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Introduction to relativistic quantum mechanics

So far, we have confined our discussions to Schrödinger equation & its related phenomenon.

Since the Schrödinger equation is motivated by the non-relativistic energy-momentum relation : $E = \frac{p^2}{2m} + U(x)$, it belongs to non-relativistic quantum mechanics.

Here the appropriate invariance of the equation is addressed by the **Galilean** transformation :

Galilean transformation & Schrödinger eq.

$$\left.\begin{aligned} x' &= x - vt \\ t' &= t \end{aligned}\right\} \text{ Galilean transformation of coordinates}$$

probability is invariant : $|\psi'(x',t')|^2 = |\psi(x,t)|^2$ . . . ①

different functions

$\therefore\ \psi'(x',t') = e^{i\alpha(x,t)}\psi(x,t)$ $\quad \alpha(x,t)$ real. . . . ②

$\therefore$ If we start from a free particle at rest in the unprime frame, $\psi(x,t) = A_0$.

In the prime frame, this particle is still free but has momentum $p = -mv$, $E = \frac{1}{2}mv^2$.

Therefore $\psi'(x',t') \propto e^{i\frac{1}{\hbar}(px' - Et')} = e^{\frac{-i}{\hbar}(mvx - \frac{mv^2}{2}t)}$

moving towards left

To obey ①, $\psi'(x',t') = A_0 e^{\frac{-i}{\hbar}(mvx - \frac{mv^2}{2}t)}$

Now, the phase $\alpha(x,t)$ in equation ② should be independ of ψ, i.e., carry no information of particular frames.

Otherwise, there is no "universal" transformation rule on $\psi(x,t)$; different $\psi(x,t)$'s transform differently (using different α).

This violates the principle of linear superposition:

Same Hamiltonian: $\psi_1 \to \psi_1'$

$\psi_2 \to \psi_2'$

$\tilde{\alpha}\psi_1 + \tilde{\beta}\psi_2 \to \tilde{\alpha}\psi_1' + \tilde{\beta}\psi_2'$

$\therefore$ $\alpha(x,t)$ must be independent of $\psi(x,t)$!

$$\therefore \quad \psi'(x',t') = e^{\frac{-i}{\hbar}(mvx - \frac{mv^2}{2}t)}\,\psi(x,t) \qquad \text{--- ③}$$

even if $\psi(x,t)$ describes a plane wave already!

In the presence of a potential U, we have

e.g. $f(x') = U'(x')$ $\boxed{U'(x',t) = f(x)}$

$$U'(x-vt,t) = U(x,t).$$

$\Rightarrow U(x,t) = f(x-vt)$

It turns out α does not depend on U (as expected).

and is still given by ③. (exercise) another way recover by path integral

$\therefore$ The Galilean transformation only changes phases of the wave functions: $\psi'(x',t') = e^{\frac{-i}{\hbar}(mvx - \frac{mv^2}{2}t)}\,\psi(x,t)$

* ~~New~~ aspects & problems encountered in relativistic Q.M.

(i) Lorentz invariance (covariance): Obviously, when one goes to relativistic Q.M., one has to incorporate the Lorentz invariance instead of the Galilean invariance:

$$x' = \frac{x - vt}{\sqrt{1 - v^2/c^2}} \qquad y' = y$$

$$t' = \frac{t - \frac{v}{c^2}x}{\sqrt{1 - v^2/c^2}} \qquad z' = z$$

In this case, $|\psi(x,t)|^2$ is no longer invariance because of the Lorentz contraction.

In fact, $|\psi(x,t)|^2$ & the probability current form a four vector.

If one thinks everything carefully, one should discover that for the free particle case, the true invariant quantity is # of waves between two any points in space-time, i.e, $\underbrace{\vec{k}\cdot\vec{x}-\omega t}$, whose invariance governs the transformation: product of two 4-vectors $(ct, \vec{r})\cdot(\frac{E}{c}, \vec{p})$ #

$$e^{-\frac{i}{\hbar}(mvx-\frac{mv^2}{2}t)}\; e^{\underline{i(kx-\omega t)}} \qquad \frac{i}{\hbar}[px-\frac{p^2}{2m}t]$$

$$= e^{\frac{i}{\hbar}[(p-mv)x-(E-\frac{1}{2}mv^2)t]} \qquad \frac{p^2}{2m}-\frac{1}{2}mv^2-pmv+mv^2$$

$$= e^{\frac{i}{\hbar}[p'(x'+vt')-(E-\frac{1}{2}mv^2)t']} \qquad =\frac{1}{2m}(p-mv)^2$$

$$= e^{\underline{\frac{i}{\hbar}[p'x'-\frac{p'^2}{2m}t']}} \qquad p'=p-mv.$$

$\therefore$ For a plane wave of a scalar particle (spin=0), one expects its form should be

$$A\, e^{\frac{i}{\hbar}[\vec{p}\cdot\vec{x}-Et]}$$ which is the same in every frame.

(ii) Field theory is unavoidable.

In non-relatistic Q.M., we talk about the probability of finding a particle at x, which is $|\Psi(x,t)|^2$.

The underlying assumption behind the above statement is that we can measure the position of the particle, x, as accurately as we like (of course, sacrificing the accuracy of the momentum!)

This scenario is changed, however, as we go to relativistic Q.M.

In relativistics, the relation $E^2 = c^2p^2 + m^2c^4$ tells us that there is $\underbrace{\text{a minimun energy}}_{mc^2}$ to create a particle; while in non-relatisvistics, no such possibility is exhibited!

Compton wavelength:

Consider a Gaussian wave packet with Δx,

$$\therefore \Delta p \sim \frac{\hbar}{\Delta x}$$

$$\Delta E \simeq \sqrt{c^2(\Delta p)^2 + m^2c^4} \gtrsim 2mc^2 \quad \text{if} \quad \Delta p \gtrsim mc$$

$$\therefore \text{For } \Delta x \lesssim \frac{\hbar}{mc}, \quad \Delta E \gtrsim 2mc^2$$

Since when $\Delta E \gtrsim 2mc^2$, creation of particles (particle-antiparticle pair) is possible ($\Delta E + mc^2 \gtrsim 3mc^2$).

$\therefore$ This indicates that when $\Delta x \leq \frac{\hbar}{mc}$ (probing the system to localize the particle in a region narrower than $\frac{\hbar}{mc}$), the single-particle picture may fail!

The length $\frac{\hbar}{mc} \equiv \lambda\!\!\!^{-}_e$ is called Compton wavelength.

