\rho^{l+1}} \end{aligned}\right\}\ \rho \to 0$$

→ $\rho \gg l$:

$$\left.\begin{aligned} j_l(\rho) &\simeq \frac{1}{\rho}\sin\left(\rho - \frac{\pi}{2}l\right) \\ n_l(\rho) &\simeq -\frac{1}{\rho}\cos\left(\rho - \frac{\pi}{2}l\right) \end{aligned}\right\}\ \rho \to \infty$$

<u>regular soln</u>: $\psi_{Elm}(r,\theta,\varphi) = j_l(kr)\, Y_{lm}(\theta,\varphi)$, $k = \sqrt{\frac{2mE}{\hbar^2}}$

with $\displaystyle\int_0^\infty dr\, r^2\, j_l(kr)\, j_l(k'r) = \frac{\pi}{2k^2}\,\delta(k-k')$

L. Infeld's (Phys. Rev. 59, 737 (1941))

- Derivation of $R_{El}(r) = j_l(\rho),\ n_l(\rho)$:

$E \propto k^2$

inside argument

$$\left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2}\right] u_l = u_l(\rho)$$

ladder ops: $d_l = \frac{d}{d\rho} + \frac{l+1}{\rho}$

$$d_l^+ = -\frac{d}{d\rho} + \frac{l+1}{\rho}$$

$d_l d_l^+ u_l = u_l \quad \rightarrow \quad u_l$ eigenstate of $d_l d_l^+$ with $\lambda = 1$.

$$d_l^+ d_l (d_l^+ u_l) = (d_l^+ u_l)$$

use $d_l^+ d_l = d_{l+1} d_{l+1}^+$

$$\Rightarrow \underline{d_{l+1} d_{l+1}^+} (d_l^+ u_l) = (d_l^+ u_l)$$

$$\Rightarrow \underline{d_l^+ u_l = c_l u_{l+1}}$$

For $l=0 \quad -\frac{d^2}{d\rho^2} u_0 = u_0(\rho)$

$\Rightarrow u_0^A(\rho) = \sin\rho, \quad u_0^B(\rho) = -\cos\rho$

Generate all other u_l's from these via

d_l^+ : $\quad \underline{u_{l+1} = d_l^+ u_l}$

details:

$$\rho R_{\ell+1} = d_\ell^+ (\rho R_\ell) = \left(-\frac{d}{d\rho} + \frac{\ell+1}{\rho}\right)(\rho R_\ell)$$

$$\Rightarrow \quad R_{\ell+1} = \left(-\frac{d}{d\rho} + \frac{\ell}{\rho}\right) R_\ell = \rho^\ell \left(-\frac{d}{d\rho}\right) \frac{R_\ell}{\rho^\ell}$$

$$\Rightarrow \quad \frac{R_{\ell+1}}{\rho^{\ell+1}} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_\ell}{\rho^\ell}$$

$$\Rightarrow \quad R_\ell = (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell R_0(\rho)$$

$$\Rightarrow \quad R_\ell^A \equiv j_\ell(\rho) = (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \left(\frac{\sin\rho}{\rho}\right)$$

$$R_\ell^B \equiv n_\ell(\rho) = -(-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \left(\frac{\cos\rho}{\rho}\right)$$

3 Relation to Cartesian coordinates:

recall for $V(r)=0$:

$$\psi_{\vec{k}}(x,y,z) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{k}\cdot\vec{r}}, \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

39.#'s.

scalar

$$\text{vs.} \quad \psi_{k\ell m}(r,\theta,\varphi) = j_\ell(kr)\, Y_{\ell m}(\theta,\varphi)$$

39.#'s.

