

Dirac Equation for a central Field

- Assume that $\vec{A} = 0$ and $\phi(\vec{r}, t) = \phi(r)$.
The Dirac equation is then

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi, \quad H = c\vec{\alpha} \cdot \vec{p} + \beta mc^2 + V.$$

- As might be expected from the nonrel. discussion of spin, $\vec{L}$ is not a constant of the motion. In fact

$$\begin{aligned} \frac{dL_x}{dt} &= \frac{1}{i\hbar} [L_x H - H L_x] \\ &= \frac{c}{i\hbar} \vec{\alpha} \cdot [(y p_z - z p_y) \vec{p} - \vec{p} (y p_z - z p_y)] \\ &= -c (\alpha_z p_y - \alpha_y p_z) \end{aligned}$$

Let us therefore try to find another operator $\vec{S}$ such that

$$\frac{dS_x}{dt} = c (\alpha_z p_y - \alpha_y p_z)$$

$$\text{Then } \frac{d}{dt} (\vec{L} + \vec{S}) = 0.$$

Since we already know about electron spin and $\vec{S} \rightarrow \vec{\sigma}$ in the N.R. two-component limit, try calculating

$$\frac{d\Sigma_x}{dt} = \frac{1}{i\hbar} [\Sigma_x, H]$$

Σ_x commutes with α_x and β , but not with α_y and α_z . We therefore need

$$\{\Sigma_x, \alpha_y\} = 2i\alpha_z, \quad \{\Sigma_x, \alpha_z\} = -2i\alpha_y.$$

Thus $\frac{d\Sigma_x}{dt} = \frac{1}{i\hbar} 2ic(\alpha_z p_y - \alpha_y p_z)$

and $\vec{J} = \vec{L} + \frac{1}{\hbar} \Sigma$ commutes with H .

$\therefore \vec{S} = \frac{\hbar}{2} \vec{\Sigma}$ is the electron spin operator.

Approximate Reduction of the Dirac Equ'n.

Write $\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$, where ψ_1 and ψ_2 are two component wavefunctions, and $E = E' + mc^2$. The Dirac equ'n. then becomes

$$\{E' + mc^2 - \beta mc^2 - V - c\vec{\alpha} \cdot \vec{p}\} \Psi = 0$$

$$\left\{ (E' + mc^2 - V) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - mc^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - c \begin{pmatrix} 0 & \vec{\sigma} \cdot \vec{p} \\ \vec{\sigma} \cdot \vec{p} & 0 \end{pmatrix} \right\} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0$$

$$(E' - V) \psi_1 - c \vec{\sigma} \cdot \vec{p} \psi_2 = 0$$

$$(E' - V + 2mc^2) \psi_2 - c \vec{\sigma} \cdot \vec{p} \psi_1 = 0.$$

From the second equation,

$$\psi_2 = \frac{c \vec{\sigma} \cdot \vec{p}}{E' - V + 2mc^2} \psi_1$$

Substituting this in the first eqn. gives

$$E' \psi_1 = \frac{1}{2m} (\vec{\sigma} \cdot \vec{p}) \frac{1}{1 + \frac{E' - V}{2mc^2}} (\vec{\sigma} \cdot \vec{p}) \psi_1 + V \psi_1$$

For $E' - V \ll mc^2$, expand

$$\frac{1}{1 + \frac{E' - V}{2mc^2}} \approx 1 - \frac{(E' - V)}{2mc^2}$$

Use $(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p}) = p^2$

$$\begin{aligned} (\vec{\sigma} \cdot \vec{p}) V (\vec{\sigma} \cdot \vec{p}) &= V (\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p}) + (\vec{\sigma} \cdot [\vec{p}, V]) (\vec{\sigma} \cdot \vec{p}) \\ &= V p^2 + \frac{\hbar}{i} (\vec{\sigma} \cdot \nabla V) (\vec{\sigma} \cdot \vec{p}) \\ &= V p^2 + \frac{\hbar}{i} [\nabla V \cdot \vec{p} + i \vec{\sigma} \cdot \nabla V \times \vec{p}] \end{aligned}$$

Then

$$\begin{aligned} E' \psi_1 &= \left[\left(1 - \frac{E' - V}{2mc^2} \right) \frac{p^2}{2m} + V \right] \psi_1 \\ &\quad - \frac{\hbar^2}{4m^2 c^2} \nabla V \cdot \nabla \psi_1 + \frac{\hbar^2}{4m^2 c^2} \vec{\sigma} \cdot \nabla V \times \vec{p} \psi_1 \end{aligned}$$