In the atomic & molecular physics, the characteristic length $= a_0$ (Bohr radius).

$$\because \quad \frac{\lambda\!\!\!^{-}_e}{a_0} = \frac{\hbar}{mc}\frac{me^2}{\hbar^2} = \frac{e^2}{\hbar c} = \alpha \simeq \frac{1}{137}$$

$\therefore$ single-particle theory (Schrödinger eq.) is approximately good! (Field theory correction $\sim O(\alpha)$ ~~QED $\Rightarrow$ $O(\alpha^2)$~~) e.g. anamolous magnetic moment)

When the single-particle theory fails, specifying the amplitude of finding a particle specifically becomes less interesting because the particle that is found in experiments may not be the same particle as different expts perform.
because the # of particles is not conserved

Instead, it is more convenient to talk about # of particles found at (x,t). In principle, there is no limit on total # of particles. The theories that deal with infinitely many particles are called field theories.
or (degrees of freedoms)

In quantum field theories, $\Psi(x,t)$ is no longer wavefunctions (Ψ no longer describes "matter waves"), instead, $\Psi(x,t)$ is promoted to be an operator. This is called field quantization.

For example, the Schrödinger wave function $\psi(x,t)$ can be also quantized to be a boson field:

$$\underset{\substack{\uparrow \\ \text{create a particle at } (x,t)}}{\psi^{+}(x,t)}\ \underset{\substack{\uparrow \\ \text{vacuum.}}}{|0\rangle}$$

$$\therefore\ |xt\rangle = \psi^{+}(x,t)|0\rangle$$

Also $$\underbrace{[\psi(x,t),\ \psi^{+}(x',t)]}_{\text{same time}}_{\pm} = \delta(x-x')$$

$$\Leftrightarrow\ [a, a^{+}] = 1$$

(iii) difficulties with negative energy.

In classical mechanics, the relation $E^2 = c^2p^2 + m^2c^4$ permits two solutions: $E = \pm\sqrt{c^2p^2+m^2c^4}$.

This is not a problem in classical mechanics because the change of energy is continuous and we always start from mc^2, $\therefore$ the energy is always positive.

When we go to relativistic Q. M., we can no longer throw away negative energy states by simply condemning them as unphysical solutions. The transition, induced by the perturbation $Ve^{i\omega t}$ with $\omega > 2mc^2$, can always bring a positive energy state to a negative energy state!

Since there is no bound for $\sqrt{p^2c^2+m^2c^4}$, the energy of a particle will be min. if it goes to $-\infty$ energy state.

It is this difficulty that bothered early physicists working in this field.

Facing this problem, as we shall see, Dirac simply assumes that states, from $E = -mc^2$ to $-\infty$, are filled, so that by Pauli's exclusion principle, the transition to negative states is forbidden.

This proposal actually brings us back to quantum field theory because the negative energy states are full of other particles! (even though this proposal eventually is abandoned)

Note that in non-relativistic Q.M., we are always staying on positive energy branch:

$$E = \sqrt{m^2c^4 + p^2c^2} = mc^2 + \frac{p^2}{2m} + \cdots$$

no such difficulty arises!

Single-particle theories (essentially, 1st quantization)

Early work concentrated on respecting Lorentz covariance

These work lead to some equations which respect Lorentz covariance but because they are constructed in "single-particle" fashion, the difficulties of negative energy & non-positivity of ρ (see below) still exist.

The followings are two representatives:

* Klein-Gordon equation

Historically, this equation was also considered by Schrödinger himself too, but it was abandoned because the probability thus defined is not positive definite (see below).

From $E^2 = p^2c^2 + m^2c^4$, substitute E by $i\hbar\frac{\partial}{\partial t}$ & $\vec{p}$ by $\frac{\hbar}{i}\vec{\nabla}$, we obtain the Klein-Gordon equation:

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = (-\hbar^2c^2\nabla^2 + m^2c^4)\,\psi \quad \text{--- ①}$$

By construction, $\psi = e^{i(\vec{k}\cdot\vec{r} - \omega t)}$ is the plane wave solution.

Note that this is second-order in time

$\therefore$ At $t=0$, we can arbitrary assign ψ_0 & $\left.\frac{\partial\psi}{\partial t}\right|_0$ ---①'

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Now $\because$ $-\hbar^2 \frac{\partial^2\psi^*}{\partial t^2} = (-\hbar^2 c^2 \nabla^2 + m^2c^4)\,\psi^* \quad \cdots ②$

$$\psi^* \times ① - \psi \times ② \Rightarrow -\hbar^2 \frac{\partial}{\partial t}\left[\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right]$$
$$= -\hbar^2 c^2\, \vec{\nabla}\cdot\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]$$

$\therefore$ We can identify

$$\vec{j} = \frac{-i\hbar}{2m}\left[\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right]$$
$$\rho = \frac{i\hbar}{2mc^2}\left[\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right]$$

for completeness one has to include ECO

As a result of ①′, ρ can be made negative!
(Note that $\rho<0$ corresponds to $\omega<0$, i.e. negative E solutions)
It was because of this difficulty, the Klein-Gordon equation was postponed 7 years until Pauli & Weisskopf re-interpretated the Klein-Gordon equation as a field equation and found that it describes (complex) spin zero charged particles (for example, K^-, π^- mesons) and ρ is the net charge density which of course can be negative!

↳ ECO, antiparticle
∴ charge is opposite! (particle, $q>0$)

* The Dirac equation.

This is what we will be mainly discussing.
As hinted by two-component formulation of spin, one knows that the wave function needs to be at least two-component for spin-$\frac{1}{2}$ particles!

* The fact that the Klein-Gordon eq. needs two initial conditions is later realized as: one needs two initial conditions for particle/antiparticle

So, we will consider the most general situation when

$$\Psi = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix}$$ has N components.

To avoid the problem that the Klein-Gordon eq. has, the equation must be first order in time.

To be Lorentz covariance, it also must be first order in $\frac{\partial}{\partial x_i}$ so that $\vec{x}$ & t are equally treated!

* For a free particle, the most general eq. that is linear in Ψ may be written as

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{\hbar c}{i} \left[\alpha_1 \frac{\partial \Psi}{\partial x} + \alpha_2 \frac{\partial \Psi}{\partial x_2} + \alpha_3 \frac{\partial \Psi}{\partial x_3} \right] + \beta m c^2 \Psi$$

where $\alpha_1, \alpha_2, \alpha_3$ & β are $N \times N$ matrices!

We can write the above eq. as

$$i\hbar \frac{\partial \Psi}{\partial t} = (c\,\vec{\alpha} \cdot \vec{p} + \beta m c^2)\,\Psi \equiv \hat{H}\,\Psi$$

where $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$.

$$\Psi_E \sim e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - Et)}$$

$\therefore$ We get $E\,\mathbb{I} = c\,\vec{\alpha}\cdot\vec{p} + \beta m c^2 = c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta m c^2$

To compare with $E^2 = m^2c^4 + p^2c^2$,

We require :

$$(c\vec{\alpha}\cdot\vec{p} + \beta mc^2)^2 = E^2 \mathbb{I}$$

$$\shortparallel$$

$$c^2\alpha_x^2 p_x + c^2\alpha_y^2 p_y^2 + c^2\alpha_z^2 p_z^2 + \beta^2 m^2 c^4$$

$$\left.\begin{aligned} &+ c^2(\alpha_x\alpha_y + \alpha_y\alpha_x)\, p_x p_y + \cdots \\ &+ mc^3\, p_x(\alpha_x\beta + \beta\alpha_x) + \cdots \end{aligned}\right\} \text{cross-terms}$$

$$\therefore \left.\begin{aligned} &\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = \mathbb{I} \\ &\alpha_i\alpha_j + \alpha_j\alpha_i = 0 \qquad i \neq j \\ &\alpha_i\beta + \beta\alpha_i = 0 \end{aligned}\right\} \cdots (3)$$

$\because \hat{H}$ is Hermitian, $\therefore$ α_i, β are hermitian matrices.

