Lecture 13 — 10/23

$(\varepsilon \equiv E - mc^2)$

- $\dfrac{c^2}{2mc^2+\varepsilon-V} \propto \dfrac{1}{2m}\left(1 - \dfrac{\varepsilon - V}{2mc^2}\right)$

- $(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) \equiv \vec{A}\cdot\vec{B} + i\vec{\sigma}(\vec{A}\times\vec{B})$

$$\Rightarrow (\vec{\sigma}\cdot\vec{p})\, f(r)\, (\vec{\sigma}\cdot\vec{p}) =$$

$$= f(r)(\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\vec{p}) - i\hbar \frac{f'(r)}{r}(\vec{\sigma}\cdot\vec{r})(\vec{\sigma}\cdot\vec{p}) =$$

$$= f(r)\vec{p}^{\,2} - i\hbar\frac{f'(r)}{r}\left(\vec{r}\cdot\vec{p} + i\vec{\sigma}(\vec{r}\times\vec{p})\right)$$

with $f(r) = \dfrac{1}{2m}\left(1 - \dfrac{\varepsilon - V(r)}{2mc^2}\right)$

$$\boxed{\hbar\vec{\sigma} \equiv 2\vec{S}\ ;\ \vec{r}\times\vec{p} = \vec{L}}$$

definition of quantity with dimension of $\hbar$ (ang. mom.)

$\Rightarrow$ call "spin"

$\vec{s}$: single e^-
$\vec{S}$: all e^-

Why factor of 2?

↳ such that $\vec{s}$ spin commutation relations can be satisfied

↳ there are (at least) 2 spin components $\Rightarrow$

$$2s+1 \stackrel{!}{=} 2$$

$$\left[\left(1 - \frac{\varepsilon - V(r)}{2mc^2}\right)\frac{p^2}{2m} - i\hbar\frac{1}{4m^2c^2}\frac{V'(r)}{r}(\vec{r}\cdot\vec{p}) + \frac{1}{2m^2c^2}\frac{V'(r)}{r}\vec{S}\cdot\vec{L}\right]\psi_+ = (\varepsilon - V(r))\psi_+$$

with $\varepsilon - V(r) \approx \dfrac{p^2}{2m}$

higher spins?

$\Rightarrow \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}$ for higher-dim. Paulis

$$\Rightarrow \boxed{H = \underbrace{\frac{p^2}{2m} - \frac{p^4}{8m^2c^2}}_{\text{two lowest terms of } \sqrt{p^2c^2+m^2c^4}-mc^2} + V(r) + H_{LS} + H_D}$$

H_D : "Darwin term"

$i\frac{V'}{r}\underline{r}\cdot\underline{p}$ not hermitian (because $\psi_+ - \psi_-$ coupling neglected) $\Rightarrow$ symmetrize (Darwin)

$$i\frac{V'}{r}\vec{r}\cdot\vec{p}\,\psi \longrightarrow \frac{1}{2}\left(i\frac{V'}{r}\vec{r}\cdot\vec{p} - i\vec{p}\cdot\vec{r}\,\frac{V'}{r}\right)\psi$$

$$= -\hbar\,\psi\,\vec{\nabla}^2 V(r)$$

$$\Rightarrow \boxed{H_D = \underset{\uparrow \atop \text{general } V(r)}{\frac{\hbar^2}{8m^2c^2}}\,\vec{\nabla}^2 V(r) = \underset{\uparrow \atop \text{Coulomb pot.}}{\frac{\pi\hbar^2 Ze^2}{2m^2c^2(4\pi\epsilon_0)}}\,\delta^3(\vec{r})}$$

<u>Remarks</u> : ① only relevant for $l=0$

② <u>interpretation</u>: Uncertainty of $V(r)$: ΔV

$$\Delta V \approx \vec{\nabla}^2 V \langle \delta r_i \rangle \langle \delta r_j \rangle \approx \frac{1}{8}\lambda_c^2\,\vec{\nabla}^2 V$$

$\lambda_c = \frac{\hbar}{mc}$ $(= \alpha a_B)$ "Compton wavelength"

$\rightarrow$ Compton wavelength uncertainty.

"Zitterbewegung" - q.fluct's ≙ interactions of e^- w/ virtual e^--hole pairs.

$$\boxed{H_{LS} = \frac{1}{2m^2c^2}\frac{V'}{r}\vec{L}\cdot\vec{S} = \frac{Ze^2}{2m^2c^2(4\pi\epsilon_0)}\frac{1}{r^3}\vec{L}\cdot\vec{S}}$$

"spin-orbit coupling"

$$E_{\text{spin-orbit}} = \frac{1}{2m^2c^2}\,\frac{Ze^2}{4\pi\varepsilon_0}\left\langle \frac{1}{r^3}\right\rangle \langle \vec{L}\cdot\vec{S}\rangle$$

$$\left\langle \frac{1}{r^3}\right\rangle \to \frac{1}{l(l+\frac{1}{2})(l+1)}\,\frac{Z^3}{(n a_B)^3}$$

$$\langle \vec{L}\cdot\vec{S}\rangle = \frac{\hbar^2}{2}\begin{cases} l & \text{for } j = l+\frac{1}{2} \\ -(l+1) & \text{for } j = l-\frac{1}{2}\end{cases}$$

$$\Rightarrow \Delta\langle \vec{L}\cdot\vec{S}\rangle = \hbar^2 (l+\tfrac{1}{2})$$
(for $s = \pm\frac{\hbar}{2}$)

$$E_{\text{spin-orbit}} = \frac{\hbar^2}{4m^2c^2}\,\frac{e^2}{4\pi\varepsilon_0}\,\frac{1}{l(l+1)}\,\frac{Z^3}{(n a_B)^3} = \frac{(Z\alpha)^2}{n^3 l(l+1)} E_n$$

$$\Rightarrow \boxed{E_{nj} = E_n\left(1 - \frac{(Z\alpha)^2}{2n^2} - \frac{(Z\alpha)^4}{2n^4}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right)}$$

sorted by orders of α

"relativistic corrections"

