Spin of Dirac Particles

Let's discuss spin in more detail. In the Heisenberg picture we get:

\[
\frac{d\hat{A}}{dt} = \frac{i}{\hbar} [\hat{A}, \hat{H}]
\]

For a free Dirac particle \( \hat{H} = c \cdot \alpha \cdot \hat{p} + \beta m c^2 \) let's introduce a time evolution for this particle with an angular momentum \( \hat{\mathbf{L}} \):

\[
-i\hbar \frac{\partial \hat{L}^a}{\partial t} = [\hat{H}, \hat{L}^a] = \hat{c} \left( \hat{L}_x, \hat{L}_y, \hat{L}_z \right)
\]

Consider only one component, say \( \hat{L}_3 \):

\[
-i\hbar \frac{\partial \hat{L}_3}{\partial t} = [\hat{H}, \hat{L}_3] = \sum_{\kappa=1}^{3} \gamma_\kappa \frac{\alpha_{\kappa} \cdot \hat{p}_\kappa + \beta m c^2}{\kappa}
\]

\[
\frac{x_1 p_3 - x_3 p_1}{\hbar} = \mathbf{L}_3
\]

Recall \( \alpha_\kappa \) and \( \beta \) are matrices, and

\[
\left[ \beta m c^2, x_1 p_3 - x_3 p_1 \right] = 0 \quad \beta \text{ is a matrix}
\]

\( x \) and \( p \) are scalars

\[
-i\hbar \frac{\partial \hat{L}_3}{\partial t} = \sum_{\kappa=1}^{3} \gamma_\kappa \frac{\alpha_{\kappa} \cdot \hat{p}_\kappa}{\kappa} - \sum_{\kappa=1}^{3} \gamma_\kappa \frac{\alpha_{\kappa} \cdot \hat{p}_\kappa}{\kappa} + i\hbar c \sum_{\kappa=1}^{3} \delta_{\kappa 1} \hat{L}_1 + i\hbar c \sum_{\kappa=1}^{3} \delta_{\kappa 3} \hat{L}_3
\]

\[
= -i\hbar c \left( x_1 p_2 - x_2 p_1 \right) = -i\hbar \left( \alpha_{\kappa} \cdot \hat{p} \right)_{3} \text{ 3rd component}
\]
Here I used \([p_i, x_j] = -i\hbar \delta_{ij}\) \([p_i, p_j] = 0\) the same we can derive for \([L_2, \text{ } L_1]\) in other words:

\[
\frac{dL_1}{dt} = C(\alpha \times p) \neq 0
\]

thus \(\vec{L}\) is not a constant of motion.

We should construct a new operator to cancel out \(-C(\alpha \times p)\) and hence if a good operator is:

\[
\vec{L} + \vec{A} = \text{ is conserved if } \frac{d\vec{A}}{dt} = -C(\alpha \times p)
\]

We now can demonstrate that

\[
\vec{A} = \frac{\hbar}{2} \sigma^* \text{ where } \sigma^* = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}
\]

For this purpose we calculate

\[
-i\hbar \frac{d\sigma_3^*}{dt} = [\vec{A}, \sigma_3^*] =
\]

\[
\begin{bmatrix}
\sum m_\nu c^2 \cos \alpha_\nu \rho_\nu + \beta \sqrt{m c^2} & \sigma_3^* \\
\sigma_3^* & 0
\end{bmatrix} = 2i C(\alpha, p\mathbf{c} - \mathbf{p}\alpha_2)
\]

Show this again we use

\[
[\beta \sqrt{mc^2}, \sigma_3^*] = 0
\]

\[
[\alpha_3, \sigma_3^*] = 0 \quad \sigma_1^* \sigma_3^* = -\sigma_3^* \sigma_1^* \quad \text{(I used sympy)}
\]
that is: \[ \frac{\hbar}{2} \frac{d^2 \sigma_3^*}{dt^2} = -C (\alpha \times p) \] component

the same for \( \sigma_1^* \) and \( \sigma_2^* \), in short

\[ \frac{d}{dt} \frac{\hbar}{2} \sigma_3^* = -C (\alpha \times p) \]

