Lecture 5 – Sizes of Relativistic Corrections

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1. Time Reversal on Spinors
2. Schrödinger Corrections

1. Time Reversal on Spinors

$\Theta\chi = -i\sigma_2\chi^*$

where $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$; $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Suppose $\hat{n}\cdot\vec{\sigma}\chi = \chi$ for χ spin-up in the $\hat{n}$-direction

$$\hat{n}\cdot\vec{\sigma}(\Theta\chi) = -i\hat{n}\cdot\vec{\sigma}\sigma_2\chi^*$$

want to commute $\vec{\sigma}$ past σ_2

$$\vec{\sigma}\sigma_2 = -\sigma_2\vec{\sigma}^*$$

$$= +i\sigma_2\underbrace{\hat{n}\cdot\vec{\sigma}^*\chi^*}_{\chi^*}$$

$$= -\Theta\chi$$

↑ χ now spin-down and negative

2. Schrödinger Corrections, con't

$i\partial_t\psi = \mathcal{H}\psi$ $(\hbar = c = 1)$

$$= (\alpha^i p_i c + \beta mc^2)\psi$$

*where both α and β both commute with p

→ For non-zero p, how do we obtain $E^2 = p^2c^2 + m^2c^4$?

Assume: $\psi = e^{-iEt}e^{i\vec{p}\cdot\vec{x}}\psi_0$ ← $\psi(x=0, t=0)$

$i\partial_t\psi = E\psi$

$(i\partial_t)^2\psi = E^2\psi = \mathcal{H}^2\psi$

$$= (\alpha^i p_i + \beta m)(\alpha^j p_j + \beta m)\psi$$

$$= [\alpha^i\alpha^j p_i p_j + \underbrace{(\alpha^i\beta + \beta\alpha^i)mp_i}_{\text{this term must} = 0} + \beta^2 m^2]\psi$$

then, in order to match the E^2 equation:

$$\left.\begin{aligned} &\alpha^i\alpha^j + \alpha^j\alpha^i = 2\delta^{ij} \\ &\alpha^i\beta + \beta\alpha^i = 0 \\ &\quad\uparrow \alpha^i \,\&\, \beta \text{ anti-commute} \\ &\beta^2 = 1 \end{aligned}\right\} \text{4×4 matrices}$$

these relations can be used to solve:

- The Weyl Equation - a relativistic wave equation for describing massless spin-1/2 particles composed of two spinors
  - the signs of the spinors correspond to the chirality of Ψ or handedness (left/right)

Consider velocity in the Heisenberg representation:

$$v^i = \frac{dx^i}{dt} = -i[x^i, \mathcal{H}]$$

the only thing $\hat{x}$ does not commute with in the Hamiltonian is the $\vec{p}$-factor

$$= -i[x^i, \alpha^i \cdot p_j + \beta m]$$

$= \alpha^i$, where the α-matrix is just the velocity matrix

Look at the $\vec{p}=0$ eigenstate $E^2 = p^2c^2 + m^2c^4 \rightarrow E = \pm mc^2$

$$i\partial_t \Psi = m\beta\Psi$$

$$i\partial_t \begin{pmatrix} \Psi_+ \\ \Psi_- \end{pmatrix} = m \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} \begin{pmatrix} \Psi_+ \\ \Psi_- \end{pmatrix}$$

$\Rightarrow \begin{pmatrix} \Psi_+ \\ 0 \end{pmatrix}$ is an $E = mc^2$ eigenstate with $\Psi_+ =$ constant, $|+\rangle$

- What is the velocity of this eigenstate?

$$\langle + | v^i | + \rangle = (\Psi_+ \;\; 0) \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} \begin{pmatrix} \Psi_+ \\ 0 \end{pmatrix}$$

$$= (\Psi_+ \;\; 0) \begin{pmatrix} 0 \\ \sigma^i \Psi_+ \end{pmatrix} = 0$$

as expected that a particle with no momentum would probably have no velocity

How do we calculate these quantum fluctuations?