"fine structure"

f) Lamb shift

Dirac $\Rightarrow$ $({}^2S_{1/2}, {}^2P_{1/2})$, $({}^2P_{3/2}, {}^2D_{3/2})$, $({}^2D_{5/2}, {}^2F_{5/2})$...

pairs are all degenerate!

But: measurement of Lamb, Retherford (1947)

$$\delta_L = E(2\,{}^2S_{1/2}) - E(2\,{}^2P_{1/2}) \approx 1058\,\text{MHz}\cdot\hbar$$

"Lamb shift"

Reason: interaction of atom with vacuum fluctuations of electromagnetic field.

$$\langle E\rangle = 0 \qquad \langle E^2\rangle \neq 0$$

- Brief derivation

$$\Delta V = V(\vec{r}+\delta\vec{r}) - V(\vec{r}) =$$

$$= \delta\vec{r}\cdot\vec{\nabla}V + \frac{1}{2}(\delta\vec{r}\cdot\vec{\nabla})^2 V + \ldots$$

for isotropic fluctuations:

$$\langle \vec{\delta r} \rangle_{vac} = 0$$

$$\langle (\vec{\delta r} \cdot \vec{\nabla})^2 \rangle = \frac{1}{3} \langle (\vec{\delta r})^2 \rangle \, \vec{\nabla}^2$$

$$\langle \Delta V \rangle = \frac{1}{6} \underbrace{\langle \vec{\delta r}^2 \rangle_{vac}}_{1} \; \underbrace{\left\langle \vec{\nabla}^2 \frac{-e}{4\pi\epsilon_0 r} \right\rangle_{atom}}_{2}$$

1 $\quad m \ddot{\vec{\delta r}} = -e \vec{E}_k$, $\quad \sim e^{i\nu t}$

relevant $\nu > \frac{\pi c}{a_B}$ (for $\Delta r = a_B$)

$\Delta r \cdot \Delta k \gtrsim 1/2$

($\leftarrow$ min freq. of e^-)

max ν: $\nu_{compl.} = \frac{mc^2}{\hbar}$)

$$\Rightarrow \vec{\delta r} = \frac{e}{mc^2 k^2} \vec{\mathcal{E}}_k \left(a_k e^{-i\nu t + i k \delta r} + cc \right)$$

$$|\vec{\mathcal{E}}_k| = \sqrt{\frac{\hbar c k}{2\epsilon_0 \Omega_q}}$$

Ω_q: quantization volume

$$\Rightarrow \vec{\delta r}^2 = \sum_k \left(\frac{e}{mc^2 k^2} \right)^2 \frac{\hbar c k}{2\epsilon_0 \Omega_q} \approx \qquad \Big| \; \sum_k \to \frac{\Omega_q}{(2\pi)^3} \int d^3k$$

$$= 2 \frac{\Omega_q}{(2\pi)^3} 4\pi \int k^2 dk \left(\frac{e}{mc^2 k^2} \right)^2 \frac{\hbar c k}{2\epsilon_0 \Omega_q} =$$

$$= \frac{1}{2\epsilon_0 \pi^2} \frac{e^2}{\hbar c} \left(\frac{\hbar}{mc} \right)^2 \int dk \, \frac{1}{k}$$

limits?

$\nu_{min} = \frac{\pi c}{a_B}$, $\quad \nu_{max} = \frac{mc^2}{\hbar}$

$$\Rightarrow \langle (\vec{\delta r})^2 \rangle_{vac} \approx \frac{1}{2\epsilon_0 \pi^2} \frac{e^2}{\hbar c} \left(\frac{\hbar}{mc} \right)^2 \ln \frac{4\epsilon_0 \hbar c}{e^2}$$

② $\Rightarrow -\frac{e^2}{4\pi\epsilon_0}(-4\pi)\langle\delta(\vec{r})\rangle_{atom}$

$$= \begin{cases} \frac{e^2}{\epsilon_0{}^2}|\psi(0)|^2 & \text{for } l=0 \\ 0 & \text{for } l>0 \end{cases}$$

$$|\psi_{2s}(0)|^2 = \frac{1}{8\pi a_0^3}$$

$$\langle\Delta V\rangle_{2s} = \frac{1}{6}\frac{e^2}{\epsilon_0}\frac{1}{8\pi a_0^3}\frac{1}{2\pi^2\epsilon_0}\frac{e^2}{\hbar c}\left(\frac{\hbar}{mc}\right)^2 \ln\frac{4\epsilon_0\hbar c}{e^2}$$

$$= \alpha^5 mc^2 \frac{1}{6\pi}\ln\frac{1}{\pi\alpha} \approx 1\,\text{GHz}$$