

Lecture 8

①

Spin of Dirac Particles

In the Heisenberg picture we get

$$\frac{dA}{dt} = \frac{i}{\hbar} [A, H]$$

For a free Dirac particle $H = c \cdot \alpha \cdot p + \beta mc^2$
Let's introduce a time evolution for this particle with an angular momentum \vec{L} :

$$-i\hbar \frac{\partial}{\partial t} \vec{L} = [H, \vec{L}]$$

↳ (L_x, L_y, L_z)

Consider only one component; say L_z

$$-i\hbar \frac{\partial L_z}{\partial t} = [H, L_z] = \left[\sum_{k=1}^3 c \alpha_k p_k + \beta mc^2, \underbrace{x_1 p_2 - x_2 p_1}_{=L_z} \right]$$

recall α_k and β are matrices, and

$$[\beta mc^2, x_1 p_2 - x_2 p_1] = 0 \leftarrow \text{can you tell why?}$$

$$-i\hbar \frac{\partial L_z}{\partial t} = \left[\sum c \alpha_k p_k, x_1 p_2 - x_2 p_1 \right] - \sum c \alpha_k p_k, x_2 p_1] = -i\hbar c \sum \alpha_k \delta_{k_1 p_2} + i\hbar c \sum \alpha_k \delta_{k_2 p_1} = -i\hbar c (\alpha_1 p_2 - \alpha_2 p_1) = -i\hbar (\alpha \times p)_3 \text{ -d component}$$

Here I used $[p, x] = -i\hbar$ $[p_i, p_j] = 0$
 the same we can derive for L_2 and L_1
 in other words:

$$\frac{d\vec{L}}{dt} = c(\alpha \times p) \neq 0$$

so L is not a constant of motion

We should construct a new operator to cancel out $-c(\alpha \times p)$ and make it a good operator, i.e.

$$L + A = \text{is conserved if } \frac{dA}{dt} = -c(\alpha \times p)$$

We now can demonstrate that

$$\bar{A} = \frac{\hbar}{2} \cdot \vec{\sigma}^* \quad \text{where } \vec{\sigma}^* = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$$

For this purpose we calculate

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

$$= [\sum (\alpha_k \cdot p_k + \beta mc^2), \sigma_3^*] = 2i (\alpha_1 p_1 - p_1 \alpha_1)$$

again we use

$$[\beta mc^2, \sigma_3^*] = 0$$

↑
scalar

$$[\alpha_3, \sigma_3^*] = 0$$

$$\sigma_1^* \sigma_3^* = -\sigma_3^* \sigma_1^*$$

and $\sigma_1^* \sigma_2^* = -i\sigma_3^*$ (show this with Pauli matrices)

that is : $\frac{\hbar}{2} \frac{d\sigma_3^*}{dt} = -c(\alpha \times p)_3$ ③

the same for σ_1^* and σ_2^* , in short

$$\frac{d}{dt} \frac{\hbar}{2} \vec{\sigma}^* = -c(\alpha \times \vec{p})$$

Combining this with the expression for \vec{L}

$$\frac{d\vec{L}}{dt} = c(\alpha \times \vec{p}) \Rightarrow \frac{d}{dt} \left(\vec{L} + \frac{\hbar}{2} \vec{\sigma}^* \right) = 0$$

↑
Spin
angular
moment

Thus a new quantity :

$$\vec{J} = \vec{L} + \frac{\hbar}{2} \vec{\sigma}^*$$

is conserved $\frac{d\vec{J}}{dt} = 0$

and the Dirac particle has spin $\frac{\hbar}{2} \sigma^*$

Dirac PARTICLE IN A POTENTIAL

To solve a problem of a Dirac particle in the potential V we 1st modify the equation to include the potential.

Intuitively we can write down:

$$\begin{aligned}
 H &= c\alpha \cdot \vec{p} + \beta mc^2 + V = \\
 &= -i\hbar c \frac{d}{dz} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \\
 &+ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + V(z)
 \end{aligned}$$

where we select $\alpha = \alpha_2$

for $H\psi = E\psi \Rightarrow$

$$\left[i\hbar c \frac{\partial}{\partial z} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + mc^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + V \right] \begin{pmatrix} u \\ w \end{pmatrix} = E \begin{pmatrix} u \\ w \end{pmatrix} \Rightarrow \text{multiplying those matrices}$$

$$\begin{cases}
 -i\hbar c w' + V(mc^2 + V) = Eu \\
 \hbar c u' - w(mc^2 + V) = Ew
 \end{cases}$$

Recall $\psi_1 = \begin{pmatrix} u_1 \\ w_1 \end{pmatrix}$ and $\psi_2 = \begin{pmatrix} u_2 \\ w_2 \end{pmatrix}$
 these are two bound state solutions