Must be same, expandable in terms of each other.

pick $\vec{p} = \hbar k \hat{z}$ (axis choice)

fixed $E \propto k^2$:

$$\Rightarrow e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} C_{m\ell}\, j_\ell(kr)\, Y_{\ell m}(\theta,\varphi)$$

degenerate eigenstates expansion

φ independent $\Rightarrow$ $C_{m\ell} = 0$ for $m \neq 0$

physically: particle moving along z has $L_z = m = 0$

using $Y_{\ell 0}(\theta) = \left(\frac{2\ell+1}{4\pi}\right)^{1/2} P_\ell(\cos\theta)$

$$\Rightarrow e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} C_\ell\, j_\ell(kr)\, P_\ell(\cos\theta)$$

C_ℓ's can be found using orthonormality of P_ℓ's $\left(\int_{-1}^{1} P_\ell(u) P_{\ell'}(u)\, du = \left(\frac{2}{2\ell+1}\right)\delta_{\ell\ell'}\right)$

$\Rightarrow C_\ell = i^\ell (2\ell+1)$

$$\Rightarrow \boxed{e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta)}$$

$\xrightarrow{kr\to\infty} \frac{1}{kr}\sin\left(kr - \frac{\pi}{2}\ell\right)$ → corresponds to A & B's specific

- Facts about spherical Bessel fncs:

→ $$j_\ell(z) = \frac{1}{2i^\ell} \int_0^\pi e^{iz\cos\theta} P_\ell(\cos\theta)\,\cos\theta\,d\theta$$ ← arise in 3D

→ $$j_0(z) = \frac{\sin z}{z}$$

→ relation to Bessel fnc $J_n(z)$

$$j_n(z) = \sqrt{\frac{\pi}{2}}\,\frac{1}{\sqrt{z}}\,J_{n+1/2}(z)$$

where,

$$J_n(z) = \frac{1}{2\pi i^n} \int_0^{2\pi} d\phi\, e^{iz\cos\phi}\, e^{in\phi}$$ ← arise in 2D

4. The isotropic harmonic oscillator:

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 r^2$$

- recall: in Cartesian coordinates:

$$\psi_{n_x n_y n_z}(x,y,z) = H_{n_x}\left(\frac{x}{r_0}\right) H_{n_y}\left(\frac{y}{r_0}\right) H_{n_z}\left(\frac{z}{r_0}\right) e^{-r^2/2r_0^2}$$

$$E_n = (\underbrace{n_x + n_y + n_z}_{\equiv n} + 3/2)\hbar\omega$$

Spherical coordinates:

$$\psi_{Elm} = \frac{1}{r} u_{El}(r) Y_{lm}(\theta,\varphi)$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} u_{El}(r) + \left(\frac{1}{2}m\omega^2 r^2 + \frac{\hbar^2 l(l+1)}{2mr^2}\right) u_{El}(r) = E_l u_{El}(r)$$

in units of $r_0 = \sqrt{\frac{\hbar}{m\omega}}$, i.e. $\hat{r} = r/r_0$

$r \to \infty \qquad u(r) \sim e^{-\hat{r}^2/2}$

$\Rightarrow$ take $u(r) = v(\hat{r})\, e^{-\hat{r}^2/2}$

$$v'' - 2\hat{r}v' + [2\underset{\uparrow}{\varepsilon} - 1 - \underbrace{\frac{l(l+1)}{\hat{r}^2}}]v = 0$$

$E/\hbar\omega$ — distinguishes from pure 1d h.o.

take $v(\hat{r}) = \underset{\uparrow}{\hat{r}^{l+1}} \sum_{n=0}^{\infty} c_n \hat{r}^n$

since know that $u(\hat{r}) \xrightarrow[r\to 0]{} \hat{r}^{l+1}$

→ Series soln

→ recursion for C_n terminates if

$$E_n = (\underbrace{2k+l}_{n} + 3/2)\hbar\omega \quad , \quad k = 0, 1, 2, \ldots \in \mathbb{Z}$$

n – principle q. #.

same as via Cartesian coord.

• Degeneracy:

at each n there are $n/2+1$, or $(n+1)/2$ l's.

$l = n - 2k = n, n-2, n-4, \ldots, 1$, or 0.

AND for every l there are $2l+1$ m-states.

take n = even (we'll see that's same as odd)

$$N_n = \sum_{k=0}^{n/2} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \delta_{n,\, l+2k}$$

$$= \sum_{k=0}^{n/2} \sum_{l=0}^{\infty} (2l+1)\delta_{n,l+2k} = \sum_{k=0}^{n/2} \left[2(n-2k)+1\right]$$

$$= \sum_{k=0}^{n/2} (2n+1) - 4 \underbrace{\sum_{k=0}^{n/2} k}_{\frac{\frac{n}{2}\left(\frac{n}{2}+1\right)}{2}}$$

$$= (2n+1)\left(\frac{n}{2}+1\right) - n\left(\frac{n}{2}+1\right)$$

$$\boxed{N_n = \left(\frac{n}{2}+1\right)(n+1)} \quad ✓ \quad \frac{(n+1)(n+2)}{2} \quad ✓$$

