Lecture $\boxed{28}$, Nov. 4 (Wed.) & part $\textcircled{I}$ of lecture $\boxed{29}$, Nov. 6 (Fri.)

$\boxed{\text{Outline}}$ for today (& Fri.)

- finish general features of radial solutions
- Onto specific examples:
  - 3 d free particle (also ∞ spherical well)
  - 3 d isotropic SHO (general/anisotropic in HW 6.3)

  from spherical coordinates/angular momentum viewpoint (vs. Cartesian earlier)

- One-electron atom (Coulomb potential)

General features of $u_{E\ell}(r)$

- $\boxed{r \to 0}$ studied earlier: $u_{E\ell} \propto r^{\ell+1}$

Other asymptotics: $\boxed{r \to \infty}$

Assume $\boxed{V(r) \to 0 \text{ as } r \to \infty}$

$\Rightarrow V_{eff}(r) \longrightarrow 0$ also, since
$\ell(\ell+1)\hbar^2/(2mr^2) \longrightarrow 0$ as $r \to \infty$

$\Rightarrow$ need $\boxed{E < 0}$ for bound states
($E \geq 0$ will "escape" potential)

$$\Rightarrow \frac{d^2 u_E}{dr^2} = \kappa^2 u_E, \quad \kappa^2 = -\frac{2mE}{\hbar^2} > 0$$

no "ℓ"

$(\kappa > 0)$

(as $r \to \infty$)

i.e., $u_E \propto e^{-\kappa r} + e^{+\kappa r}$

can't normalize: volume element also $\to \infty$, so drop

- Use $\rho \equiv \kappa r$ (dimensionless):

combining $r \to 0$ and $r \to \infty$ limits

$$u_{E\ell}(\rho) = \underbrace{\rho^{\ell+1}}_{\text{(short-distance)}} \times \underbrace{w(\rho)}_{\text{"well-behaved"}} \times \underbrace{e^{-\rho}}_{\text{(long-distance)}}$$

so that $w(\rho)$ satisfies

$$\frac{d^2 w}{d\rho^2} + 2\left(\frac{\ell+1}{\rho} - 1\right)\frac{dw}{d\rho} + \left[\frac{V}{E} - \frac{2(\ell+1)}{\rho}\right] w = 0$$

solution for w depends on $V(r = \rho/\kappa)$, e.g., use for Coulomb potential

Warm-up with free 3d particle and ∞ spherical well

(done earlier using Cartesian) Since $V = 0$, just use original radial equation [can we use for all r, since $V = \boxed{0}$? No: due to "E" term in DE, "A-B" solution still valid only for $r \to 0$]

$u = A r^{\ell+1} + B r^{-\ell}$,

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

$$\left[\rho = \kappa r, \quad E \equiv \hbar^2 \kappa^2 / (2m)\right]$$

— Solutions are spherical Bessel:

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

$\longrightarrow \rho^\ell$ as $\rho \to 0$ ("sensible")

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

$\longrightarrow \rho^{-\ell-1}$ as $\rho \to 0$ (problematic)

$\Rightarrow$ keep only j_ℓ ($\propto r^\ell$): matches earlier general discussion: $j_\ell \sim A \ldots$ of u, $n_\ell \sim B \ldots$

[$j_0(\rho) = \sin\rho/\rho$; $j_1(\rho) = \frac{\sin\rho}{\rho} - \frac{\cos\rho}{\rho}$ ...]