Combining this with the expression for \( \sigma \)

\[ \frac{dL}{dt} = C (\alpha \times p) \implies \frac{1}{m} \frac{d}{dt} (L + \frac{\hbar}{2} \sigma_3^*) = 0 \]

Thus a new quantity:

\[ \tilde{J} = L + \frac{\hbar}{2} \sigma_3^* \]

is conserved \( \frac{d\tilde{J}}{dt} = 0 \)

and the Dirac particle has spin \( \frac{\hbar}{2} \sigma_3^* \)

**Dirac Particle in a Potential**

To solve a problem of a Dirac particle in the potential \( V \), we first modify the equation to include the potential. Intuitively, we can write down:
\[ H = c \alpha \cdot \overrightarrow{p} + mc^2 + V(x) = \]
\[ = -i \hbar c \frac{\partial}{\partial t} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + V(x) \]

where we selected \( \alpha = \alpha_2 \)

for \( H \psi = E \psi \Rightarrow \)

\[ \left[ i \hbar c \frac{\partial}{\partial t} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + mc^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + V \right] \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \]

\[ \Rightarrow \text{multiplying those matrices} \]

\[ \left\{ \begin{array}{l}
- i \hbar c \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E_1 \psi_1 \\
\frac{d}{dt} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + V \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} E_2 \psi_1 \\ \psi_2 \end{pmatrix}
\end{array} \right. \]

Recall \( \psi_1 = \begin{pmatrix} \varphi_1 \\ w_1 \end{pmatrix} \) and \( \psi_2 = \begin{pmatrix} \varphi_2 \\ w_2 \end{pmatrix} \)

those are two bound state solutions

So we have \( k \) equ. for those components
\[-\hbar c \psi_1 - (m c^2 + V) \psi_1 = \varepsilon_1 \psi_1 \]
\[-\hbar c \psi'_1 - (m c^2 + V) \psi_1 = \varepsilon_1 \psi'_1 \]
\[-\hbar c \psi'_2 + (m c^2 + V) \psi_2 = \varepsilon_2 \psi_2 \]
\[-\hbar c \psi_2 - (m c^2 + V) \psi_2 = \varepsilon_2 \psi_2 \]
\[
\begin{align*}
\hbar c (\psi_1 \psi'_2 - \psi'_1 \psi_2) &= (\varepsilon_1 - \varepsilon_2) \psi_1 \psi_2 \\
\hbar c (\psi'_1 \psi_2 - \psi_1 \psi'_2) &= (\varepsilon_1 - \varepsilon_2) \psi'_1 \psi'_2
\end{align*}
\]

or
\[
\hbar c \frac{d}{dz} (\psi_1 \psi_2 - \psi_1 \psi_2) = (\varepsilon_1 - \varepsilon_2) \psi'_1 \psi'_2
\]

if \( \varepsilon_1 = \varepsilon_2 \) \implies \frac{d}{dz} (\psi_1 \psi_2 - \psi_2 \psi_1) = 0

cost. If \( z \to \infty \)
so the constant = 0

that is: \( \frac{\psi_1}{\psi_2} = \frac{\psi_2}{\psi_1} \), returning

or \( \frac{\psi_1}{\psi_2} = \frac{\psi_2}{\psi_1} \Rightarrow \psi_1 \propto \psi_2 \)

meaning they represent the same state and meaning also they are NON-DEGENERATE

and also \( \langle \psi_1 | \psi_2 \rangle = \int_{-\infty}^{\infty} \psi_1^{*} \psi_2 dz \)
Recall
\[ \frac{\hbar}{c} \frac{d}{dz} (\psi_1 \psi_2^* - \psi_1^* \psi_2) = (E_1 - E_2) \psi_1^* \psi_2 \]

\[ \psi_1^* \psi_2 = \frac{\hbar c}{E_1 - E_2} \frac{d}{dz} (\psi_1 \psi_2 - \psi_1^* \psi_2) \Rightarrow \int \cdots \]

\[ \frac{1}{E_1 - E_2} \left( \psi_1 \psi_2 - \psi_1^* \psi_2 \right) \bigg|_\infty^{-\infty} = 0 \]

or \( \psi_1 \) and \( \psi_2 \) are orthogonal.

