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Lecture XXXIII

Relativsitic Quantum Mechanics

3.1 Dirac Equation Summary and notation

We found that the two component spinors transform according to $A = e^{\pm}\sigma \cdot \xi/2$ where $\pm$ refers to the two independent transformations that are relatd by parity, the direction of the vector χ is parallel to the velocity, and $|\xi|$ is the rapidity, $\tanh\xi = v$. Two distinct transformations produce two distinct spinors that are equivalent in the respt frame. To transform from one to the other, transform to the rest frame with A_+ and then back to the moving frame with A_-.

$$\begin{aligned}
\chi_+ &= e^{\sigma\cdot\xi/2}\zeta \quad \chi_- = e^{-\sigma\cdot\xi/2}\zeta \\
&\to e^{-\sigma\cdot\xi}\chi_+ = \chi_- \\
&\to (E - \sigma\cdot\mathbf{p}) = m\chi_- \\
&\to (E + \sigma\cdot\mathbf{p}) = m\chi_+
\end{aligned}$$

$\chi_\pm$ are eigenkets of helicity with eigenvalues $\lambda = \pm\hbar/2$. In the ultra-relativistic limit $\chi_\pm$ are decoupled and never mix. Helicity is conserved. And in the low energy limit, $\chi_+ = \chi_-$. The coordinate state representation is

$$\begin{aligned}
(i\frac{\partial}{\partial t} + i\sigma\cdot\nabla)\phi_+(\mathbf{r},t) &= m\phi_-(\mathbf{r},t) \\
(i\frac{\partial}{\partial t} - i\sigma\cdot\nabla)\phi_-(\mathbf{r},t) &= m\phi_+(\mathbf{r},t)
\end{aligned}$$

where

$$\phi_\pm(\mathbf{r},t) = \int d^3p e^{-iEt}e^{i\mathbf{p}\cdot\mathbf{r}}\chi_\pm(p)$$

Define

$$\begin{pmatrix}\phi_+\\ \phi_-\end{pmatrix} \to \begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix}$$

$$A = \begin{pmatrix}A_+ & 0\\ 0 & A_-\end{pmatrix} = \begin{pmatrix}e^{\sigma\cdot\xi/2} & 0\\ 0 & e^{-\sigma\cdot\xi/2}\end{pmatrix}$$

$$\Sigma^i = \begin{pmatrix}\sigma_i & 0\\ 0 & -\sigma_i\end{pmatrix}$$

Then the Dirac equation is written

$$\begin{aligned}
(\frac{\partial}{\partial t} + \Sigma^i\frac{\partial}{\partial x^i} + im\gamma^0)\psi &= 0 \qquad (3.1)\\
&\text{or}\\
\begin{pmatrix}i\frac{\partial}{\partial t} + i\sigma\cdot\nabla & -m\\ -m & i\frac{\partial}{\partial t} - i\sigma\cdot\nabla\end{pmatrix}\begin{pmatrix}\phi_+\\ \phi_-\end{pmatrix} &= 0
\end{aligned}$$

Define

$$\gamma_0 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$$

Then ${\gamma^0}^2 = I$ and

$$\gamma^0 \Sigma^i = \gamma^i = \begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix}$$

Then multiply Equation 3.1 from the left by γ^0 and we have

$$\begin{aligned}
\gamma^0(\frac{\partial}{\partial t} + \Sigma^i \frac{\partial}{\partial x^i} + im\gamma^0)\psi &= 0 \\
(\gamma^0 \frac{\partial}{\partial t} + \gamma^i \frac{\partial}{\partial x^i} + im)\psi &= 0 \\
(\gamma^0 \partial_0 + \gamma^i \partial_i + im)\psi &= 0 \\
(\gamma^\mu \partial_\mu + im)\psi &= 0 \\
(i\gamma^\mu \partial_\mu - m)\psi &= 0
\end{aligned}$$

Just as σ transforms as a three vector, $\gamma^\mu = (\gamma^0, \gamma)$ transforms like a four vector.