Onto ∞ spherical well:

$$V(r) = \begin{cases} 0 & \text{for } r < a \\ \infty & \text{for } r > a \end{cases}$$

$\Rightarrow$ wavefunction $[\propto j_\ell(\rho)] = 0$ $\boxed{\text{at } r = a}$

i.e., for given ℓ, $\boxed{j_\ell(ka)=0}$

$\Rightarrow ka =$ zeroes of j_ℓ

[e.g., $\underbrace{\ell = 0}_{j_0(\rho)=\frac{\sin\rho}{\rho}} \Rightarrow ka = \pi, 2\pi, 3\pi$]

$\boxed{ka=0}$ "absent", since $j_0(0) \rightarrow 1$

$$\Rightarrow E_{\ell=0} = \frac{\hbar^2}{2ma^2}\left[\pi^2, (2\pi)^2, (3\pi)^2\right]$$

(Numerically for $\ell > 0$)

In general, different ℓ's not degenerate (unless different order spherical Bessel functions — coincidentally — have same zero), cf. 3D isotropic SHO or one-electron atom below

$\boxed{\text{Isotropic}}$ SHO in 3d :

$$H = |\vec{p}|^2/(2m) + \frac{1}{2} m\omega^2 r^2$$

spectrum already obtained in HW 6.3 using cartesian, in fact for anisotropic case :

$$H = H_x + H_y + H_z$$

(sum of independent SHO in each dimension, that too different ω in general ... but here same ω :

$H_i \; (i = x, y, z) = a_i^\dagger a_i + 1/2 \ldots$

... eigenstate labeled by $|n_x, n_y, n_z\rangle$

with energy eigenvalues :

$$\frac{E}{\hbar\omega} = \underbrace{n_x + 1/2}_{\text{SHO} - x} + \underbrace{n_y + 1/2}_{\ldots y} + \underbrace{n_z + 1/2}_{\ldots z}$$

$= (N + 3/2)\hbar\omega$, $N = n_x + n_y + n_z$

Degeneracy : (1). $N = 0$: $n_x = n_y = n_z = 0$

only $\boxed{1}$ state

(2). $N = 1$: $\boxed{3}$ states (one $n = 1$, others 0)

(3). $N = 2$: one $n = 2$, other $\underbrace{}_{2\ n\text{'s}}$ 0 $\Rightarrow$ 3 states

or 1 $n = 0$, other 2 n's $= 1 \Rightarrow$ 3 states : $\boxed{\text{total} = 6}$

— "Check" using spherical coordinates (angular momentum eigenstates)

— dimensionless variables :

$$E = \frac{1}{2}\hbar\omega\lambda \quad \text{and} \quad r = \sqrt{\frac{\hbar}{m\omega}}\,\rho$$

["similar" to 1 d SHO : why not use $\rho = \kappa r$ of general strategy ?! No because $V \not\to 0$ for $r \to \infty$]

$\Rightarrow$ radial equation :

$$\boxed{\frac{d^2u}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2}u + (\lambda - \rho^2)u = 0}$$

Factor out short & long distance:

$$u(\rho) = \underbrace{f(\rho)}_{\text{well-behaved (as } r \to 0 \text{ or } \infty)} \times \underbrace{\rho^{\ell+1}}_{\text{short distance}} \underbrace{e^{-\rho^2/2}}_{\text{long... (like 1 d)}}$$

like general case

$(r^2 V \to 0$ as $r \to 0)$

[why not $e^{-\rho}$? $V(r) \not\to 0$ as $r \to \infty$]

$\Rightarrow$ DE (differential equation) for $f(\rho)$ (fixed ℓ):

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

$\boxed{\text{Goal}}$: For given ℓ, what values of λ are "needed" to get "reasonable" solution for u?

– Try series solution for $f = \sum_{n=0}^{\infty} a_n \rho^n$

– (You know the drill!) Plug into DE;

set coefficient of each power of $\rho = 0$

(0). ρ^0 gives $2(\ell+1)a_1 = 0$

{only middle term of DE: $2[(\ell+1)-\cancel{\rho}^2](a_1 + 2a_2\cancel{\rho} + \dots)$}

$\ell \geq 0 \Rightarrow (\ell+1) \geq 1 \ (\neq 0)$ so that $a_1 = 0$

(from 3rd term)

(from 1st, middle terms)

(1). a_2 related to a_0, λ by ρ^1 coefficient $= 0$

$$\rho^1 2a_2 + 2(\ell+1)\rho^1(2a_2) + [\lambda - (2\ell+3)] \times \rho^1 a_0 = 0$$

