Lecture $\boxed{29}$, Nov. 6 (Fri.): part II

Outline for Coulomb potential (one-electron atom)

- solving radial part of wavefunction, thus energy values
- properties of energy levels
- onto spin-orbit interaction: motivation for addition of angular momenta as next topic (sec. 3.8)

$\boxed{\text{Summary}}$ of radial equation solving:

$$\langle x' | E \ell m \rangle = \boxed{R_{E\ell}(r)} \underbrace{Y_\ell^m(\theta, \phi)}_{|\vec{L}|^2,\ L_z \text{ eigenstate}}$$

requiring "sensible" solution determines energy levels

$R_{E\ell}(r) = u_{E\ell}(r)/r$ makes it "1 d" Schroedinger wave equation, with

$$V_{eff}(r) = V(r) + \left.\frac{\ell(\ell+1)\hbar^2}{2mr^2}\right\}$$ angular momentum barrier

(1). Short-distance $(r \to 0)$ behaviour:

for $r^2 V(r) \to 0$ as $r \to 0$ (e.g., 3d isotropic SHO; 1-electron atom)

$\Rightarrow$ angular momentum barrier (+ sensible solution) dictates $u_{E\ell}(r) \propto r^{\ell+1}$ (for $r \to 0$)

(2) Long-distance: for $V(r) \to 0$, thus $V_{eff} \to 0$ as $r \to \boxed{\infty}$, bound states for $E < 0$ ... useful: $\rho = \kappa r$, $\kappa = \frac{-2mE}{\hbar^2}$

$$\Rightarrow u_{E\ell}(\rho) \propto e^{-\rho} \ldots$$

(applies to Coulomb, but not to 3d SHO...)

Combining 2 asymptotics,

$$u_{E\ell}(\rho) = \underbrace{\rho^{\ell+1}}_{\text{short...}} \times \underbrace{w(\rho)}_{\text{depends on } V} \times \underbrace{e^{-\rho}}_{\text{long...}}$$

$$\boxed{\text{Coulomb potential (also classical gravity)}}$$

- One-electron atom with charge of nucleus $= -ze$ $(e<0)$ $\Rightarrow V = -\dfrac{ze^2}{r}$

- goal (general): solve for radial function, getting energy eigenvalues

- Satisfies both $V(r)$ conditions: $\to 0$ as $r \to \infty$ & $r^2 V \to 0$ as $r \to 0$ so that

$$u_{E\ell}(\rho) = \rho^{\ell+1}\, w(\rho)\, e^{-\rho}$$

- Use $\rho_0 = \sqrt{2m/-E}\left(\dfrac{ze^2}{\hbar}\right) = \sqrt{\dfrac{2mc^2}{-E}}\, z\alpha$

$\left[\alpha = e^2/(\hbar c) \simeq \dfrac{1}{137} \text{ fine structure constant}\right]$

- General equation for $w(\rho)$ becomes

$$\boxed{\rho\frac{d^2 w}{d\rho^2} + 2(\ell+1-\rho)\frac{dw}{d\rho} + \left[\rho_0 - 2(\ell+1)\right] w = 0}$$

- Goal (specifically): for given ℓ, what ρ_0 (or E) will give "reasonable" solution?

– Solve by series ansatz: see sec. 4.2.1 of (3rd edition of) $\boxed{\text{Griffiths}}$

where $\omega \to v$ in Eq. 4.61

– Summary (like 3d isotropic SHO):

(1). Plug series into DE: set net coefficient of ρ^n in DE $= 0$ ...

(2). recursion relations for coefficients in ω ...

(3). Require normalizability of $\omega(\rho)$ ... $\Rightarrow$ series must terminate ... $\Rightarrow$ $\boxed{\text{condition}}$ on $\boxed{\rho_0}$ ... and $\omega(\rho)$ is polynomial

Result: $\rho_0 = 2n$ ($n = 0, 1, 2 \ldots$ principal quantum number)

($l = 0, 1 \ldots (n-1)$)

i.e., $$\boxed{E = -\frac{1}{2} \frac{mc^2 Z^2 \alpha^2}{n^2} = -13.6\,\text{eV} \frac{Z^2}{n^2}}$$

– $\omega(\rho)$ (polynomial, defined by recursion formula, up to normalization) are (associated) Lauguerre

$$= \boxed{L^{2\ell+1}_{n-\ell}}(2\rho)$$, where (mathematically)