For a central potential,

$$\nabla V \cdot \nabla = \frac{dV}{dr} \frac{\partial}{\partial r} \quad \text{and} \quad \nabla V = \frac{1}{r} \frac{dV}{dr} \vec{r}$$

also $E' - V \approx \frac{p^2}{2m}$
 so that $\frac{E' - V}{2mc^2} \frac{p^2}{2m} \approx \frac{p^4}{8m^3c^2}$

The final result is

$$E' \psi_1 \approx \left(\frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + V - \frac{\hbar^2}{4m^2c^2} \frac{dV}{dr} \frac{\partial}{\partial r} + \frac{1}{2m^2c^2} \frac{1}{r} \frac{\partial V}{\partial r} \vec{L} \cdot \vec{S} \right) \psi_1 \quad \text{with } \vec{S} = \frac{\hbar}{2} \vec{\sigma}.$$

Interpretation

- The second term represents the variation of mass with velocity

$$E' = E - mc^2 = (c^2 p^2 + m^2 c^4)^{1/2} - mc^2$$

$$\approx \frac{p^2}{2m} - \frac{p^4}{8m^3c^2}.$$

- The last term is the spin-orbit interaction. For a Coulomb potential

$$V = -\frac{Ze^2}{r}$$

$$\frac{1}{r} \frac{\partial V}{\partial r} = \frac{Ze^2}{r^3}.$$

- The second-last term is characteristic of the Dirac equation, and has no classical analogue.

Separation of the Dirac Equation

Our aim is to obtain the radial part of the Dirac eqn., just as we did in the N.R. case. This can be done exactly without approximation. Start from

$$(\vec{\alpha} \cdot \vec{p} + \beta m c^2 + V(r)) \psi = E \psi.$$

$$\text{Recall that } (\vec{\alpha} \cdot \vec{A})(\vec{\alpha} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + i \vec{\Sigma} \cdot \vec{A} \times \vec{B}$$

$$\begin{aligned} \text{and write } (\vec{\alpha} \cdot \vec{p}) &= \frac{1}{r^2} (\vec{\alpha} \cdot \vec{r})(\vec{r} \cdot \vec{p}) (\vec{\alpha} \cdot \vec{p}) \\ &= \frac{1}{r^2} (\vec{\alpha} \cdot \vec{r}) [\vec{r} \cdot \vec{p} + i \vec{\Sigma} \cdot \vec{L}] \end{aligned}$$

For later convenience, write this in the form

$$(\vec{\alpha} \cdot \vec{p}) = \underbrace{\frac{1}{r} (\vec{\alpha} \cdot \vec{r})}_{\alpha_r} \underbrace{\frac{1}{r} [\vec{r} \cdot \vec{p} - i \hbar]}_{P_r} + \underbrace{i \hbar (\frac{1}{r} + \vec{\Sigma} \cdot \vec{L})}_{\frac{i \hbar}{r} \beta k}$$

$$= \alpha_r P_r + \frac{i \hbar}{r} \alpha_r \beta k$$

define $i \hbar k = \beta (\hbar + \vec{\Sigma} \cdot \vec{L})$ since $\beta^2 = 1$.

all the above operators commute with k

$$[\alpha_r, k] = 0, \quad [\beta, k] = 0, \quad [P_r, k] = 0$$

$$[\alpha_r, P_r] \neq 0$$

Thus k is a constant of the motion.
To see what it is, calculate

$$\begin{aligned} \hbar^2 k^2 &= (\vec{S} \cdot \vec{L})^2 + 2\hbar \vec{S} \cdot \vec{L} + \hbar^2 \\ &= L^2 + i \vec{S} \cdot \vec{L} \times \vec{L} + 2\hbar \vec{S} \cdot \vec{L} + \hbar^2 \\ &= L^2 + \hbar \vec{S} \cdot \vec{L} + \hbar^2 \quad (\text{since } \vec{L} \times \vec{L} = i\hbar \vec{L}) \\ &= \left(\vec{L}^2 + \frac{\hbar}{2} \vec{S} \right)^2 + \frac{1}{4} \hbar^2 \quad (\text{since } \vec{S} \cdot \vec{S} = 3) \end{aligned}$$

Since $\vec{J} = \vec{L} + \frac{\hbar}{2} \vec{S}$ and $\vec{J}^2$ has eigenvalues $\hbar^2 j(j+1)$, k^2 has eigenvalues $(j + \frac{1}{2})^2$
 $= j(j+1) + \frac{1}{4}$

Thus $k = \pm 1, \pm 2, \pm 3, \dots$

- As we will see, the energy for a Coulomb field depends only on k^2 , and is thus degenerate.