Also, $\because \beta^2 = 1$, $\alpha_i = -\beta\alpha_i\beta$

$$\therefore tr(\alpha_i) = -tr(\beta\alpha_i\beta) = -tr(\alpha_i\beta^2)$$
$$= -tr(\alpha_i)$$

$\therefore tr(\alpha_i) = 0$

$\because \alpha_i^2 = \mathbb{I}$ $\therefore$ eigenvalues of $\alpha_i = \pm 1$

this combined with $tr(\alpha_i) = 0 \Rightarrow$ dim. of α_i must be even !

(exercise 1.8.8.)

The case $N=2$ (N=0 too!) is ruled out because σ_i are matrices satisfying $\sigma_i\sigma_j + \sigma_j\sigma_i = 0$, $\sigma_i^2 = \mathbb{I}$; there exists no 4th matrix β to anticommute with σ_i ! (Ex 14.3.8) (unless $m=0$)

$\therefore$ The min dim to realize $\alpha_x, \alpha_y, \alpha_z$ & β is 4!

The followings are particular representations that are frequently used:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}.$$

see over

[In fact, because the Lorentz group is $SU(2) \otimes SU(2)$, the min nontrivial representation of $SU(2)$ is $N=2$,

$\therefore$ the min. " " of Lorentz group is

$N=4$ ($N=2$ is ruled out to be a candidate as argued above).]

The resulting eq. is called the Dirac equation!

Note that since during the derivation, one inevitably has to use $E^2 = p^2c^2 + m^2c^4$, negative energy solutions are actually built into the equation. As we shall see, the Dirac eq. does not escape the "threat" of negative energy solutions!

However, since it's first order in time, it overcomes the problem of negative probability density:

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar}{i} c \sum_{k=1}^{3} \alpha_k \frac{\partial}{\partial x^k} \psi + \beta m c^2 \psi \quad \cdots (4)$$

$$-i\hbar \frac{\partial \psi^+}{\partial t} = -\frac{\hbar}{i} c \sum_{k=1}^{3} \frac{\partial \psi^+}{\partial x^k} \alpha_k + \beta m c^2 \psi^+ \quad \cdots (5)$$

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Dirac matrices

$$\gamma^0 = \beta, \quad \vec{\gamma} = \beta \vec{\alpha}$$

$$\gamma^\mu = (\gamma^0, \vec{\gamma}) \qquad \gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu} I$$

Can be proved that

if $\gamma'^\mu \gamma'^\nu + \gamma'^\nu \gamma'^\mu = 2g^{\mu\nu} I$ too

$$\gamma'^\mu = \underset{\substack{\uparrow \\ \text{unitary matrix}}}{U} \gamma^\mu U^+$$

R.H. Good. Rev. Mod. Phys. 27, 187 (1955)

$$\therefore \left(i\hbar \gamma'^\mu \frac{\partial}{\partial x^\mu} - mc \right) \psi' = 0$$

$$\left(i\hbar \gamma^\mu \frac{\partial}{\partial x^\mu} - mc \right) \psi = 0$$

$$U^+ \psi' = \psi$$

$\therefore$ Choosing one particular representation is enough!

$$\not{\partial} \equiv \gamma^\mu \underbrace{\frac{\partial}{\partial x^\mu}}_{\partial_\mu} = \gamma^0 \frac{\partial}{c\partial t} + \vec{\gamma} \cdot \vec{\nabla}$$

Among other representations, the Majorana representation is special: make the Dirac eq. real

$$\tilde{\alpha}_1 = -\alpha_1, \quad \tilde{\alpha}_2 = \beta, \quad \tilde{\alpha}_3 = -\alpha_3, \quad \tilde{\beta} = \alpha_2$$

$$\left(\underbrace{\hbar \frac{\partial}{\partial t} + \tilde{\vec{\alpha}} \cdot \vec{\nabla} + i \tilde{\beta} mc}_{\text{real !}} \right) \psi = 0$$

$$\psi^{+} (4) - (5)\psi$$

$$\Rightarrow \; i\hbar \frac{\partial}{\partial t}(\psi^{+}\psi) = \frac{\hbar c}{i}\sum_{k=1}^{3}\frac{\partial}{\partial x^k}(\psi^{+}\alpha_k\psi)$$

i.e. $\frac{\partial}{\partial t}(\psi^{+}\psi) + \nabla\cdot(c\psi^{+}\vec{\alpha}\psi) = 0$

We identify $\rho = \psi^{+}\psi$

$\vec{J} = c\psi^{+}\vec{\alpha}\psi$

$\because \rho = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2$

$\therefore$ ρ is positive definite! can be interpretated as probability density.

In the rest frame

$$i\hbar\frac{\partial\psi}{\partial t} = \beta mc^2\psi = \begin{pmatrix} mc^2 & 0 & 0 & 0 \\ 0 & mc^2 & 0 & 0 \\ 0 & 0 & -mc^2 & 0 \\ 0 & 0 & 0 & -mc^2 \end{pmatrix}\psi$$

$\therefore$ we have four solutions

$$\psi^1 = e^{-\frac{i}{\hbar}mc^2t}\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad \psi^2 = e^{\frac{-i}{\hbar}mc^2t}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$

$$\psi^3 = e^{\frac{i}{\hbar}mc^2t}\begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad \psi^4 = e^{\frac{i}{\hbar}mc^2t}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

$\left.\begin{array}{l}\psi^1 \,\&\, \psi^2 \Rightarrow \text{positive energy} \\ \psi^3 \,\&\, \psi^4 \Rightarrow \text{negative} \quad '' \end{array}\right\}$ one sees that negative energy solutions persist!

This situation persists even when the particle is not in the rest frame!

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General plane wave solutions

If we write $\psi_E = \begin{pmatrix} \chi \\ \Phi \end{pmatrix} e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - Et)}$, χ & Φ are two-component spinors.