So we have 4 eqns for those components

$$\begin{pmatrix} \psi_2^* \\ \psi_1^* \end{pmatrix} \begin{cases} -\hbar c w_1' + (mc^2 + V) \psi_1 = E_1 w_1 \\ \hbar c \psi_1' - (mc^2 + V) w_1 = E_1 \psi_1 \\ -\hbar c w_2' + (mc^2 + V) \psi_2 = E_2 \psi_2 \\ \hbar c \psi_2' - (mc^2 + V) w_2 = E_2 w_2 \end{cases}$$

$$\begin{cases} \hbar c (\psi_1 w_2' - w_1' \psi_2) = (E_1 - E_2) \psi_1 \psi_2 \\ \hbar c (\psi_1' w_2 - w_1 \psi_2') = (E_1 - E_2) \psi_1 w_2 \end{cases}$$

→ $\hbar c \frac{d}{dz} (\psi_1 w_2 - w_1 \psi_2) = (E_1 - E_2) \psi_1^* \psi_2$

① if $E_1 = E_2 \Rightarrow \frac{d}{dz} (\psi_1 w_2 - \psi_2 w_1) = 0$

↓
const.

We assume that ψ and $w \rightarrow 0$ if $z \rightarrow \infty$
so the constant = 0

that is: $\frac{\psi_1}{w_1} = \frac{\psi_2}{w_2}$, return in g .

or $\frac{\psi_1}{\psi_2} = \frac{w_1}{w_2} \Rightarrow \psi_1 \propto \psi_2$

meaning they represent the same state
meaning also they are NON-DEGENERATE
and also $\langle \psi_1 | \psi_2 \rangle = \int_{-\infty}^{\infty} \psi_1^* \psi_2 dz =$

recall $\frac{d}{dz} (\psi_1 \psi_2 - w_1 \psi_2) = (E_1 - E_2) \psi_1 \psi_2$ (6)

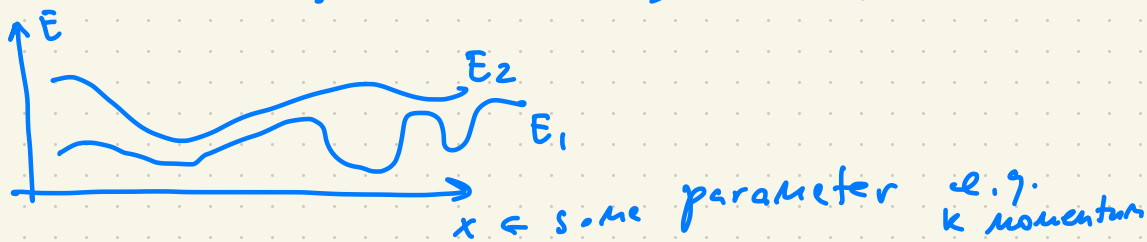
$\psi_1 \psi_2^* = \frac{\hbar c}{E_1 - E_2} \frac{d}{dz} (\psi_1 \psi_2 - w_1 \psi_2) \Rightarrow \int \dots$

$\frac{1}{E_1 - E_2} (\psi_1 \psi_2 - w_1 \psi_2) \Big|_{-\infty}^{\infty} = 0$

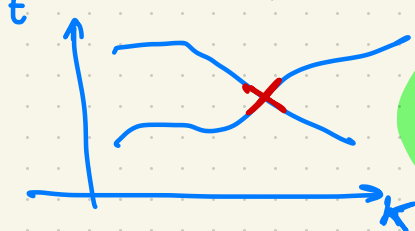
or ψ_1 and ψ_2 are orthogonal

+ non-degenerate
This means that level crossing cannot occur!

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



and for the levels to cross

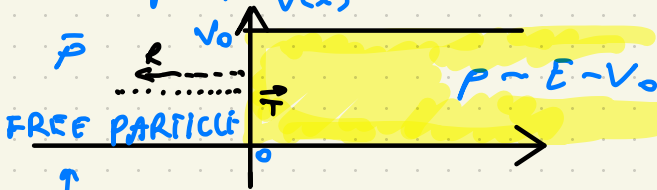


This requires a SINGULAR behavior in $\langle \psi_1 | \psi_2 \rangle$ when $E_1 = E_2$

Klein "Paradox"

(verified in graphene)