3.2 Current density

Go back to coordinate representation

$$\begin{aligned} i\partial_t\phi_+ &= -i\sigma\cdot\nabla\phi_+ + m\phi_- && (3.2)\\ i\partial_t\phi_- &= i\sigma\cdot\nabla\phi_+ + m\phi_+ && (3.3)\\ & && (3.4)\end{aligned}$$

The complex conjugates are

$$\begin{aligned} -i\partial_t\phi_+^* &= i\nabla\cdot(\phi_+^*\sigma) + m\phi_-^* && (3.5)\\ -i\partial_t\phi_-^* &= -i\nabla\cdot(\phi_-^*\sigma) + m\phi_+^* && (3.6)\\ & && (3.7)\end{aligned}$$

Now multiply Equations 3.2 and 3.3 from the right by ϕ_+^* and ϕ_-^* respectively and Equations 3.5 and 3.6 from the right by ϕ_+ and ϕ_- and add and we have

$$\begin{gathered} i\partial_t(\phi_+^*\phi_+) = -i\nabla\cdot(\phi_+^*\sigma\phi_+) + m(\phi_-\phi_+^* - \phi_-^*\phi_+)\\ i\partial_t(\phi_-^*\phi_-) = i\nabla\cdot(\phi_-^*\sigma\phi_-) + m(\phi_+\phi_-^* - \phi_+^*\phi_-)\end{gathered}$$

(We have used

$$\begin{aligned} (M\Theta)_\alpha^* &= (M_{\alpha\beta}\Theta_\beta)^* = M_{\alpha\beta)}\Theta_\beta^*\\ &= \Theta_\beta^* M_{\beta\alpha}^\dagger = (\Theta^* M^\dagger)_\alpha\\ \to (\sigma\phi)_\alpha^* &= (\phi^*\sigma)_\alpha)\end{aligned}$$

The continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0$$

suggests

$$\rho = \phi_+^*\phi_+ + \phi_-^*\phi_-$$

and

$$\mathbf{j} = \phi_+^*\sigma\phi_+ - \phi_-^*\sigma\phi_-$$

Note that there is no mixing of left and right states. More notation.

$$j^\mu = (\rho, \mathbf{j}), \qquad \partial_\mu j^\mu = 0$$

Also

$$\rho = \psi^*\psi = \psi^*\gamma^0\gamma^0\psi = \bar\psi\gamma^0\psi$$

where $\bar\psi = \psi^*\gamma^0$ is the Pauli adjoint. Then

$$\mathbf{j} = \psi^*\begin{pmatrix}\sigma & 0\\ 0 & -\sigma\end{pmatrix}\psi = \psi^*\gamma^0\gamma^i\psi = \bar\psi\gamma\psi$$

and

$$j^\mu = \bar\psi\gamma^\mu\psi$$

Coupling term is $\bar\psi\gamma^\mu\psi A^\mu$

3.3 Fermion magnetic moment

First we introduce the EM field by the usual strategy, $p \to p - \frac{e}{c}A$ or in coordinate space $i\partial_\mu \to i\partial_\mu - eA_\mu$. Then the Dirac equation becomes

$$i\gamma^\mu(\partial_\mu - eA_\mu)\psi = m\psi$$

In terms of the left and right handed spinors

$$[(i\partial_0 - eV) + \sigma\cdot(-i\nabla - e\mathbf{A})]\phi_+ \quad = \quad m\phi_-$$

$$[(i\partial_0 - eV) - \sigma\cdot(-i\nabla - e\mathbf{A})]\phi_- \quad = \quad m\phi_+$$

or more compactly

$$\begin{aligned}(P_0 - \sigma\cdot\mathbf{P})\phi_+ &= m\phi_- \\ (P_0 + \sigma\cdot\mathbf{P})\phi_- &= m\phi_+\end{aligned}$$

Take the sum and difference and define

$$\begin{aligned}\tilde{\Psi} &= \frac{1}{\sqrt{2}}(\phi_+ + \phi_-) \\ \tilde{\Phi} &= \frac{1}{\sqrt{2}}(\phi_+ - \phi_-)\end{aligned}$$

Then

$$P_0\tilde{\Psi} - \sigma\cdot\mathbf{P}\tilde{\Phi} = m\tilde{\Psi} \tag{3.8}$$

$$P_0\tilde{\Phi} - \sigma\cdot\mathbf{P}\tilde{\Psi} = -m\tilde{\Phi} \tag{3.9}$$

Now define

$$\tilde{\Phi} = e^{-imt}\Phi, \qquad \tilde{\Psi} = e^{-imt}\Psi$$

Substitution into the above gives

$$P^0\Psi - \sigma\cdot\mathbf{P}\Phi = 0 \tag{3.10}$$

$$P^0\Phi - \sigma\cdot\mathbf{P}\Psi = -2m\Phi \tag{3.11}$$

Now that last equation can be rewritten

$$-\sigma\cdot\mathbf{P}\Psi = (-i\partial^0 + eV - 2m)\Phi \sim -2m\Phi \tag{3.12}$$

in the non-relativistic limit. Then substitution into the next to last gives

$$P^0\Psi - \frac{1}{2m}\sigma\cdot\mathbf{P}\sigma\cdot\mathbf{P}\Psi = (P^0 - \frac{1}{2m}(\sigma\cdot\mathbf{P})^2)\Psi = 0$$