The Dirac eq. becomes

$$E\begin{pmatrix} \chi \\ \Phi \end{pmatrix} = (c\vec{\alpha}\cdot\vec{p} + \beta mc^2)\begin{pmatrix} \chi \\ \Phi \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} E-mc^2 & -\vec{\sigma}\cdot\vec{p}c \\ -\vec{\sigma}\cdot\vec{p}\cdot c & E+mc^2 \end{pmatrix}\begin{pmatrix} \chi \\ \Phi \end{pmatrix} = 0$$

$$\left.\begin{aligned} \chi &= \frac{c\vec{\sigma}\cdot\vec{p}}{E-mc^2}\Phi \\ \Phi &= \frac{c\vec{\sigma}\cdot\vec{p}}{E+mc^2}\chi \end{aligned}\right\rangle \quad \frac{c^2(\vec{\sigma}\cdot\vec{p})^2}{E^2-m^2c^4} = 1 \Rightarrow E^2 = m^2c^4 + c^2p^2$$

$$E = \pm\sqrt{c^2p^2+m^2c^4}$$

Let $E_p \equiv \sqrt{c^2p^2+m^2c^4}$

take

$$\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \Phi = \frac{c\vec{\sigma}\cdot\vec{p}}{E_p+mc^2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{c}{E_p+mc^2}\begin{pmatrix} P_z & P_x - iP_y \\ P_x+iP_y & -P_z \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{cP_z}{E_p+mc^2} \\ \frac{cP_+}{E_p+mc^2} \end{pmatrix} \qquad P_\pm \equiv P_x \pm iP_y .$$

after normalization :

$$\psi^1 = \sqrt{\frac{E_p+mc^2}{2mc^2}}\begin{pmatrix} 1 \\ 0 \\ \frac{cP_z}{E_p+mc^2} \\ \frac{cP_+}{E_p+mc^2} \end{pmatrix} e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - Et)}$$

which is continuously connected to $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{\frac{i}{\hbar}mc^2t}$, $\therefore E = +\sqrt{c^2p^2+m^2c^4} = E_p$

Note that the normalization condition is

$$\int d^3\vec{r}\ \psi_1^+(r,t)\,\psi_1(r,t) = \text{Lorentz invariant}.$$

where $\psi_1^+\psi_1 = \frac{E_p+mc^2}{2mc^2}\left(1+\frac{c^2p^2}{(E_p+mc^2)^2}\right)$

$$= \frac{1}{2mc^2}\,\frac{E_p^2+2mc^2E_p+(mc^2)^2+c^2p^2}{E_p+mc^2}$$

$$= \frac{1}{2mc^2}\,\frac{2E_p(E_p+mc^2)}{E_p+mc^2} = \frac{E_p}{mc^2} = \gamma\ \left(=\frac{1}{\sqrt{1-v^2/c^2}}\right)$$

Which is to compensate the Lorentz contraction of $d^3\vec{r}$!

Similarly, $\chi \Rightarrow \begin{pmatrix}0\\1\end{pmatrix} \Rightarrow$ we get

$$\psi^2 = \sqrt{\frac{E_p+mc^2}{2mc^2}}\begin{pmatrix}0\\1\\ \frac{cp_-}{E_p+mc^2}\\ \frac{-cp_z}{E_p+mc^2}\end{pmatrix} e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-Et)}, \quad E=E_p$$

$\Phi \Rightarrow \begin{pmatrix}1\\0\end{pmatrix}$ $\quad \chi \Rightarrow \frac{c}{E_p+mc^2}\,\vec{\sigma}\cdot\vec{p}\begin{pmatrix}1\\0\end{pmatrix}$ $\left[=\frac{c}{(-E_p)-mc^2}(-\vec{\sigma}\cdot\vec{p})\begin{pmatrix}1\\0\end{pmatrix}!\right]$

($E=-E_p$, $\vec{p}\to-\vec{p}$ so that $e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-Et)}$

becomes $e^{\frac{-i}{\hbar}(\vec{p}\cdot\vec{r}-Et)}$ to be able to

connect with $e^{\frac{i}{\hbar}mc^2t}$!)

$$\psi^3 = \sqrt{\frac{E_p+mc^2}{2mc^2}}\begin{pmatrix}\frac{cp_z}{E_p+mc^2}\\ \frac{cp_+}{E_p+mc^2}\\ 1\\ 0\end{pmatrix} e^{\frac{-i}{\hbar}(\vec{p}\cdot\vec{r}-E_pt)}$$

$\Phi \Rightarrow \begin{pmatrix}1\\0\end{pmatrix}$, $\quad \psi^4 = \sqrt{\frac{E_p+mc^2}{2mc^2}}\begin{pmatrix}\frac{cp_-}{E_p+mc^2}\\ \frac{-cp_z}{E_p+mc^2}\\ 0\\ 1\end{pmatrix} e^{\frac{-i}{\hbar}(\vec{p}\cdot\vec{r}-E_pt)}$

$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\bar{u} = u^{+}\gamma^{0}$

$$\psi^{\alpha} = u^{\alpha} e^{+\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - Et)} \qquad \psi^{\alpha} = v^{\alpha} e^{-\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - Et)}$$

$$\bar{u}^{\alpha} u^{\alpha'} = \delta_{\alpha\alpha'} \qquad \alpha = 1,2$$

$$\bar{v}^{\alpha} \bar{v}^{\alpha'} = -\delta_{\alpha\alpha'}$$

$$\bar{u}^{\alpha} v^{\alpha'} = 0$$

General solution

$$\psi(\vec{r}, t) = \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{\sqrt{2E_k}} \sum_{\alpha=1,2} \left\{ b_\alpha(k)\, u^{\alpha}(k)\, e^{-ik\cdot r} + d_\alpha^{+}(k)\, v^{\alpha}(k)\, e^{ik\cdot r} \right\}$$

$d^3\vec{k}$

not Lorentz invariant

such ~~normalization~~ $\cancel{\int \psi^{+}(r,t)\psi(r,t)\, d^3\vec{r}}$

$\cancel{\propto \int d^3\vec{k} \frac{1}{2E_k}}$

$$\int \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{2E_k} = \int \frac{d^4k}{(2\pi)^4} 2\pi\, \delta(k^2 - m^2) \Big|_{k^0 > 0}$$

$$\delta((k^0 - E_k)(k^0 + E_k))$$

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$$u^1 = \sqrt{\frac{E_p+mc^2}{2mc^2}} \begin{pmatrix} 1 \\ 0 \\ \frac{cP_z}{E_p+mc^2} \\ \frac{cP_+}{E_p+mc^2} \end{pmatrix} \qquad u^2 = \sqrt{\frac{E_p+mc^2}{2mc^2}} \begin{pmatrix} 0 \\ 1 \\ \frac{cP_-}{E_p+mc^2} \\ \frac{-cP_z}{E_p+mc^2} \end{pmatrix}$$

$$u^{2\dagger} u^1 = 0$$

$$u^{1\dagger} u^1 = \gamma \qquad u^{2\dagger} u^2 = \gamma$$

$$v^1 = \sqrt{\frac{E_p+mc^2}{2mc^2}} \begin{pmatrix} \frac{cP_z}{E_p+mc^2} \\ \frac{cP_+}{E_p+mc^2} \\ 1 \\ 0 \end{pmatrix} \qquad v^2 = \sqrt{\frac{E_p+mc^2}{2mc^2}} \begin{pmatrix} \frac{cP_-}{E_p+mc^2} \\ \frac{-cP_z}{E_p+mc^2} \\ 0 \\ 1 \end{pmatrix}$$

$$v^{1\dagger} v^1 = \gamma \qquad v^{2\dagger} v^2 = \gamma$$

$$v^{1\dagger} v^2 = 0$$

But $v^{1\dagger} u^1 \neq 0$ why?