Lecture 12

Hydrogen Atom
(orbital part)

$\ominus$ m_e

$\oplus$ m_p $\quad V_{Coulomb}(r) = -\dfrac{e^2}{r}$

$$H = \frac{p_p^2}{2m_p} + \frac{p_e^2}{2m_e} - \frac{e^2}{|\vec{r}_p - \vec{r}_e|}$$

go to com & relative coord.

$$H = \underbrace{\frac{P_{cm}^2}{2(m_p+m_e)}}_{H_{cm}} + \underbrace{\frac{p^2}{2\mu} - \frac{e^2}{r}}_{H_{rel}}$$

$$\mu = \frac{m_p\, m_e}{m_p + m_e} \simeq m_e \,, \quad \text{since } \frac{m_e}{m_p} \simeq \frac{1}{2000}$$

$H_{cm} \rightarrow$ free motion of whole atom $\Rightarrow e^{i\vec{K}_{cm}\cdot\vec{R}}$

In CM reference frame (or for $\vec{K}_{cm} = 0$)

$$\hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{e^2}{r} \longrightarrow \text{rot. invnt} \Rightarrow \text{spherical coord.}$$

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

$$\hat{H}\,\psi_{E,l,m}(r,\theta,\varphi) = E_{E,l}\,\psi_{Elm}(r,\theta,\varphi)$$

$$\psi_{E,l,m}(r,\theta,\varphi) = R_{El}(r)\,Y_{lm}(\theta,\varphi)$$

where radial eqn:

$$\underbrace{\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)}_{\frac{1}{r}\frac{d^2}{dr^2}r} R + \frac{2\mu}{\hbar^2}\left(E + \frac{e^2}{r} - \frac{l(l+1)\hbar^2}{2\mu r^2}\right)R = 0$$

$$\Rightarrow \quad \psi_{E,l,m} = \frac{u_{El}(r)}{r}\,Y_{lm}(\theta,\varphi)$$

where,

$$\left[\frac{d^2}{dr^2} + \underbrace{\frac{2\mu}{\hbar^2}\Big(E}_{\equiv -r_E^{-2} = -\kappa_E^2} + \frac{e^2}{r} - \frac{l(l+1)\hbar^2}{2\mu r^2}\Big)\right]u_{El} = 0$$

$$\frac{d^2 u_l(\rho)}{d\rho^2} - u_l + \frac{\lambda_E}{\rho}u_l - \frac{l(l+1)}{\rho^2}u_l = 0$$

$$\lambda_E = e^2 r_E \frac{2\mu}{\hbar^2} = \frac{(e^2/r_E)}{(\hbar^2/2\mu r_E^2)} = \frac{E_{coul}(r_E)}{E_{KIN}(r_E)}$$

<u>Note:</u> E is inside r_E inside $\rho = r/r_E$

i.e. "shape" of $u_l(\rho)$ only depends on l & inside λ

$$\lambda_E = e^2\sqrt{\frac{2\mu}{\hbar^2|E|}} \Rightarrow |E| = \frac{e^4\,2\mu}{\hbar^2}\frac{1}{\lambda_E^2} = 4\frac{E_{Ry}}{\lambda_E^2}$$

Look at limits $\rho \to 0$, $\rho \to \infty$.

$\rho \to 0$: $\frac{d^2 u_{E\ell}}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} u_{E\ell} = 0$

$\Rightarrow u_\ell(\rho) \sim \rho^{\ell+1}$ (as for any $V(r) \ll \frac{1}{r^2}$ $_{r \to 0}$

$\rho \to \infty$ $\frac{d^2 u_\ell}{d\rho^2} - u_\ell = 0$

$\Rightarrow u_\ell(\rho) \sim e^{-\rho}$

$$u_\ell(\rho) = e^{-\rho} \overbrace{\rho^{\ell+1} \underbrace{v_\ell(\rho)}}^{f_\ell(\rho)}$$