- The radial part of the Dirac equation is thus

$$\left[c \alpha_r p_r + \frac{i\hbar c}{r} \alpha_r \beta k + \beta m c^2 + V \right] \psi = E \psi(r)$$

$$\begin{aligned} \text{with } p_r &= \vec{p} \cdot \frac{\vec{r}}{r} = \hbar \nabla \cdot \vec{p} = \frac{\hbar}{r} (\vec{r} \cdot \vec{p} - i\hbar) \\ &= -i\hbar \left(\frac{d}{dr} + \frac{1}{r} \right) \end{aligned}$$

$$\text{and } \hbar k = \beta (\vec{S} \cdot \vec{L} + \hbar)$$

- Since we now have just a single α -matrix α_r instead of $\alpha_1, \alpha_2, \alpha_3$, a simpler representation is possible than 4×4 matrices.

The commutators are

$$[\alpha_r, K] = 0, \quad [\beta, K] = 0$$

$$\alpha_r \beta + \beta \alpha_r = 0, \quad \alpha_r^2 = \beta^2 = 1.$$

Choose $K = k \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

then $\alpha_r = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y$

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z$$

and $\psi(r) = \begin{pmatrix} F(r)/r \\ G(r)/r \end{pmatrix}.$

The radial Dirac equation is then

$$(\bar{E} - mc^2 - V)F + \hbar c \frac{dG}{dr} + \frac{\hbar c k}{r} G = 0$$

$$(\bar{E} + mc^2 - V)G - \hbar c \frac{dF}{dr} + \frac{\hbar c k}{r} F = 0.$$

Following Schiff, define

$$A_1 = \frac{mc^2 + \bar{E}}{\hbar c}, \quad A_2 = \frac{mc^2 - \bar{E}}{\hbar c}, \quad \rho = Ar$$

with $A = (A_1 A_2)^{1/2} = \frac{(m^2 c^4 - \bar{E}^2)^{1/2}}{\hbar c}$

The radial Dirac equation is then

$$\left(\frac{d}{d\rho} + \frac{k}{\rho} \right) G - \left(\frac{A_2}{A} + \frac{V}{\hbar c A} \right) F = 0$$

$$\left(\frac{d}{d\rho} - \frac{k}{\rho} \right) F - \left(\frac{A_1}{A} - \frac{V}{\hbar c A} \right) G = 0$$

The Hydrogen atom

- For a Coulomb potential

$$V(r) = -\frac{Ze^2}{r}$$

Put $\gamma = Ze^2/\hbar c$. Then $\frac{V}{\hbar c A} = -\frac{\gamma}{\rho}$
 $= \alpha Z$

Since the asymptotic form of the Dirac equation is the same as the Schrödinger equation, put

$$F(\rho) = f(\rho) e^{-\rho}, \quad G(\rho) = g(\rho) e^{-\rho}$$

Then

$$g' - g + \frac{k g}{\rho} - \left(\frac{A_2}{A} - \frac{\gamma}{\rho} \right) f = 0$$

$$f' - f - \frac{k f}{\rho} - \left(\frac{A_1}{A} + \frac{\gamma}{\rho} \right) g = 0$$

Look for power series solutions in the form

$$f = \rho^s (a_0 + a_1 \rho + \dots)$$

$$g = \rho^s (b_0 + b_1 \rho + \dots)$$

This gives the pair of individual equations

$$(s+k)b_0 + \gamma a_0 = 0$$

$$(s-k)a_0 - \gamma b_0 = 0$$

$$\begin{vmatrix} (s+k) & \gamma \\ (s-k) & -\gamma \end{vmatrix} = 0 \quad \text{gives } s = (k^2 - \gamma^2)^{1/2}$$

Recall that $k = \pm 1, \pm 2, \dots$ and $\gamma = \frac{Ze^2}{\hbar c} = \alpha Z$

$$\therefore s \approx 1 - \frac{1}{2} \gamma^2 \quad \text{for } k = \pm 1$$

$$\begin{aligned} \text{and } \psi_1(r) &\sim \frac{1}{r} F(r) \sim r^{-1/2} \gamma^2 \\ &= e^{-1/2 \gamma^2 \ln r} \approx 1 - \frac{1}{2} \gamma^2 \ln r. \end{aligned}$$

Thus $\psi(r)$ has a weak logarithmic singularity at the origin.