Recall $(c\vec{\alpha}\cdot\vec{p} + \beta mc^2)\, u^1 = E_p u^1$

$(-c\vec{\alpha}\cdot\vec{p} + \beta mc^2)\, v^1 = -E_p v^1$

↑
extra "−"

$$\therefore v^{1\dagger} \underbrace{(-c\vec{\alpha}\cdot\vec{p} + \beta mc^2)^\dagger}_{= -c\vec{\alpha}\cdot\vec{p} + \beta mc^2} = -E_p v^{1\dagger}$$

∴ One can't apply the same trick to show $v^\dagger u^1 = 0$.

For this reason, one introduces

$$\bar{u} = u^{+} \gamma^{0}, \quad \bar{v} = v^{+} \gamma^{0}$$

$$\because \gamma^{0} \vec{\alpha} = -\vec{\alpha} \gamma^{0}, \quad \gamma^{0} \beta = \beta \gamma^{0}$$

$\therefore$ From $v^{+}(-c\vec{\alpha}\cdot\vec{p} + \beta mc^{2}) = -E_p v^{+}$

$\uparrow \times \gamma^{0}$ $\quad\quad \uparrow \gamma^{0}$

$$\Rightarrow v^{+}\gamma^{0}(c\vec{\alpha}\cdot\vec{p} + \beta mc^{2}) = -E_p v^{+} \gamma^{0}$$

$$\therefore \bar{v}(c\vec{\alpha}\cdot\vec{p} + \beta mc^{2}) = -E_p \bar{v}$$

$$\therefore \bar{v} u = 0 \, !$$

Since the orthogonality among $u^{\alpha}, u^{\alpha'}$ ($v^{\alpha}, v^{\alpha'}$) only involves either χ or Φ, it applies to $\bar{u}/u$ as well, i.e.,

$\bar{u}^{\alpha} u^{\alpha'} = \delta_{\alpha\alpha'}$ $\quad$ changes $u^{\alpha +} u^{\alpha} = \delta$

$\bar{v}^{\alpha} v^{\alpha'} = \delta_{\alpha\alpha'}$ $\quad$ to $\bar{u}^{\alpha} u^{\alpha} = 1$

$\bar{v}^{\alpha} u^{\alpha'} = 0$

$$\bar{u}' u' = \frac{E_p + mc^2}{2mc^2}\left(1 - \frac{c^2 p^2}{(E_p+mc^2)^2}\right) = \frac{E_p^2 + 2mc^2 E_p + (mc^2)^2 - c^2 p^2}{2mc^2(E_p+mc^2)}$$

$E_p^2 - c^2p^2 = m^2c^4$

$$= 1$$

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Electromagnetic interaction & non-relativistic limit

Classical $\quad H = \underbrace{\left[(\vec{P} - \frac{q\vec{A}}{c})^2 c^2 + m^2 c^4 \right]^{\frac{1}{2}}} + q\phi$

which suggests

$$i\hbar \frac{\partial \psi}{\partial t} = \overbrace{\left[c\vec{\alpha} \cdot (\underbrace{\vec{P} - \tfrac{q}{c}\vec{A}}_{\vec{\pi}}) + \beta mc^2 + q\phi \right]} \psi \quad , \quad q = -|e|$$

Let $\quad \psi = \begin{pmatrix} \chi \\ \Phi \end{pmatrix} e^{-\frac{i}{\hbar}Et} \qquad$ (positive E !)

$$\Rightarrow \begin{bmatrix} E - mc^2 - q\phi & -c\vec{\sigma}\cdot\vec{\pi} \\ -c\vec{\sigma}\cdot\vec{\pi} & E + mc^2 - q\phi \end{bmatrix} \begin{pmatrix} \chi \\ \Phi \end{pmatrix} = 0$$

$$\therefore \quad \Phi = \frac{c\vec{\sigma}\cdot\vec{\pi}}{E + mc^2 - q\phi} \chi$$

$$\chi = \frac{c\vec{\sigma}\cdot\vec{\pi}}{E - mc^2 - q\phi} \Phi$$

In the non-relativistic limit, $E = mc^2 + E_s$, $\; 0 < E_s << mc^2$.

$$\because \; O(\vec{\sigma}\cdot\vec{\pi}) \sim O(v) \cdot m$$

$$\therefore |\Phi| \sim \left| \frac{cmv}{2mc^2} \chi \right| = \frac{1}{2} \frac{v}{c} |\chi|$$

$$\therefore \; \underset{\substack{\uparrow \\ \text{small}}}{|\Phi|} << \underset{\substack{\uparrow \\ \text{large}}}{|\chi|} \quad \text{component.}$$

In general, in this limit, $\; \Phi \simeq \frac{\vec{\sigma}\cdot\vec{\pi}}{2mc} \chi$

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$$\underbrace{(E - mc^2 - q\phi)}_{E_s}\chi = c\vec{\sigma}\cdot\vec{\pi}\,\Phi \quad --- \ ①$$

$$\simeq \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m}\chi$$

$$\therefore E_s\chi = \left[\frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})^2 + q\phi\right]\chi$$

$$\Updownarrow$$

$$i\hbar\frac{\partial}{\partial t}\psi_s = \left[\frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})^2 + q\phi\right]\psi_s, \quad \psi_s = \chi e^{-\frac{i}{\hbar}E_s t}$$

Using $(\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b}) = a\cdot b + i\vec{\sigma}\cdot(\vec{a}\times\vec{b})$

$$\Rightarrow (\vec{\sigma}\cdot\vec{\pi})(\vec{\sigma}\cdot\vec{\pi}) = \pi^2 + i\vec{\sigma}\cdot\underbrace{(\vec{\pi}\times\vec{\pi})}_{\parallel}$$

$$-\frac{q}{c}(\vec{P}\times\vec{A}) = i\hbar\frac{q}{c}\nabla\times\vec{A} = \frac{q}{c}i\hbar\vec{B}$$

$$= \pi^2 - \frac{q\hbar}{c}\vec{B}\cdot\vec{\sigma}$$

$$\therefore i\hbar\frac{\partial}{\partial t}\psi_s = \left[\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 \underbrace{- \frac{q\hbar}{2mc}\vec{\sigma}\cdot\vec{B}}_{\parallel} + q\phi\right]\psi_s$$

$$-\underbrace{\frac{q}{mc}}_{\parallel}\vec{S}\cdot\vec{B}$$

$$\left(\frac{q}{2mc}\vec{S}\right)\cdot 2$$

$$\Uparrow$$

$$\underline{g_s = 2\,!}$$

$$\vec{\mu} = \frac{\overset{-e}{\overset{\parallel}{q}}}{mc}\vec{S} = -g_s\frac{\mu_b}{\hbar}\vec{S} \qquad , e>0 \qquad \mu_b = \frac{|e|\hbar}{2mc}$$