$u_\ell'' - u_\ell + \frac{\lambda}{\rho} u_\ell - \frac{\ell(\ell+1)}{\rho^2} u_\ell = 0$ will try power series $= \sum_{n=0}^{\infty} c_n \rho^n$

$\Rightarrow$

$$f_\ell'' - 2 f_\ell' + \left(\frac{\lambda}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right) f_\ell = 0$$

$$f_\ell(\rho) = \rho^{\ell+1} v_\ell(\rho)$$

$$\rho v_\ell'' + 2(\ell+1-\rho) v_\ell' + (\lambda - 2\ell - 2) v_\ell = 0$$

(take $\rho = \alpha x \Rightarrow \frac{1}{\alpha} x v_\ell'' + \left(\frac{2\ell+2}{\alpha} - 2x\right) v_\ell' + (\lambda - 2\ell - 2) v_\ell = 0$

choose $\alpha = \frac{1}{2} \Rightarrow x v_\ell'' + (2\ell+2-x) v_\ell' - (\ell+1-\lambda/2) v_\ell = 0$)

$$\Rightarrow \rho = \frac{1}{2} x$$

$$x\, v_\ell''(x) + (2\ell+2-x)\, v_\ell'(x) - (\ell+1-\lambda/2)\, v_\ell = 0$$

Confluent Hypergeometric eqn with solns

$$x y'' + (b-x) y' - a y = 0$$

with soln: $${}_1F_1(a,b;x) = 1 + \frac{a}{b}x + \frac{a(a+1)}{b(b+1)}\frac{x^2}{2!} + \dots$$

(Bessel's, error, $\Gamma(x)$, Hermite, Laguerre fncs are special cases of ${}_1F_1(a,b;x)$)

To terminate at a finite polynomial choose $-a = k \in \mathbb{Z}$. (otherwise $\sim e^{+2\rho} = v_\ell(\rho)$)

$$v_\ell(x) = {}_1F_1(\underbrace{\ell+1-\lambda/2}_{=-k}, 2\ell+2; x) =$$

$\rightarrow$ (Associated) Laguerre polynom.

$$\Rightarrow \lambda = \underbrace{2k+2\ell+2}_{\equiv 2n} \qquad v_\ell(\rho) = L^{2\ell+1}_{n-\ell-1}(2\rho)$$

More explicitly $\quad v_\ell(\rho) = \sum_{s=0}^{\infty} \rho^s c_s$

$$\sum_{s=0}\Big[s(s-1)c_s\rho^{s-1} + 2(\ell+1)s c_s \rho^{s-1} - 2s c_s \rho^s + (\lambda-2\ell-2)\rho^s c_s\Big] = 0$$

$$\sum_{s=0}\Big[\big((s+1)s + 2(\ell+1)(s+1)\big)c_{s+1} - (2s+2\ell+2-\lambda)c_s\Big]\rho^s = 0$$

$$\Rightarrow \frac{c_{s+1}}{c_s} = \frac{2s+2\ell+2-\lambda}{\underbrace{s(s+1)+2(s+1)(\ell+1)}_{(s+1)(s+2\ell+2)}} \underset{s\to\infty}{\simeq} \frac{2}{s} \Rightarrow \underline{e^{2\rho}}$$

must terminate (radial q. #) to get $e^{-\rho} \cdot$ polynomial (ρ).

$$\Rightarrow \quad \lambda = 2(k+l+1) \equiv 2n \quad \leftarrow \text{principle q. \#.}$$

$$\Rightarrow \quad \boxed{E_n = -\underbrace{\left(\frac{\mu e^4}{2\hbar^2}\right)}_{(E_{Ry} \simeq 13.6\,eV)}\frac{1}{n^2}}, \quad n = 1, 2, \ldots \in \mathbb{Z}$$

$$n = k + l + 1 = 1, 2, 3, \ldots$$

$$l = n - k - 1 \leq n - 1$$

i.e. for given n

$$l = \underbrace{n-1,\ n-2,\ n-3,\ \ldots,\ 0}_{n \text{ states}}.$$

$k=0$, $k=1$, ..., $k=n-1$

- Degeneracy:

→ E_n is (not only independent of m, guaranteed by rot. invnce, indep. of L_z, but it is also) independent of l! extra symm "accidental degeneracy"

$$\rightarrow D_n = \sum_{l=0}^{n-1} (2l+1) = 2\,\frac{n(n-1)}{2} + n$$

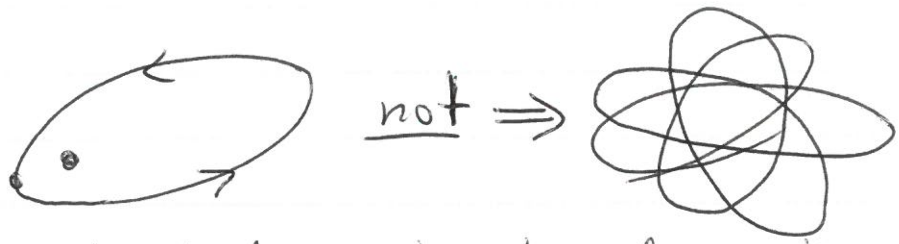
$$\boxed{D_n = n^2}$$

- Notation: $l = 0, 1, 2, 3, \ldots \Rightarrow s, p, d, f, \ldots$

$\Rightarrow$ 1s $(n=1, l=0)$, 2s, 2p $(n=2;\ l=0, l=1)$, etc.

→ "Accidental" Degeneracy:

Special form of $V(r) = \frac{1}{r}$ has extra symmetry. Even classically well-known and is responsible for closed planetary orbits (elliptic)



"culture": perturbations to $\frac{1}{r}$ from other planets cause precession of perihelion of Mercury; 42"/century unaccounted for by Newton's gravity but is by Einstein's GR

Extra symmetry → generator

Runge-Lenz vector: $\left(\vec{n} = \frac{1}{m}\vec{p}\times\vec{L} - \frac{e^2}{r}\vec{r}\right.$ classically)

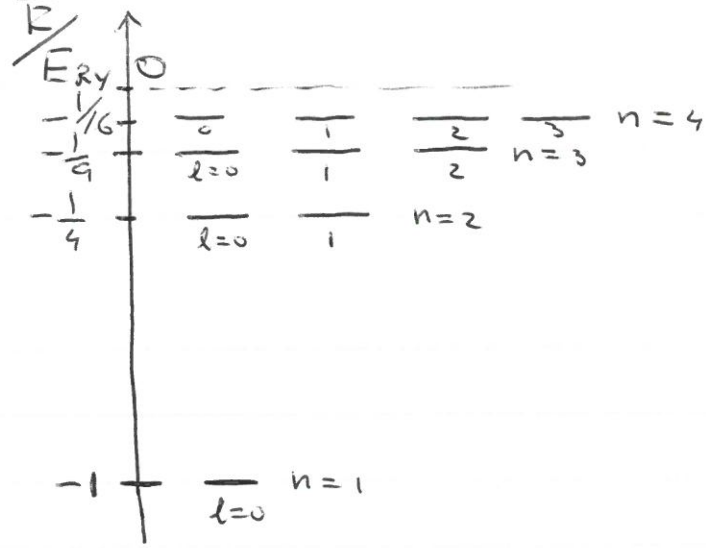
$$\hat{\vec{N}} = \frac{1}{2m}\left(\vec{p}\times\vec{L} - \vec{L}\times\vec{p} - \frac{e^2}{r}\vec{r}\right)$$

with $[H, \vec{N}] = 0 \Rightarrow \frac{d\vec{N}}{dt} = 0$, $\vec{N}$ → conserved

but since N_x, N_y, N_z do not commute, pick N_z ⇒ $N_\pm = N_x \pm i N_y$ raise/lower ladder ops. ⇒ extra degeneracy due to N_z independence, with $N_\pm$ raise lower $N_z = \ell$.

- Similar to harm. oscill. $H = \vec{p}^2 + \vec{r}^2$; can rotate $\vec{z} \equiv \vec{p} + i\vec{r} \Rightarrow$ SU(3) $\underset{?}{\Leftrightarrow}$ O(4)

→ <u>spectrum</u>



→ <u>eigenfncs</u>:

$$v_\ell(\rho) = {}_1F_1(n-\ell-1, 2\ell+2; 2\rho) = L^{2\ell+1}_{n-\ell-1}(2\rho)$$

$$\Rightarrow \quad R_{n\ell}(\rho) = e^{-\rho}\rho^{\ell} L^{2\ell+1}_{n-\ell-1}(2\rho)$$