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



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

$$E\psi = (c\alpha_x p_x + \beta mc^2)\psi \quad \text{or}$$

$$i\hbar \frac{\partial \psi}{\partial t} + i\hbar c \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \frac{\partial \psi}{\partial x} - mc^2 \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \psi = 0$$

or in the χ -component form:

$$i\hbar \frac{\partial \chi_1}{\partial t} + i\hbar c \frac{\partial \chi_4}{\partial x} - mc^2 \chi_1 = 0$$

$$i\hbar \frac{\partial \chi_2}{\partial t} + i\hbar c \frac{\partial \chi_3}{\partial x} - mc^2 \chi_2 = 0$$

$$i\hbar \frac{\partial \chi_3}{\partial t} + i\hbar c \frac{\partial \chi_2}{\partial x} - mc^2 \chi_3 = 0$$

$$i\hbar \frac{\partial \chi_4}{\partial t} + i\hbar c \frac{\partial \chi_1}{\partial x} - mc^2 \chi_4 = 0$$

Note: χ_1 couples only to χ_3
and χ_2 to χ_4 .

b/c of this let's into a 2-component 8
spinor, with $\Psi_u = \Psi_1$ or Ψ_2

$$\Psi_D = \Psi_3 \text{ or } \Psi_4$$

for stationary states we get:

$$\left. \begin{array}{l} \text{with } \Psi_1' + (E + mc^2)\Psi_4 = 0 \\ \text{with } \Psi_3' + (E - mc^2)\Psi_2 = 0 \end{array} \right\} \begin{array}{l} \text{with } \Psi_2' + (E + mc^2)\Psi_1 = 0 \\ \text{with } \Psi_4' + (E - mc^2)\Psi_3 = 0 \end{array}$$

in terms of Ψ_u and Ψ_e we
can rewrite it as a single equation

$$\left\{ \begin{array}{l} i\hbar c \Psi_u' + (E + mc^2)\Psi_e = 0 \\ i\hbar c \Psi_e' + (E - mc^2)\Psi_u = 0 \end{array} \right.$$

rename $\Psi_u = u$ and $\Psi_e = w$

$$\left\{ \begin{array}{l} i\hbar c u' + (E + mc^2)w = 0 \quad \checkmark \\ i\hbar c w' + (E - mc^2)u = 0 \quad \checkmark \end{array} \right.$$

$\frac{d}{dx} u$ and using w' from w

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

$$w' = \frac{u (E - mc^2)}{i\hbar}$$

$u'' + \frac{p^2}{\hbar^2} u = 0$ where $p^2 \equiv c^2 (E^2 - m^2 c^4)$
and putting u'' into $\bullet w = -\frac{i\hbar c}{E + mc^2} \cdot u'$

For $\psi'' + \frac{p^2}{\hbar^2} \psi = 0$

(9)

$\psi = A e^{ipx/\hbar} + B e^{-ipx/\hbar}$

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

Based on this we can write down:

$\psi_L(x) = A (e^{ipx/\hbar} + R e^{-ipx/\hbar})$

$w_L(x) = A (a e^{ipx} - aR e^{-ipx/\hbar})$
 $a \equiv c p / (E + mc^2)$

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

The w.f. for $x < 0$ is:

$\Psi_L = \begin{pmatrix} \psi_L \\ w_L \end{pmatrix} = A \left[\begin{pmatrix} 1 \\ a \end{pmatrix} e^{ipx/\hbar} + R \begin{pmatrix} 1 \\ -a \end{pmatrix} e^{-ipx/\hbar} \right] \equiv A \left[u_+ e^{ipx/\hbar} + R u_- e^{-ipx/\hbar} \right]$ where $u_{\pm} = \begin{pmatrix} 1 \\ \pm a \end{pmatrix}$

for $x > 0$ there is no reflected wave

so $\Psi_R = \begin{pmatrix} \psi_R \\ w_R \end{pmatrix} = D \bar{u} e^{ipx/\hbar}$

(10)

here $\bar{u} = \begin{pmatrix} 1 \\ b \end{pmatrix}$ $\bar{p} = p(E - V_0) = \frac{1}{c} [(E - V_0)^2 - m^2 c^4]^{1/2}$

and $b = \frac{c\bar{p}}{(E - V_0 + mc^2)}$

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

$$\begin{cases} \psi_{<}(0) = \psi_{>}(0) \\ \psi'_{<}(0) = \psi'_{>}(0) \end{cases}$$

for $\psi_{<}$ $D\bar{u} e^{i\bar{p}x/\hbar} = A [u_+ e^{ipx/\hbar} + Ru_- e^{-ipx/\hbar}]$ at $x=0$

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

$\Rightarrow \begin{cases} A(1+R) = D \\ Aa(1-R) = bD \end{cases} \Rightarrow R = \frac{a-b}{b+a}$
 $T = \frac{2a}{a+b}$

Behavior of the w.f. depends on V_0 (11)

Consider ① $E > V_0 + mc^2$

② $V_0 - mc^2 < E < V_0 + mc^2$

③ $E < V_0 - mc^2$

① $E > V_0 + mc^2 \Rightarrow$
 $E^2 > m^2 c^4 + V_0^2 + 2mc^2 V_0 \Rightarrow$
 $E^2 - m^2 c^4 > 0$
 $p^2 c^2 = E^2 - m^2 c^4$ also $> 0 \Rightarrow$
 p is real

Since $E - V_0 > mc^2$ $(E - V_0)^2 >$
 $> m^2 c^4$ or

$$\bar{p} = \sqrt{(E - V_0)^2 - m^2 c^4} > 0$$

\Rightarrow and \bar{p} is real

as such if

$$E > V_0 + mc^2$$

ALL like NRQM!