$g_s = 2$

$B=0$

To $O\left(\frac{v^4}{c^4}\right)$: $\quad \frac{-p^4}{8m^3c^2}$, $\quad \frac{e^2}{2m^2c^2r^3}\vec{S}\cdot\vec{L}$, $\quad \frac{e^2\hbar^2\pi}{2m^2c^2}\delta^3(\vec{r})$ (fine structure)

$\Uparrow$ Darwin term

($\cancel{v^2}$ $\frac{v^2}{c^2}$ actually)

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Date The above is correct to ~~$O(\frac{v^2}{c^2})$~~ $O(\frac{v^2}{c^2})+O(\frac{v^4}{c^4})$

To $O(\frac{v^4}{c^4})$:

$$\frac{1}{E+mc^2-q\phi} \overset{E=mc^2+E_s}{=} \frac{1}{2mc^2+E_s-q\phi} = \frac{1}{2mc^2}\left[1+\frac{E_s-q\phi}{2mc^2}\right]^{-1}$$

$$= \frac{1}{2mc^2}\left[1-\frac{E_s-q\phi}{2mc^2}\right]+\cdots = \frac{1}{2mc^2}-\frac{E_s-q\phi}{(2mc^2)^2}$$

$$\therefore \quad \Phi = \left[\frac{c\vec{\sigma}\cdot\vec{\pi}}{2mc^2} - \frac{E_s-q\phi}{(2mc^2)^2}c\vec{\sigma}\cdot\vec{\pi}\right]\chi$$

$$① \Rightarrow \quad E_s\chi = \left[\frac{\pi^2}{2m}+q\phi-\vec{\mu}\cdot\vec{B}-\frac{(\vec{\sigma}\cdot\vec{\pi})(E_s-q\phi)(\vec{\sigma}\cdot\vec{\pi})}{4m^2c^2}\right]\chi \cdots ②$$

$$[\underbrace{(E_s-q\phi)}_{=\frac{\pi^2}{2m}+\cdots},\ \vec{\sigma}\cdot\vec{\pi}] = \vec{\sigma}\cdot[-q\phi,\vec{\pi}]$$

$$= \vec{\sigma}\cdot[-q\phi,\vec{p}]$$

$$= \vec{\sigma}\cdot[\vec{p},q\phi]$$

$$\therefore \quad (E_s-q\phi)\vec{\sigma}\cdot\vec{\pi} = (\vec{\sigma}\cdot\vec{\pi})\frac{\pi^2}{2m}+\vec{\sigma}\cdot[\vec{p},q\phi]$$

$$② \Rightarrow \quad E_s\chi = \left\{\frac{\pi^2}{2m}+q\phi-\vec{\mu}\cdot\vec{B}-\underbrace{(\vec{\sigma}\cdot\vec{\pi})^2\frac{\pi^2}{8m^3c^2}}_{=\frac{\pi^4}{8m^3c^2}-\frac{q\hbar}{c}(\vec{B}\cdot\vec{\sigma})\frac{\pi^2}{8m^3c^3}}-\underbrace{\frac{(\vec{\sigma}\cdot\vec{\pi})\,\vec{\sigma}\cdot[\vec{p},q\phi]}{4m^2c^2}}_{(A)}\right\}\chi$$

$(\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b}) = i\vec{\sigma}\cdot(\vec{a}\times\vec{b})+\vec{a}\cdot\vec{b}$

$A=0 \quad \frac{p^4}{8m^3c^2} \Leftarrow$ relativistic correction to kinetic term : $\sqrt{p^2c^2+m^2c^4}-mc^2$

$$(A) = \frac{-i\vec{\sigma}\cdot\vec{\pi}\times[\vec{\pi},q\phi]}{4m^2c^2} - \frac{\vec{\pi}\cdot[\vec{\pi},q\phi]}{4m^2c^2} \qquad = \frac{p^2}{2m}-\frac{p^4}{8m^3c^2}+\cdots$$

$q\phi=\frac{-e^2}{r}$. $[\vec{\pi},q\phi]=\frac{\hbar}{i}\nabla(\frac{-e^2}{r})$, $A=0$. $-i\vec{\sigma}\cdot\vec{\pi}\times[\vec{\pi},q\phi] = \frac{-\hbar e^2\vec{\sigma}\cdot\vec{p}\times\vec{r}}{r^3}$

$$\Rightarrow \frac{\hbar e^2}{4m^2c^2r^3}\vec{\sigma}\cdot\vec{r}\times\vec{p} = \frac{e^2}{2m^2c^2r^3}\vec{S}\cdot\vec{L} \quad (\text{spin-orbital interaction})$$

$(\vec{p}\times\vec{r}=-\vec{r}\times\vec{p})$ $\Uparrow$ Thomas factor , the last term $\Rightarrow$ Darwin term

$-\frac{\vec{\pi}\cdot[\vec{\pi}, q\phi]}{4m^2c^2} = \frac{-1}{8m^2c^2}\left(\frac{\hbar}{i}\right)^2 \nabla^2 \frac{-e^2}{r}$

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Systematic expansion of the Dirac equation.

$$= \frac{-\hbar^2 e^2}{4m^2c^2}\nabla^2 \underbrace{\frac{1}{r}}_{-4\pi\delta(r)}$$

$$\int \psi^+ \psi \, d^3r = \text{constant}$$

$$= \int \left(|\chi|^2 + |\Phi|^2 \right) d^3\vec{r} \qquad \vec{A}, \phi = 0$$

$$\Phi = \frac{c\vec{\sigma}\cdot\vec{p}}{E+mc^2-V}\chi \cong \frac{\vec{\sigma}\cdot\vec{p}}{2mc}\chi$$

$$\therefore |\Phi|^2 = \chi^+ \frac{(\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\vec{p})}{4m^2c^2}\chi = \chi^+ \frac{p^2}{4m^2c^2}\chi$$

$$\therefore \int \chi^+ \left(1 + \frac{p^2}{4m^2c^2}\right) \chi \, d^3\vec{r} = \text{const.}$$

to $O(\frac{v^2}{c^2})$ $\left(\frac{p^2}{c^2} = O(\frac{v^2}{c^2})\right)$, we have

$$\int \left[\left(1 + \frac{p^2}{8m^2c^2}\right)\chi\right]^+ \left[\left(1 + \frac{p^2}{8m^2c^2}\right)\chi\right] = \text{Const.}$$

$\chi_s \equiv \left(1 + \frac{p^2}{8m^2c^2}\right)\chi$ to $O(\frac{v^2}{c^2})$ is the right wavefunction with constant total probability!