Laguerre polyn: $L^k_p(x) = (-1)^k \left(\frac{d^k}{dx^k}\right) L^0_{p+k}(x)$

$$L^0_p(x) = e^x \frac{d^p}{dx^p}\left(e^{-x}x^p\right)$$

→ physical scales

Bohr radius : $a_0 = \frac{\hbar^2}{\mu e^2}$ ← size of $n=1$ state, Hydrogen atom

$$\Rightarrow \quad \underline{\rho = r/r_E = \frac{r}{a_0 n}} \qquad \approx \begin{cases} r^{n-1}e^{-r/na_0}, & r \gg a_0 n \\ r^\ell, & r \ll a_0 n \end{cases}$$

$$\Rightarrow \boxed{R_{n\ell}(r) \sim e^{-r/na_0}\left(\frac{r}{na_0}\right)^{\ell} L^{2\ell+1}_{n-\ell-1}\left(2\frac{r}{na_0}\right)}$$

$$\langle r \rangle_{n\ell m} = \frac{1}{2}a_0\left[3n^2 - \ell(\ell+1)\right]$$ ← "size" of $n\ell$ orbital

why $r_n \sim n^2$? $\langle E \rangle \simeq \langle V \rangle \sim -e^2\left\langle \frac{1}{r} \right\rangle \sim -\frac{E_{RY}}{n^2}$

$$\Rightarrow \underline{\langle r \rangle_n \sim n^2 a_0}$$

- Numbers, Experments etc:

$m_e c^2 \simeq 0.5\ \text{MeV}$
$m_p c^2 \simeq 1000\ \text{MeV}$ $\Rightarrow \mu \simeq m_e$.

$\rightarrow a_0 \simeq \frac{1}{2}\ \text{Å} = \frac{\hbar^2}{me^2} = \frac{\hbar}{mc}\alpha^{-1} = \lambda_e 137$

$\hbar c \simeq 2000\ \text{eV}\cdot\text{Å}$

$\alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}$.

$\rightarrow E_{Ry} = \frac{me^4}{2\hbar^2} = \frac{1}{2}mc^2\alpha^2 << mc^2$

$\simeq \left(\frac{1}{137}\right)^2 \frac{1}{4}\ \text{MeV}$

$\simeq \underline{13.6\ \text{eV}}$

justifies nonrelativistic single particle approach.

Note: $\lambda\!\!\!^{-}_e = \frac{\hbar}{mc} = \alpha a_0 << a_0 \Rightarrow e$ location is well defined.

e - Compton

(otherwise to localize a particle below its Compton length require photon of energy $> mc^2 \Rightarrow$ qft!)

$\Delta E_{phot} = \frac{\hbar}{\Delta X} c \simeq mc^2$

$\Rightarrow \underline{\Delta X \simeq \frac{\hbar}{mc} = \lambda\!\!\!^{-}_{comp.}}$

$\rightarrow V_{e \text{ in ground state}} = \alpha c \simeq \frac{1}{137} c \Rightarrow$

$\Rightarrow E \simeq -\frac{1}{2}mv^2 \simeq \underline{-mc^2\alpha^2}$. ✓

Experimentally excellent agreement ;

reproduce spectrum of emitted E&M (photon) radiation

$$\omega_{nn'} = \frac{E_n - E_{n'}}{\hbar} = \frac{E_{Ry}}{\hbar}\left(\frac{1}{n'^2} - \frac{1}{n^2}\right)$$

$n' = 1$ — Lyman series. (ground to excited states)

$n' = 2$ — Balmer series $|nlm\rangle \to |2lm\rangle$

$n' = 3$ — Paschen series. $\uparrow n > 2$.

$$\omega_{21} \simeq \frac{13.6\,eV}{\hbar}\left(1 - \frac{1}{4}\right) \simeq \frac{10}{\hbar}\,eV \Rightarrow 1200\mathring{A}$$

corrections :

→ $m_e \neq \mu$.

→ $K = mc^2\left[\sqrt{1 + \frac{p^2}{m^2c^2}} - 1\right] \neq \frac{p^2}{2m}$.

→ other relativistic corrections from Dirac eqn $\mathcal{O}(\alpha^2)$

→ quantum treatment of E&M radiation QED. → Lamb shift