which leads us to

$$
\begin{aligned}
0 &= (i\partial_0 - eV - \frac{1}{2m}(P^2 - i\sigma\cdot(\mathbf{P}\times\mathbf{P}))\Psi \\
&= (i\partial_0 - eV - \frac{1}{2m}(P^2 - i\sigma_k\epsilon_{ijk}P_iP_j))\Psi \\
&= (i\partial_0 - eV - \frac{1}{2m}(P^2 - i\frac{1}{2}\sigma_k\epsilon_{ijk}[P_i,P_j]))\Psi \\
&= (i\partial_0 - eV - \frac{1}{2m}(P^2 + e\frac{1}{2}\sigma_k\epsilon_{ijk}[\nabla_iA_j - \nabla_jA_i]))\Psi \\
&= (i\partial_0 - eV - \frac{1}{2m}(P^2 + e\sigma\cdot\mathbf{B}))\Psi \\
\rightarrow \quad & (\frac{1}{2m}(-i\nabla - e\mathbf{A})^2 + \frac{e}{2m}\sigma\cdot\mathbf{B} + eV)\Psi = i\partial_0\Psi
\end{aligned}
$$

The fermion magnetic moment $\mu = \frac{e}{2m}\sigma = \frac{ge}{2m}\mathbf{s} \rightarrow g = 2$.

3.4 Fine Structure Hamiltonian

Let's write an approximation of the Dirac equation to order $(v/c)^4$. We begin with a pair of coupled equations for the two spinors. In the non-relativistic limit we solve for Φ in terms of Ψ and then write an equation with only Ψ which is the solution to the Schrodinger equation when $v = 0$. We are trying to derive the fine structure hamiltonian in the Schrodinger limit, since we will in the end still rely on perturbation theory and that depends on knowing the unperturbed energies for $H_0 = \frac{p^2}{2m} + eV$. Refering back to equations 3.10 and 3.11, in the non-relativistic limit, Equation 3.11 become

$$\Phi \sim \frac{\sigma \cdot \mathbf{P}}{2m}\Psi \tag{3.13}$$

Substitution back into 3.11 gives Φ to next higher order

$$\Phi = \left(-\frac{P^0}{2m}\frac{\sigma \cdot \mathbf{P}}{2m} + \frac{\sigma \cdot \mathbf{P}}{2m}\right)\Psi$$

and then substituting into 3.10

$$\begin{aligned} P^0\Psi &= \sigma \cdot \mathbf{P}\left(-\frac{P^0}{2m}\frac{\sigma \cdot \mathbf{P}}{2m} + \frac{\sigma \cdot \mathbf{P}}{2m}\right)\Psi & (3.14) \\ &= \sigma \cdot \mathbf{P}\left(-\frac{P^0\sigma \cdot \mathbf{P}}{4m^2} + \frac{\sigma \cdot \mathbf{P}}{2m}\right)\Psi & (3.15) \end{aligned}$$

Our goal here is to derive the Schrodinger equation to order $(v/c)^6$. But Ψ is not the same as ψ. After all

$$\int |\psi|^2 d^3r = \int d^3r(|\Psi|^2 + |\Phi|^2) \approx \int d^3r(|\Psi|^2 + |\Psi^* \frac{\sigma \cdot \mathbf{P}}{2m}\frac{\sigma \cdot \mathbf{P}}{2m}\Psi|)$$

Therefore, in order that ψ be properly normalized

$$\begin{aligned} \psi &= (1 + \frac{1}{2}\left(\frac{\sigma \cdot \mathbf{P}}{2m}\right)^2)\Psi \\ &\text{and} \\ \Psi &= (1 - \frac{1}{2}\left(\frac{\sigma \cdot \mathbf{P}}{2m}\right)^2)\psi \end{aligned}$$

and substitution into 3.15 gives an equation for the Schrodinger wave function

$$P^0(1 - \frac{1}{2}\left(\frac{\sigma \cdot \mathbf{P}}{2m}\right)^2)\psi = \sigma \cdot \mathbf{P}\left(-\frac{P^0\sigma \cdot \mathbf{P}}{4m^2} + \frac{\sigma \cdot \mathbf{P}}{2m}\right)(1 - \frac{1}{2}\left(\frac{\sigma \cdot \mathbf{P}}{2m}\right)^2)\psi$$