Suppose we find $E_s \chi = \hat{H}\chi$

$$\Rightarrow E_s \left[1 + \frac{p^2}{8m^2c^2}\right]^{-1} \chi_s = \hat{H} \left[1 + \frac{p^2}{8m^2c^2}\right]^{-1} \chi_s$$

$$\therefore E_s \chi_s = \left(1 + \frac{p^2}{8m^2c^2}\right) \hat{H} \left(1 - \frac{p^2}{8m^2c^2}\right) \chi_s$$

need only accurate To v^2

$$= \left(\hat{H} + \left[\frac{p^2}{8m^2c^2}, \hat{H}\right]\right) \chi_s$$

$\left[-\frac{p^6}{8m^3c^2}, \frac{p^2}{8m^2c^2}\right] = 0$. $\left[\vec{L}, \frac{p^2}{8m^2c^2}\right] = 0$ ∴ the second term

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does not change $\vec{S}\cdot\vec{L}$ term & Kinetic correction term.

The term $-\dfrac{\vec{\pi}\cdot[\vec{\pi}, q\phi]}{4m^2c^2}$ is changed:

$$\frac{1}{8m^2c^2}\left[\vec{p}\cdot[\vec{p}, q\phi] + [\vec{p}, q\phi]\cdot\vec{p}\right] \quad --- (*)$$

$$H_D = \left[\frac{p^2}{8m^2c^2}, q\phi\right] - \vec{p}\cdot\frac{[\vec{p}, q\phi]}{4m^2c^2}$$

$\uparrow \frac{v^2}{c^2}$ $\uparrow v^2$ $\uparrow v^4/c^2$ (no need to consider $\left[\frac{p^2}{8m^2c^2}, -\frac{\vec{p}\cdot[\vec{p}, q\phi]}{4m^2c^2}\right]$

$$= \frac{-1}{8m^2c^2}[\vec{p}\cdot[\vec{p}, V]] \qquad V = q\phi = \frac{-e^2}{r}$$

$$= \frac{\hbar^2}{8m^2c^2}\nabla^2 V = \frac{e^2\hbar^2\pi}{2m^2c^2}\delta^3(\vec{r}) \ : \ \text{Darwin term}$$

only affect s-wave state!

explanation: Come from smeared average around $\vec{r}$ over the Compton wavelength range $\frac{\hbar}{mc}$

$$\overline{V(r)} = V(r) + \sum_i \overline{\frac{\partial V}{\partial r_i}\delta r_i} + \frac{1}{2!}\overline{\sum_i\sum_j \frac{\partial^2 V}{\partial r_i \partial r_j}\cdot \delta r_i \delta r_j} + \ldots$$

$$= V(r) + \frac{1}{6}\underbrace{(\delta r)^2}_{\sim\left(\frac{\hbar}{mc}\right)^2}\nabla^2 V + O(\delta r^3)$$

$\overline{\delta x}^2 = \frac{1}{3}\delta r^2$

$\vec{p}\cdot[\vec{p}, q\phi]$ has two terms $\Rightarrow \left[\vec{p}\cdot[\vec{p}, q\phi]\right] + [\vec{p}, q\phi]\underline{\vec{p}(\psi)}$

acting on

Combined with the 2nd term in $(*)$ $\Rightarrow \dfrac{1}{4m^2c^2}[\vec{p}, q\phi]\vec{p}$ which gets

cancelled with $-\dfrac{\vec{\pi}\cdot[\vec{\pi}, q\phi]}{4mc^2} = -\dfrac{1}{4mc^2}(\vec{\pi}[\vec{\pi}, \phi q]] \doteq \dfrac{1}{4mc^2}[\vec{\pi}, \phi q]\vec{\pi}$

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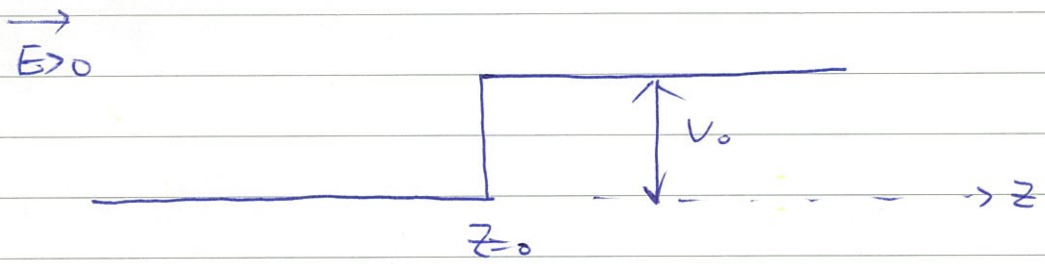
2012/5/7 revised

Klein paradox, negative energy & positrons

As we have seen, the Dirac equation is still plagued with negative energy solutions.

The problem associated with negative energy solutions shows up in the simplest problem — transimission across a step potential



For convenience, one chooses the step to be in the xy direction and considers that the electron incidents along z direction with a positive energy $E=E_p$

$$V(z)=0 \quad z<0, \qquad V(z)=V_0 \quad z>0$$

For $z\leq 0$, by using plane wave solutions, one has

$$\psi = A\begin{pmatrix} 1 \\ 0 \\ \frac{cp}{E_p+mc^2} \\ 0 \end{pmatrix} e^{\frac{i}{\hbar}(pz-E_p t)} + B\begin{pmatrix} 1 \\ 0 \\ \frac{-cp}{E_p+mc^2} \\ 0 \end{pmatrix} e^{-\frac{i}{\hbar}(pz+E_p t)}$$

where $E_p=\sqrt{c^2p^2+m^2c^4}>0$, A is the incident amplitude and B is the reflection amplitude.