$\rightarrow$ Calculate variance

$\langle + | \vec{v} \cdot \vec{v} | + \rangle = 3c^2$, "Zitterbewegung"

$\vec{v} \cdot \vec{v} = \vec{\alpha} \cdot \vec{\alpha}$

this does not violate relativity because we're not certain of values

$$\begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} = \begin{pmatrix} \vec{\sigma}\cdot\vec{\sigma} & 0 \\ 0 & \vec{\sigma}\cdot\vec{\sigma} \end{pmatrix} = 3\mathbb{1}$$

a fact of v, no matter what state you're in

How large should these corrections be?
(Schwabl ch.12)
The Dirac equation → applies relativistic corrections to atomic energy levels

$\underline{H}_1$ - kinetic energy
$\underline{H}_2$ - spin-orbit
$\underline{H}_3$ - Darwin term

- for the kinetic energy term

$$E = \sqrt{p^2+m^2} = m\sqrt{1+p^2/m^2}$$

$$= m\left(1+\frac{1}{2}\frac{p^2}{m^2} - \frac{1}{8}\frac{p^4}{m^4}+\dots\right)$$

$$= mc^2 + \overbrace{\frac{p^2}{2m}}^{\text{classical contribution}} \underbrace{- \frac{1}{8}\frac{p^4}{m^3c^2}}_{H_1 \sim \frac{v^2}{c^2}\frac{p^2}{2m}} + \dots$$

whether or not H_1 is a small correction depends on the value of this ratio

estimate v^2/c^2:

$$E_n = \frac{-mZ^2e^4}{2\hbar}\cdot\frac{1}{n^2}$$ — the Coulomb energy levels

<u>Virial Theorem</u>: $2\langle T\rangle = k\langle U\rangle$ for $U \sim r^k$
kinetic energy

$\rightarrow 2\langle T\rangle = -\langle U\rangle$ for Coulomb

$$E = \langle T+U\rangle = \underbrace{-\langle T\rangle}_{\text{energy above just } -1 * KE}$$

$$\therefore \frac{1}{2}m\langle v^2\rangle = \frac{mZ^2e^4}{2\hbar^2}\cdot\frac{1}{n^2}$$

average of v^2 — α — the fine structure constant

$$\frac{\langle v^2\rangle}{c^2} = \frac{Z^2}{n^2}\left(\frac{e^2}{\hbar c}\right)^2$$

* the fine structure constant

$$\alpha \equiv \frac{e^2}{\hbar c} \approx \frac{1}{137}$$

$$\frac{\langle v^2 \rangle}{c^2} = \left(\frac{Z\alpha}{n}\right)^2$$

Look at the energy eigenstates of the unperturbed Hamiltonian:

spin degree of freedom

$$\mathcal{H}_0 |n,\ell,m\rangle|m_s\rangle = E_n |n,\ell,m\rangle|m_s\rangle$$

Is H_1 degenerate on this $\mathcal{H}_0$ n-subspace?

$\langle n,\ell',m'|H_1|n,\ell,m\rangle = 0$ unless $\ell'=\ell$ and $m'=m$

$\sim p^4 = (\vec{p}\cdot\vec{p})^2$

a scalar operator, which cannot change angular momentum -- $[p^4, L^2] = [p^4, L_z] = 0$

$\rightarrow H_1$ is already diagonal in the basis in which we know the eigenstates

$\therefore \Delta_1 E_n = \langle n,\ell,m|H_1|n,\ell,m\rangle$

- trick for evaluating $\langle p^4 \rangle$

$$\mathcal{H}_0 = \frac{p^2}{2m} + U$$

Coulomb potential

$$p^2 = 2m(\mathcal{H}_0 - U)$$

$$\langle p^4 \rangle = 4m^2 \langle (\mathcal{H}_0 - U)^2 \rangle$$

$$= 4m^2 \langle \mathcal{H}_0^2 - \mathcal{H}_0 U - U\mathcal{H}_0 + U^2 \rangle$$

$$= 4m^2 (E_n^2 - 2E_n \underbrace{\langle U \rangle}_{2E_n} + \langle U^2 \rangle)$$

this is the only thing we have to calculate

$$U = \frac{-Ze^2}{r}$$ — so all we need to calculate is $\langle \frac{1}{r^2} \rangle$

$$\rightarrow \Delta_1 E_n = \frac{-(mc^2)(Z\alpha)^4}{2n^4}\left(\frac{n}{\ell+\frac{1}{2}} - \frac{3}{4}\right)$$