The rest of the analysis parallels that for the non-relativistic case. The requirement that the power series for f and g terminate after n' terms (i.e. $a_{n'+1} = 0, b_{n'+1} = 0$) gives

$$E = mc^2 \left[1 + \frac{\gamma^2}{(s+n')^2} \right]^{-1/2}$$

Expanding the square root gives

$$E = mc^2 \left[1 - \frac{\gamma^2}{2n'^2} - \frac{\gamma^4}{2n'^4} \left(\frac{n}{|k|} - \frac{3}{4} \right) + O(r^6) \right]$$

where $n = n' + |k|$ corresponds to the usual principal quantum no.

i.e. $n = 1, 2, 3, \dots$

$|k| = 1, 2, 3, \dots$

$n' = n - |k|$ is (no. of terms - 1) in radial function.

$$\text{A}f \quad \Delta E(n, |k|) = -\frac{mc^2 \gamma^4}{2n^4} \left(\frac{n}{|k|} - \frac{3}{4} \right)$$

$$\text{then } \Delta E(n, 1) = -\frac{mc^2 \gamma^4}{2n^4} \left(n - \frac{3}{4} \right)$$

$$\Delta E(n, n) = -\frac{mc^2 \gamma^4}{2n^4} \left(1 - \frac{3}{4} \right)$$

$$\Delta E(n, n) - \Delta E(n, 1) = \frac{mc^2 \gamma^4}{2n^4} (n-1)$$

is the fine structure splitting.

Allowed Energy Levels

- Normally, both $\pm k$ values are allowed. However, $n' \neq 0$ is a special case. The indicial equations

$$(s+k)b_0 + \gamma d_0 = 0$$

$$(s-k)a_0 - \gamma b_0 = 0$$

give $\frac{b_0}{a_0} = -\left(\frac{\gamma}{s+k}\right)$. Since $s = [k^2 - \gamma^2]^{1/2} < |k|$

$$\frac{b_0}{a_0} < 0 \text{ for } k > 0$$

$$\frac{b_0}{a_0} > 0 \text{ for } k < 0.$$

For $n'=0$, $q = b_0 p^s$, $t = a_0 p^s$

$$q' = \frac{s}{p} q \quad t' = \frac{s}{p} t$$

The p^{-1} terms in the Dirac eq'n. are

$$\left. \begin{aligned} p^{-1} [(s+k)b_0 + \gamma a_0] &= 0 \\ p^{-1} [(s-k)a_0 - \gamma b_0] &= 0 \end{aligned} \right\} \text{indicial eq'n.}$$

The p^0 terms are

$$\left. \begin{aligned} -b_0 - \frac{A_2}{A} a_0 &= 0 \\ -a_0 - \frac{A_1}{A} b_0 &= 0 \end{aligned} \right\} \Rightarrow \frac{b_0}{a_0} < 0.$$

$\therefore$ only the $k > 0$ sol'n. exists for $n'=0$.

- what is the connection between k and l ?
So far, we only know that $k^2 = (j + \frac{1}{2})^2$.
In the N.R. limit,

$$h k = \beta (\vec{\Sigma} \cdot \vec{L} + t) \rightarrow \vec{\sigma} \cdot \vec{L} + t$$

$$\text{Use } j^2 = (\vec{L} + \frac{t}{2} \vec{\sigma})^2 = L^2 + \frac{t^2}{4} \sigma^2 + t \vec{L} \cdot \vec{\sigma}$$

$$\begin{aligned} \text{to obtain } t \vec{\sigma} \cdot \vec{L} &= j^2 - L^2 - \frac{t^2}{4} \sigma^2 \\ &= (j(j+1) - l(l+1) - \frac{3}{4}) t^2 \end{aligned}$$

$$\therefore k = j(j+1) - l(l+1) + \frac{1}{4} = \begin{cases} l+1 & j = l + \frac{1}{2} \\ -l & j = l - \frac{1}{2} \end{cases}$$

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$$n = 1$$

$$n' = n - |k|$$

we only have $k^{\pm} = 1, n' = 0$

$$n = 2$$

n'	k	l	j		
0	2	1	$\frac{3}{2}$	$2 P_{3/2}$	$\text{--- } P_{3/2}$
1	-1	1	$\frac{1}{2}$	$2 P_{1/2}$	
1	1	0	$\frac{1}{2}$	$2 S_{1/2}$	$\text{--- } S_{1/2} \text{ --- } P_{1/2}$

$$n = 3$$

n'	k	l	j		
0	3	2	$\frac{5}{2}$	$2 D_{5/2}$	$\text{--- } d_{5/2}$
1	-2	2	$\frac{3}{2}$	$2 D_{3/2}$	
1	2	1	$\frac{3}{2}$	$2 P_{3/2}$	$\text{--- } P_{3/2} \text{ --- } d_{3/2}$
2	-1	1	$\frac{1}{2}$	$2 P_{1/2}$	
2	1	0	$\frac{1}{2}$	$2 S_{1/2}$	$\text{--- } S_{1/2} \text{ --- } P_{1/2}$

QED corrections lift the exact degeneracy of states with the same j . These are terms of order $\alpha^3 Z^4 \ln \alpha$