Let's expand and rearrange that last

$$\begin{aligned} P^0\psi &= \sigma \cdot \mathbf{P}\left(-\frac{P^0\sigma \cdot \mathbf{P}}{4m^2} + \frac{\sigma \cdot \mathbf{P}}{2m}\right)(1 - \frac{1}{2}\left(\frac{\sigma \cdot \mathbf{P}}{2m}\right)^2)\psi + P^0\frac{1}{2}\left(\frac{\sigma \cdot \mathbf{P}}{2m}\right)^2\psi \\ &= \frac{(\sigma \cdot \mathbf{P})^2}{2m} - \frac{(\sigma \cdot \mathbf{P})^4}{16m^3} + \frac{1}{8m^2}([P^0, (\sigma \cdot \mathbf{P})^2] + (\sigma \cdot \mathbf{P})^2P^0) - \frac{\sigma \cdot \mathbf{P}}{4m^2}([P^0, \sigma \cdot \mathbf{P}] + \sigma \cdot \mathbf{P}P^0)\psi \\ &= \frac{(\sigma \cdot \mathbf{P})^2}{2m} - \frac{(\sigma \cdot \mathbf{P})^4}{16m^3} + \frac{1}{8m^2}([P^0, (\sigma \cdot \mathbf{P})^2]) - \frac{\sigma \cdot \mathbf{P}}{4m^2}([P^0, \sigma \cdot \mathbf{P}]) - \frac{(\sigma \cdot \mathbf{P})^2}{8m^2}P^0)\psi \end{aligned}$$

As we are interested in a hydrogen atom, we know that $P^0 = i\partial_t - eV$ and as we are in an energy eigenstate $i\partial_t\psi = E\psi$. Also $\sigma \cdot \mathbf{P} = \sigma \cdot \mathbf{p}$.

$$\begin{aligned}
(E-eV)\psi &= (\frac{(\sigma\cdot\mathbf{p})^2}{2m} - \frac{(\sigma\cdot\mathbf{p})^4}{16m^3} + \frac{1}{8m^2}([eV,(\sigma\cdot\mathbf{p})^2]) - \frac{\sigma\cdot\mathbf{p}}{4m^2}([eV,\sigma\cdot\mathbf{p}]) - \frac{(\sigma\cdot\mathbf{p})^2}{8m^2}(E-eV))\psi \\
&= (\frac{(\mathbf{p})^2}{2m} - \frac{(\mathbf{p})^4}{16m^3} + \frac{e}{8m^2}(\nabla^2 V) - e\frac{\sigma\cdot\mathbf{p}}{4m^2}(\sigma\cdot[V,\mathbf{p}]) - \frac{(\sigma\cdot\mathbf{p})^2}{8m^2}(E-eV))\psi \\
&= (\frac{(\mathbf{p})^2}{2m} - \frac{(\mathbf{p})^4}{16m^3} + \frac{e}{8m^2}(\nabla^2 V) + \frac{e}{4m^2}(\mathbf{p}\cdot[\mathbf{p},V] - i\sigma\cdot(\mathbf{p}\times[\mathbf{p},V]) - \frac{(\sigma\cdot\mathbf{p})^2}{8m^2}(E-eV))\psi \\
&= (\frac{(\mathbf{p})^2}{2m} - \frac{(\mathbf{p})^4}{16m^3} + \frac{e}{8m^2}(\nabla^2 V) + \frac{e}{4m^2}(-\nabla^2 V - i\sigma\cdot(-i\mathbf{p}\times\nabla V)) - \frac{(\sigma\cdot\mathbf{p})^2}{8m^2}(E-eV))\psi \\
&= (\frac{(\mathbf{p})^2}{2m} - \frac{(\mathbf{p})^4}{16m^3} + \frac{e}{8m^2}(\nabla^2 V) + \frac{e}{4m^2}(-\nabla^2 V - i\sigma\cdot(-i\mathbf{p}\times\frac{1}{r}\frac{dV}{dr}\mathbf{r})) - \frac{(\sigma\cdot\mathbf{p})^2}{8m^2}(\frac{p^2}{2m}))\psi \\
&= (\frac{(\mathbf{p})^2}{2m} - \frac{(\mathbf{p})^4}{16m^3} - \frac{e^2}{8m^2}\delta^3(\mathbf{r}) + \frac{e}{4m^2}(\sigma\cdot\mathbf{L}\frac{1}{r}\frac{dV}{dr}) - (\frac{\mathbf{p}^4}{16m^3}))\psi \\
&= (\frac{(\mathbf{p})^2}{2m} - \frac{(\mathbf{p})^4}{8m^3} - \frac{e^2}{8m^2}\delta^3(\mathbf{r}) + \frac{e}{4m^2}(\sigma\cdot\mathbf{L}\frac{1}{r}\frac{dV}{dr}))\psi
\end{aligned}$$

The second term is the "relativistic" correction. The third, the Darwin term, and the last, the spin orbit coupling. Note that the factor of two that in the nonrelativistic approach comes from the Thomas precession is already there.