+ non-degeneracy

This means that level crossing cannot occur!

When the potential varies smoothly, the w.f. also vary smoothly.

\[ \begin{array}{c}
\text{E} \\
\text{E}_2 \\
\downarrow \\
\text{E}_1 \\
\end{array} \]

\( \psi_1^* \psi_2 \) as some parameter e.g. momentum

and for the levels to cross

\[ \text{this require a behavior in } |\langle \psi_1 | \psi_2^* \rangle| \]

When \( E_1 = E_2 \) AND SINGULAR POTENTIAL!
Klein "Paradox"

(verified in graphene)

Consider a scattering process by the step potential \( V(x) \).

\[ \Psi \sim E - V_0 \]

**FREE PARTICLE**

1st we construct the plane wave solution of Dirac's free electron in 1D:

\[ E \psi = \left( c \alpha \cdot p + \beta mc^2 \right) \psi \quad \text{or} \quad i \hbar \frac{\partial \psi}{\partial t} + i \hbar c \Sigma \frac{\partial \psi}{\partial x} - mc^2 \begin{pmatrix} \bar{\Sigma} & 0 \\ 0 & \bar{\Sigma} \end{pmatrix} \psi = 0 \]

or in the \( \tau \)-component form:

\[ i \hbar \frac{\partial \psi_1}{\partial t} + i \hbar c \frac{\partial \psi_1}{\partial x} - mc^2 \psi_1 = 0 \]

\[ i \hbar \frac{\partial \psi_2}{\partial t} + i \hbar c \frac{\partial \psi_2}{\partial x} - mc^2 \psi_2 = 0 \]

\[ i \hbar \frac{\partial \psi_3}{\partial t} + i \hbar c \frac{\partial \psi_3}{\partial x} - mc^2 \psi_3 = 0 \]

\[ i \hbar \frac{\partial \psi_4}{\partial t} + i \hbar c \frac{\partial \psi_4}{\partial x} - mc^2 \psi_4 = 0 \]

**Note:** \( \psi_1 \) couples only to \( \psi_3 \) and \( \psi_2 \) to \( \psi_4 \).
6/c of this let's introduce a 2-component spinor, with $\Psi_0 = \psi_1$ or $\psi_2$
$\Psi_2 = \psi_3$ or $\psi_4$

for stationary states we get:

$$i\hbar c \psi_1' + (E + mc^2) \psi_4 = 0$$
$$i\hbar c \psi_3' + (E - mc^2) \psi_2 = 0$$

in terms of $\psi_2$ and $\psi_0$ we can rewrite it as a single equation:

$$i\hbar c \psi_0' + (E + mc^2) \psi_2 = 0$$
$$i\hbar c \psi_2' + (E - mc^2) \psi_0 = 0$$

rename $\psi_0 = \psi$ and $\psi_2 = w$

$$i\hbar c \psi' + (E + mc^2) w = 0$$
$$i\hbar c w' + (E - mc^2) \psi = 0$$

$$\frac{d}{dx} \psi$$

and using $w'$ from $w$

$$i\hbar c w'' + (E + mc^2) w' = 0$$

$$w' = \frac{\psi'}{\left(\frac{\hbar c}{E + mc^2}\right)}$$

$$\psi'' + \frac{\hbar^2}{E + mc^2} \psi = 0$$

where $p^2 = c^2 \left(\frac{E^2}{E + mc^2} - 1\right)$

and putting $w''$ into $w = -\frac{i\hbar c}{E + mc^2} \cdot \psi'$
For $\psi'' + \frac{p^2}{\hbar^2} \psi = 0$

- $\psi = A e^{i p x / \hbar} + B e^{-i p x / \hbar}$

and $w = -\frac{(i \hbar c)}{E + mc^2} \cdot \psi$

Based on this we can write down:

$U^- (x) = A \left( e^{i p x / \hbar} + R e^{-i p x / \hbar} \right)$

$W^- (x) = A \left( e^{i p x / \hbar} - a R e^{-i p x / \hbar} \right)$

From solution for $<$ we set the solution for $>$ by replacing $E$ by $E - V_0$

The W.F. for $x < 0$ is:

$\psi^- = \begin{pmatrix} U^- \\ \omega_2 \end{pmatrix} = A \int \begin{pmatrix} 1 \\ (a) \end{pmatrix} e^{i p x / \hbar} +

+ R \begin{pmatrix} -1 \\ -a \end{pmatrix} e^{-i p x / \hbar} \int = A \left[ U_+ e^{i p x / \hbar} + R \right.$

$U_- e^{-i p x / \hbar} \left. \right] \quad \text{where} \quad U_+ = \begin{pmatrix} 1 \\ a \end{pmatrix}$

for $x > 0$ there is no reflected wave

so $\psi^+ = \begin{pmatrix} U^+ \\ \omega_2 \end{pmatrix} = D \bar{U} e^{-i p x / \hbar}$
\[
\begin{align*}
\text{here } \bar{u} &= \begin{pmatrix} 1 \\ b \end{pmatrix} \quad \bar{p} = p \left( E - V_0 \right) = \frac{1}{\sqrt{c^2 (E - V_0)^2 - m^2 c^4}} \\
\text{and } b &= \frac{c \bar{p}}{(E - V_0 + mc^2)}
\end{align*}
\]

As usual to determine those constants A, D and R we use

\[
\begin{align*}
\left\{ \begin{array}{l}
\psi_\leq (0) = \psi_\geq (0) \\
\psi^*_\leq (0) = \psi^*_\geq (0)
\end{array} \right.
\end{align*}
\]

\[
\begin{align*}
\int \bar{u} e^{i p x \hbar / \sqrt{2}} = A \int U_+ e^{i p x \hbar / \sqrt{2}} + RU_- e^{-i p x \hbar / \sqrt{2}} \quad x = 0
\end{align*}
\]

\[
A \left( U_+ + RU_- \right) = D\bar{u} \quad \Rightarrow \\
A \left[ \begin{pmatrix} 1 \\ a \end{pmatrix} + R \begin{pmatrix} 1 \\ -a \end{pmatrix} \right] = D \begin{pmatrix} 1 \\ b \end{pmatrix}
\]

\[
\begin{align*}
\Rightarrow \begin{cases}
A (1 + R) = D \\
A a (1 - R) = b D
\end{cases} \quad \Rightarrow R = \frac{a - b}{b + a} \\
T = \frac{2 a}{a + b}
\end{align*}
\]
Behavior of the w.f. depends on $v_0$.

Consider:
1. $E > v_0 + mc^2$
2. $v_0 - mc^2 < E < v_0 + mc^2$
3. $E < v_0 - mc^2$

\[ E > v_0 + mc^2 \implies E^2 > m^2 c^4 + v_0^2 + 2mc^2v_0 > 0 \]
\[ E^2 - m^2 c^4 > 0 \]
\[ p^2 c^2 = E^2 - m^2 c^4 \implies p > 0 \implies p \text{ is real} \]

Since $E - v_0 > mc^2$, $(E - v_0)^2 > m^2 c^4$, or
\[ \bar{p} = \sqrt{(E - v_0)^2 - m^2 c^4} \]
\[ \bar{p} > 0 \implies \text{and } \bar{p} \text{ is real} \]

As such if $E > v_0 + mc^2$

\[ x < 0 : e^{-ipx} \text{ incident, } e^{ipx} \text{ reflected, } e^{-2ipx} \text{ transmitted} \]

ALL LIKE NIRQM?
\[ V_0 - mc^2 < E < V_0 + mc^2 \]

in this case \( (E - V_0)^2 < mc^4 \)

or

\[ \sqrt{\left( (E - V_0)^2 - mc^4 \right)} \]

is imaginary.

Then we have for:

\[ x > 0 \]

in coming + reflected

\[ \text{exponentially decaying wave} \]

Like in NRQM.