$x < 0$: e^{ipx} incoming + e^{-ipx} reflected

$x > 0$ e^{ipx} transmitted

2 $V_0 - mc^2 < E < V_0 + mc^2$

in this case $(E - V_0)^2 < m^2 c^4$

or $\tilde{P} = [(E - V_0)^2 - m^2 c^4]^{1/2}$

is IMAGINARY

Then we have for:

$x < 0$

incoming + reflected

$x > 0$

exponentially decaying wave

LIKE IN NRQM.

Finally

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$E < V_0 - mc^2$

$E - V_0 < -mc^2 \Rightarrow$

$(E - V_0) < 0$ and

$(E - V_0)^2 > m^2 c^4 \Rightarrow$

\tilde{P} is REAL !

Meaning that we have oscillatory behaviour after the barrier !!??

Recall for NRQM no such solution is possible.

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But wait as $E_0 - V_0 + mc^2 < 0$

and thus b is negative

$$\left(b = \frac{c\bar{p} > 0}{(E - V_0 + mc^2) < 0} \Rightarrow b < 0 \right)$$

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 $V_0 \rightarrow \infty$

$$T = \frac{2p}{E+p} \neq 0 \text{ !! ??}$$

Dirac electron in the field

(14)

Electric field is described by

$A_\mu = \left(\frac{e\varphi}{c}, \vec{A} \right)$ and Dirac eqn
is simply modified as $\vec{p} \rightarrow \vec{p} - \frac{e}{c}\vec{A}$
 $E \rightarrow E - e\varphi$

$$\begin{cases} (E - e\varphi - mc^2) \psi = c (\vec{\sigma} \cdot \vec{p}) \chi \\ (E + mc^2) \chi = c (\vec{\sigma} \cdot \vec{p}) \psi \end{cases}$$

\uparrow
 $E - e\varphi$

Now we are interested in positive solutions in the form

$$E = E_0 + mc^2$$

$$(2mc^2 + E_0 - e\varphi) \chi = c \vec{\sigma} \cdot (\vec{p} - \frac{e}{c}\vec{A}) \psi$$

in a weak field E_0 and $e\varphi$ are small

$$\text{so } 2mc^2 \chi \approx c \vec{\sigma} \cdot (\vec{p} - \frac{e}{c}\vec{A}) \psi \Rightarrow$$

$$\chi \approx \frac{1}{2mc} \vec{\sigma} \cdot (\vec{p} - \frac{e}{c}\vec{A}) \psi$$

$$(E_0 - e\varphi - mc^2) \psi \approx \frac{c}{2mc} (\vec{\sigma} \cdot (\vec{p} - \frac{e}{c}\vec{A}))^2 \psi \Rightarrow$$

\uparrow
 $E_0 = E + mc^2$

$$\frac{1}{2m} \left[\sigma \cdot \left(p - \frac{e}{c} A \right) \right]^2 \psi = (\mathcal{E} - e\varphi) \psi \quad (15)$$

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

with $B = C = \left(p - \frac{e}{c} A \right) \Rightarrow i\hbar \nabla$

$$\left[\sigma \cdot \left(p - \frac{e}{c} A \right) \right]^2 = \left(p - \frac{e}{c} A \right)^2 + i\sigma \cdot \left\{ \begin{array}{l} \left(p - \frac{e}{c} A \right)_x \\ \times \left(p - \frac{e}{c} A \right) \end{array} \right\} = \left(p - \frac{e}{c} A \right)^2 - \frac{e\hbar}{c} \sigma \cdot B$$

$p \times p + \frac{e^2}{c^2} A \times A + \frac{p \times A - A \times p}{= 2p \times A} \quad p = i\hbar \nabla$

where $\bar{B} = \nabla \times \bar{A}$

thus the eqn:

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

becomes

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

\uparrow
 $B = \nabla \times A$

PAULI EQUATION

the extra term $-\frac{e\hbar}{2mc} \sigma \cdot B$ suggest

that an electron in the magn. field gains extra energy $-\bar{\mu} \cdot \bar{B} = -\frac{e\hbar}{2mc} \sigma \cdot B = -\mu_B \sigma \cdot B$

Important topic is spin-orbit
interaction: READ pp 493-495
of the text.

the END OF RQM
section! 