"physics notation"

$$L_q^{\,p}(x) \equiv (-1)^p \left(\frac{d}{dx}\right)^p L_{p+q}(x);$$

$$L_q(x) \equiv e^x/q! \, \left(d/dx\right)^q \left(e^{-x} x^q\right)$$

so that (including normalization)

$$\psi_{n\ell m}(\bar{x}) \equiv \langle \bar{x} | n\ell m \rangle = R_{n\ell}(r) Y_\ell^m(\theta, \phi),$$

$$R_{n\ell}(r) = \left(\frac{2Z}{n a_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!} \boxed{e^{-Zr/(n a_0)}}$$

$\rightarrow e^{-\rho}$ (long...

$$\times \; L^{2\ell+1}_{n-\ell-1}\left(\frac{2Zr}{n a_0}\right) \times \left(\frac{2Zr}{n a_0}\right)^\ell$$

$w(\rho)$

$\rightarrow \frac{\rho^{\ell+1}}{\rho}$ (short

where Bohr radius a_0 is natural length scale $= \hbar/(mc\alpha) \simeq 0.53\,\mathring{A}$:

$\rho = \kappa r$, with $\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$ (general)

Plug $E = -\frac{1}{2} m c^2 Z^2 \alpha^2 / n^2$ to get

$$\frac{1}{\kappa} = \frac{\hbar}{mc\alpha} \frac{n}{Z} \equiv a_0 \, n/Z$$

— Equivalently (a la $\boxed{\text{Sakurai}}$), radial equation for $w(\rho)$ written as (known) Kummer's equation, whose solution is (already) known in series form: require normalizability ... same ρ_0

[Problem 3.22 of Sakurai: 2 methods directly connected: (associated) Lauguerre polynomials (defined using generating function) solve Kummer's equation ...]

Properties of energies/radial functions

for given n $[\ell = 0, 1 \ldots (n-1)]$

(1). Wavefunctions at origin:

only $\ell = 0$ is non-vanishing

(agrees with general case: angular momentum barrier)

(2). Number of nodes: $(n-1)$ for $\ell = 0$

vs. none for $\ell = n-1$ (highest ℓ)

(3) level of degeneracy (E depends only on n, not on ℓ, m)

$$= \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{+\ell} 1 = \sum_{\ell=0}^{n-1} \underbrace{(2\ell+1)}_{\text{(usual) } \sum_m} = 2 \sum_{\ell=1}^{n-1} \ell + \overbrace{n}^{\text{number of } \ell \text{ values}}$$

(no $\ell = 0$ here)

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

[use $(1+2+\ldots n) = \dfrac{n(n+1)}{2}$]

(4) Compare to (old) $\boxed{\text{Bohr}}$ model of hydrogen atom: same energy levels [Balmer formula (empirical)] ... from quantization of angular momentum $= \hbar n$

[$\boxed{\text{1-to-1}}$ correspondence between angular momentum and energy

$\Rightarrow$ Bohr model ground state ($n = 1$) has non-zero angular momentum ($\ell = 1$)

vs. Schroedinger/Heisenberg theory:

$n = 1$ has $\ell = 0$ (zero angular momentum)

and for higher n, $\ell = 0, 1 \ldots (n-1)$ ...

($\boxed{\text{range}}$ of ℓ giving same E)

... $\boxed{\text{degeneracy}}$ in ℓ "broken" by spin-orbit interaction: so far only energy/angular momentum from (only) spatial/orbital motion included

– Enter $\boxed{\text{spin}}$ (magnetic moment) of electron (for now!): contributes to energy (Hamiltonian) if there is magnetic field ($\bar{B}$)

– $\bar{B}$ acting on electron in one-electron atom ?!

... Yes! Go to rest frame of electron,

nucleus orbiting electron $\Rightarrow$ current...

$\Rightarrow \bar{B}$ acting on electron $\propto \bar{L}$ of proton/electron

$\Rightarrow$ contribution to $H \propto \bar{B} \cdot \bar{S}$

$\propto \boxed{\bar{L} \cdot \bar{S}}$ (fine structure: E chapter 5 in Phys 623)

depends on l ;

$\Rightarrow$ motivates "adding" angular momenta