**Finally**

\[ E < V_0 - mc^2 \]

\[ E - V_0 < -mc^2 \]

\[ (E - V_0) < 0 \]

and

\[ (E - V_0)^2 > mc^4 \]

\[ \sqrt{\left( (E - V_0)^2 - mc^4 \right)} \]

is real!

**Meaning that we have oscillatory behaviour after the barrier!!??**
Recall for NRQM no such solution is possible.

But wait as $E_0 - V_0 + mc^2 < 0$ and thus $b$ is negative

\[ b = \frac{c \sqrt{p^2}}{E - V_0 + mc^2} \Rightarrow b < 0 \]

we can write down

\[ |R| = \left| \frac{a - b}{a + b} \right| > 1 \]

Klein paradox: The amplitude of the reflected wave is larger than incoming one. Or more particles gets reflected than arrived.

Also one can show the even for $V_0 \rightarrow \infty$

\[ \Gamma = \frac{2p}{E + p} \neq 0.11?? \]
Dirac electron in the field

Electric field is described by

\[ A_\mu = \left( \frac{i \varphi}{c}, A \right) \]

and Dirac eqn is simply ii modified as

\[ \nu \rightarrow \nu = \mathbf{E} \rightarrow \mathbf{E} - e \varphi \]

\[
\begin{aligned}
(E - mc^2) \mathbf{u} &= c (\sigma \cdot p) \mathbf{u} \\
(E + mc^2) \mathbf{u} &= c (\sigma \cdot p) \mathbf{u}
\end{aligned}
\]

Now we are interested in positive solutions in the form

\[ E = E + mc^2 > 0 \]

\[
(2mc^2 + E - e \varphi) \mathbf{u} = c \sigma \cdot (p - \frac{e}{c} A) \mathbf{u}
\]

in a weak field \( E \) and \( e \varphi \) are small so

\[ 2mc^2 \mathbf{u} \approx c \sigma \cdot (p - \frac{e}{c} A) \mathbf{u} \Rightarrow \]

\[ w \approx \frac{1}{2mc} \sigma \cdot (p - \frac{e}{c} A) \mathbf{u} \]

\[
(E - e \varphi - mc^2) \mathbf{u} \approx c (\sigma \cdot (p - \frac{e}{c} A))^2 \mathbf{u} \Rightarrow \]

\[ E = E + mc^2 \]
\[
\frac{1}{2m} \left[ \sigma \cdot \left( p - \frac{e}{c} A \right) \right]^2 \nu = (\mathcal{E} - e\varphi)^2
\]

Using \((\sigma \cdot B)(\sigma \cdot C) = B \cdot C + i\sigma \cdot (B \times C)\)

with \(B = C = p - \frac{e}{c} A\)

\[\left(\sigma \cdot (p - \frac{e}{c} A)\right)^2 = (p - \frac{e}{c} A)^2 + i\sigma \begin{bmatrix} (p - \frac{e}{c} A)_x \\ (p - \frac{e}{c} A)_y \\ (p - \frac{e}{c} A)_z \end{bmatrix} \times (p - \frac{e}{c} A)^2 \frac{eB}{c} B \times \frac{1}{2} \rho \times \rho \]

where \(\vec{B} = \vec{\nabla} \times \vec{A}\)

thus the eqn:

\[\frac{1}{2m} \left[ \sigma \cdot (p - \frac{e}{c} A) \right]^2 \nu = (\mathcal{E} - e\varphi)^2\]

be comes

\[\frac{1}{2m} \int \left( p - \frac{e}{c} A \right)^2 - \frac{eB}{2mc} \sigma \cdot \vec{B} + e\varphi \right]\nu = \mathcal{E}\nu
\]

\[\vec{B} = \vec{\nabla} \times \vec{B}\]

**Pauli Equation**

the extra term \(-\frac{e\hbar}{2mc} \cdot \vec{B}\) suggest

that an electron in the mag. field

gains extra energy \(-\vec{\mu} \cdot \vec{B} = -\frac{e\hbar}{2mc}\vec{\sigma} \cdot \vec{B} = -\mu_B \cdot \vec{B}\)
Important topic is spin-orbit interaction. READ pp 493-495 of the text.

the END of RQM Section!