- where we compare with the Coulomb's energy levels

$$E_n \rightarrow -(mc^2)\left(\frac{Z\alpha}{n}\right)^2$$

we multiplied by c^2/c^2 to get the fine structure correction term

$\rightarrow \Delta_1$ is smaller than E_n by a factor of

$\left(\frac{Z\alpha}{n}\right)^2$ (suppressed by an order of $Z\alpha/n$)

so we can say H_1 is simply a small perturbation.

— for H_2, the spin-orbit term

$$E = \underbrace{\left(\frac{1}{2m^2c^2}\,\frac{1}{r}\,\frac{dU}{dr}\right)}_{\text{scalar}} \overbrace{\vec{S}\cdot\vec{L}}^{\text{scalar operator}}$$

the electron spin interacts with the $\vec{B}$-field generated by the motion of the atom.

We need to find the eigenstates of $\vec{S}\cdot\vec{L}$

(same as solving the first-order secular equation)

$\vec{J} = \vec{L} + \vec{S}$

$J^2 = L^2 + S^2 + 2\vec{S}\cdot\vec{L}$

$\hookrightarrow \vec{S}\cdot\vec{L} = \frac{1}{2}(J^2 - L^2 - S^2)$

for which we know the eigenvalues

Note: $|n\ell m_\ell\rangle|m_s\rangle$ is NOT a J^2 eigenstate

$\ell \otimes s$ decomposes into $(\ell+\frac{1}{2}) \oplus (\underline{\ell-\frac{1}{2}})$

the states within each of these are what we need to solve to find the states of $\vec{S}\cdot\vec{L}$

if $j_1 > j_2$, $j_1 \otimes j_2 = (j_1+j_2) \oplus (j_1+j_2-1) \oplus \ldots \oplus (j_1 - j_2)$

direct sum

So instead, for the unperturbed Hamiltonian, we'll use:

$\mathcal{H}_0 |n j m_j \ell\rangle = E_n |n j m_j \ell\rangle$

where these <u>are</u> eigenstates of J^2

$\rightarrow \langle n j m_j \ell | \vec{S}\cdot\vec{L} | n j m_j \ell\rangle = \frac{\hbar^2}{2}\left(j(j+1) - \ell(\ell+1) - \frac{3}{4}\right)$

for the hydrogen atom...

Spin-orbit interaction term

$$H_2 = \frac{1}{2m^2c^2}\underbrace{\vec{S}\cdot\vec{L}}\,\frac{Ze^2}{r^3}$$

want to diagonalize the spin-orbit operator

– the states $|\ell \pm \frac{1}{2}, m_j, \ell\rangle$ diagonalize the operator $\vec{S}\cdot\vec{L}$

$$\vec{S}\cdot\vec{L}\,|l\pm\tfrac{1}{2},m_j,l\rangle = \frac{\hbar^2}{2}\begin{pmatrix} l^2+2l+\frac{3}{4}-\frac{3}{4}-l^2-l \\ l^2-\frac{1}{4}-\frac{3}{4}-l^2-l \end{pmatrix}|l\pm\tfrac{1}{2},m_j,l\rangle$$

$$\downarrow \qquad\qquad \downarrow \qquad\qquad \downarrow \qquad\qquad \downarrow$$

$$\langle H_2\rangle_{n,j=l\pm\frac{1}{2},l} = \frac{mc^2}{4n^3}\frac{(Z\alpha)^4}{l(l+\frac{1}{2})(l+1)}\begin{pmatrix} l \\ -l-1 \end{pmatrix}$$

↑ for the two j-values

$$\langle H_1+H_2\rangle = \frac{mc^2}{2n^2}(Z\alpha^4)\underbrace{\left\{\frac{3}{4}-\frac{n}{j+1/2}\right\}}$$

the dependence on l is gone!

→ However, the entire discussion is dependent on the spin degree of freedom