3.5 Fine Structure Hamiltonian (Sakurai's treatment) v/c

To recover the fine structure hamiltonian we need to keep terms to next order in v/c like we started to do in Equation **??** and we need to pay attention to the normalization. The solution to the Schrodinger must be normalized and Ψ and Φ are not, but rather we should have that

$$\int |\psi|^2 d^3r = \int d^3r(|\Psi|^2 + |\Phi|^2) = \int d^3r(|\Psi|^2(1 + \frac{p^2}{4m^2c^2} + \ldots)^2)$$

where we use **??** to lowest nonzero order. Now define

$$\psi = \Omega\Psi = (1 + \frac{\mathbf{p}^2}{8m^2c^2})\psi$$

so that

$$|\psi|^2 = |\Psi|^2(1 + \frac{\mathbf{p}^2}{4m^2c^2})$$

Then multiply **??** from the left by Ω^{-1} and for simplicity assume that $\mathbf{A} = 0$.

$$\Omega^{-1}(\frac{c\mathbf{p}\cdot\sigma}{(2mc^2)}(1 + \frac{eV - E_{nr}}{2mc^2})c\mathbf{p}\cdot\sigma + eV)\Omega^{-1}\psi \quad = \quad E_{nr}\Omega^{-2}\psi$$

To order $(v/c)^2$ we have

$$\left[\frac{\mathbf{p}^2}{2m} + eV - \left\{\frac{\mathbf{p}^2}{8m^2c^2}, \left(\frac{\mathbf{p}^2}{2m} + eV\right)\right\} - \frac{\sigma\cdot\mathbf{p}}{2m}\left(\frac{E_{nr} - eV}{2mc^2}\right)\sigma\cdot\mathbf{p}\right]\psi = E_{nr}\left(1 - \frac{\mathbf{p}^2}{4m^2c^2}\right)\psi$$

With some manipulation, using $\nabla V = -\mathbf{E}$ and $\nabla \times \mathbf{E} = 0$ we get

$$\left[\frac{\mathbf{p}^2}{2m} + eV - \frac{\mathbf{p}^4}{8m^3c^2} - \frac{e\hbar\sigma \cdot (\mathbf{E} \times \mathbf{p})}{4m^2c^2} - \frac{e\hbar^2}{8m^2c^2}\nabla \cdot \mathbf{E}\right]\psi = E_{nr}\psi$$

Using

$$\mathbf{E} = -\frac{1}{r}\frac{dV}{dr}\mathbf{x}$$

we get that the fourth term is

$$-\frac{e\hbar}{4m^2c^2}\frac{-1}{r}\frac{dV}{dr}\sigma \cdot (\mathbf{x} \times \mathbf{p}) = \frac{e\hbar}{4m^2c^2}\frac{1}{r}\frac{dV}{dr}\sigma \cdot \mathbf{L} = \frac{e\hbar}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\mathbf{S} \cdot \mathbf{L}$$

The last is the Darwin term. For hydrogen

$$\frac{e\hbar^2}{8m^2c^2}\nabla \cdot \mathbf{E} = \frac{e\hbar^2}{8m^2c^2}\delta^3(\mathbf{x})$$

3.6 Darwin

We associate the Darwin term with the fact that for a relativistic electron we cannot localize it better than the compton wavelength $\lambda = 1/m$. Therefore, the interaction with the Coulomb field is smeared out and becomes a bit weaker. We can estimate the size of the effect in these terms by first considering the average of the Coulomb potential over a small region of space.

$$\overline{V}(\mathbf{r}) = V(\mathbf{r}_0) + \overline{\frac{\partial V}{\partial r_i}r_i} + \overline{\frac{1}{2}\sum_{i,j}\frac{\partial^2 V}{\partial r_i \partial r_j}\delta r_i \delta r_j} + \ldots$$

$$\overline{V(\mathbf{r})} \approx \frac{1}{6}\nabla^2 V(\delta r)^2 = \frac{1}{6}e^2\delta^3(\mathbf{r})(\delta r)$$

Finally approximate $\delta r \sim 1/m$ and

$$H_D = \frac{1}{6}\frac{e^2}{m^2}\delta^3(\mathbf{r})$$

which is pretty close to what we get from the Dirac equation. Note that it will only shift the energy of $l = 0$ states, and it turns out by the same amount as the contribution from $\mathbf{L} \cdot \mathbf{S}$ when $l = 0$ and spin orbit really cannot be contributing at all.