(set a_0 by normalization)

... in general, coefficient of $\rho^{n+1} = 0$

($n = 0$ above)

$$= \underbrace{(n+2)(n+1)a_{n+2}}_{\text{from 1st DE term}} + \underbrace{2(\ell+1)(n+2)a_{n+2} - 2na_n}_{\text{from 2nd} \dots} + \underbrace{[\lambda - (2\ell+3)]a_n}_{\text{from 3rd} \dots}$$

$\Rightarrow$ recursion relation:

$$a_{n+2} = a_n \frac{(2n+2\ell+3-\lambda)}{(n+2)(n+2\ell+3)}$$

$$a_1 = 0 \Rightarrow a_{3,5,\ldots} = 0 \quad (a_{odd} = 0)$$

so, only even powers of ρ in $f(\rho)$

— More importantly, $\frac{a_{n+2}}{a_n} \to \frac{2}{n} = \frac{1}{q}$
(as $n \to \infty$)

[q is integer (even/odd), since n even]

$$a_{n+2} = \frac{2}{n}\overbrace{\left(\frac{2}{n-2}a_{n-2}\right)}^{a_n} = \underbrace{\overbrace{\frac{2}{n}}^{1/q}\,\overbrace{\frac{2}{n-2}}^{1/(q-1)}\,\underbrace{\frac{2}{n-4}}_{\frac{1}{q-2}}\cdots}$$

$$\Rightarrow a_q \longrightarrow \boxed{1/q!} \text{ as } \boxed{q} \to \infty$$

so that $f(\rho) \propto \sum_q (\rho^2)^q \times 1/q!$

$$\sim \exp(+\rho^2) \to \infty \text{ for } \rho \to \infty$$

So, require series to end
for normalizable solution

$\Rightarrow$ for given λ, ℓ, "must"

have $n = 2q$ such that

$$\left(\frac{a_{n+2}}{a_n} \propto\right) = (2n + 2\ell + 3 - \lambda) = 0$$

(a_{n+2} & subsequent a's

vanish, i.e., f is polynomial)

$\Rightarrow$ flipping, λ must be

$(2n + 2\ell + 3)$ for some (even) n
$= 2q$

energy eigenvalues, $E_{q\ell} = \hbar\omega$

$= (N + 3/2)\hbar\omega$

where $N = (2q + \ell)$, since $\ell = 0, 1, 2 \ldots$

& $(2q) = 0, 2, 4 \ldots \Rightarrow N = 0, 1, 2 \ldots$

(N is principal quantum number: nodes in radial function)

... $\boxed{\text{agrees}}$ with Cartesian way:

check degeneracies also agree:

(1). $N = 0$: $q = 0 = \ell$ ($\boxed{1}$ state)

(2). $N = 1$: $q = 0, \ell = 1$ ($\boxed{3}$ states)

(3) $N = 2$: $q = 0, \ell = 2$ (5 states)
or $q = 2, \ell = 0$ (1 state) : $\boxed{\text{total} = 6}$

(different ℓ's give same E,
unlike ∞ well, like one-electron atom)

- Also, for odd/even N,
only odd/even values of ℓ
(since $N = \underbrace{2q} + \ell$)

(sign flip/not

$\Rightarrow$ parity of wavefunction)

for $\bar{r} \to -\bar{r}$) is odd/even as per ℓ odd/even, thus N ... here

— Energy eigenstate labeled

$|\, q\; \ell\; m \rangle$ or $|N \underbrace{\ell\, m}_{\text{angular part}} \rangle$

vs. $|n_x\, n_y\, n_z\rangle$ in Cartesian ...

— More in HW 8.4 (3d : "relating" $|n_{x,y,z}\rangle$ to $|\ell, m\rangle$) & HW 8.1 (2d)

— use 3d isotropic SHO as approximation to potential well of finite depth ($V(r)$ becomes large "gradually", cf. ∞ well), e.g., nuclear shell model : protons & neutrons motion in "collective" potential due to all nucleons