According to the expression of the probability current, $\vec{J} = c\psi^{\dagger}\vec{\alpha}\psi$, we have

$$(J_z)_{inc} = c|A|^2 \left(1, 0, \frac{cp}{E_p+mc^2}, 0\right) \underbrace{\alpha_z}_{\begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}} \begin{pmatrix} 1 \\ 0 \\ \frac{cp}{E_p+mc^2} \\ 0 \end{pmatrix}$$

$$= c|A|^2 \left(1, 0, \frac{cp}{E_p+mc^2}, 0\right) \begin{pmatrix} \frac{cp}{E_p+mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$= \frac{2c^2p}{E_p+mc^2} |A|^2$$

Similarly, $(J_z)_{reflection} = c|B|^2$

$$\times \left(1, 0, \frac{-cp}{E_p+mc^2}, 0\right) \begin{pmatrix} \frac{-cp}{E_p+mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$= -\frac{2c^2p}{E_p+mc^2} |B|^2$$

For $z>0$ we have

$$\psi = D \begin{pmatrix} 1 \\ 0 \\ \frac{c\bar{p}}{E_p - V_0 + mc^2} \\ 0 \end{pmatrix} e^{\frac{i}{\hbar}(\bar{p}z - E_p t)}$$

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where $c^2\bar{p}^2 = (E_p - V_0)^2 - m^2c^4$

$$\therefore c\bar{p} = \pm\sqrt{(E_p - V_0)^2 - m^2c^4} \quad \text{---} \quad (K_0)$$

$$\therefore (J_z)_{\text{transmission}} = \frac{2c^2\bar{p}}{E_p - V_0 + mc^2}|D|^2$$

Continuity at $z=0$ (ψ is continuous across $z=0$)

$$A\begin{pmatrix}1\\0\\\frac{cp}{E_p+mc^2}\\0\end{pmatrix} + B\begin{pmatrix}1\\0\\\frac{-cp}{E_p+mc^2}\\0\end{pmatrix} = D\begin{pmatrix}1\\0\\\frac{c\bar{p}}{E_p-V_0+mc^2}\\0\end{pmatrix}$$

$$\therefore A+B = D$$

$$(A-B)\frac{cp}{E_p+mc^2} = D\frac{c\bar{p}}{E_p-V_0+mc^2}$$

$$\therefore 2A = \left[1 + \frac{\bar{p}}{p}\frac{E_p+mc^2}{E_p-V_0+mc^2}\right]D$$

$$2B = \left[1 - \frac{\bar{p}}{p}\frac{E_p+mc^2}{E_p-V_0+mc^2}\right]D$$

R = reflection coefficient $= \left|\frac{B}{A}\right|^2$

$$= \left|\frac{1-\frac{\bar{p}}{p}\frac{E_p+mc^2}{E_p-V_0+mc^2}}{1+\frac{\bar{p}}{p}\frac{E_p+mc^2}{E_p-V_0+mc^2}}\right|^2 \quad \text{----} \quad (K_1)$$

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There are several cases in which R behaves differently:

(i) $E_p - mc^2 \geq V_0$, i.e., Kinetic energy $(E_p - mc^2) \geq V_0$

$\therefore c^2\bar{p}^2 = (E_p - V_0)^2 - m^2c^4 \geq 0$ → + in Eq. (K0)

$\bar{p}$ is chosen ≥ 0, (J_c) transmission > 0

$$0 < \frac{\bar{p}}{p}\frac{E_p+mc^2}{E_p-V_0+mc^2} = \frac{\sqrt{(E_p-V_0+mc^2)(E_p-V_0-mc^2)}}{\sqrt{(E_p-mc^2)(E_p+mc^2)}}\cdot\frac{E_p+mc^2}{E_p-V_0+mc^2}$$

$$= \sqrt{\frac{E_p+mc^2}{E_p-mc^2}}\sqrt{\frac{E_p-V_0-mc^2}{E_p-V_0+mc^2}} < 1$$

$\Big(\because (E_p+mc^2)(E_p-V_0-mc^2) = (E_p^2-m^2c^4) - V_0(E_p+mc^2)$

$< (E_p^2-m^2c^4) - V_0(E_p-mc^2) = (E_p-mc^2)(E_p-V_0+mc^2) \Big)$

$\therefore R < 1$ & $R = 0$ when $E_p - mc^2 = V_0$

(ii) $E_p + mc^2 > V_0 > E_p - mc^2$, $\because (E_p - V_0)^2 < m^2c^4$

$\therefore \bar{p} =$ imaginary $\quad (c^2\bar{p}^2 = (E_p-V_0)^2 - m^2c^4 < 0)$

The numerator & denominator in eq. (K1)

are complex conjugated to each other

$\therefore R = 1$

Both (i) & (ii) have no surprises as it is consistent with the results obtained in the Schrödinger eq. as well.

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The surprise is the case (iii) $V_0 > E_p + mc^2$

In this case $E_p - V_0 < -mc^2$, $c^2\bar{p}^2 = (E_p - V_0)^2 - m^2c^4 > 0$

$\bar{p}$ is real again. However, since

$E_p - V_0 + mc^2 < 0$, (J_z) transimission $= \dfrac{2c^2\bar{p}}{E_p - V_0 + mc^2}|D|^2$

< 0 if $\bar{p}$ is positive!

Klein thought that J_z has to be positive.

Therefore, he requires

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

So that $\dfrac{2c^2\bar{p}}{E_p - V_0 + mc^2} = 2c\sqrt{\dfrac{V_0 - E_p + mc^2}{V_0 - E_p - mc^2}} > 0$

$\because$ $\dfrac{E_p + mc^2}{2c^2 p} = \dfrac{1}{2c}\sqrt{\dfrac{E_p + mc^2}{E_p - mc^2}}$

$$\therefore R = \left[\frac{1 - \sqrt{\dfrac{(V_0 - E_p + mc^2)(E_p + mc^2)}{(V_0 - E_p - mc^2)(E_p - mc^2)}}}{1 + \sqrt{\dfrac{(V_0 - E_p + mc^2)(E_p + mc^2)}{(V_0 - E_p - mc^2)(E_p - mc^2)}}}\right]^2$$

When $V_0 \to \infty$, one gets

$$R \to \left[\frac{1 - \sqrt{\dfrac{(E_p + mc^2)}{E_p - mc^2}}}{1 + \sqrt{\dfrac{E_p + mc^2}{E_p - mc^2}}}\right]^2 \quad \because E_p^2 - m^2c^4 = c^2p^2$$

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$$\sqrt{\frac{E_p+mc^2}{E_p-mc^2}} = \frac{\sqrt{E_p^2-m^2c^4}}{E_p-mc^2} = \frac{cp}{E_p-mc^2}$$

$$\therefore R \xrightarrow{V_0\to\infty} \left[\frac{1-\frac{cp}{E_p-mc^2}}{1+\frac{cp}{E_p-mc^2}}\right]^2 = \frac{1-\frac{2cp}{E_p-mc^2}+\frac{(cp)^2}{(E_p-mc^2)^2}}{1+\frac{2cp}{E_p-mc^2}+\frac{(cp)^2}{(E_p-mc^2)^2}}$$

$$\underset{\substack{\uparrow \\ c^2p^2=E_p^2-m^2c^4}}{=} \frac{1-\frac{2cp}{E_p-mc^2}+\frac{E_p+mc^2}{E_p-mc^2}}{1+\frac{2cp}{E_p-mc^2}+\frac{E_p+mc^2}{E_p-mc^2}} = \frac{E_p-cp}{E_p+cp}$$

$$T = 1-R = \frac{2cp}{E_p+cp} \neq 0$$

As an example, for $v/c = \sqrt{1/2}$

$$E_p = \sqrt{p^2c^2+m^2c^4} = \frac{mc^2}{\sqrt{1-v^2/c^2}} = \sqrt{2}mc^2$$

$$= 1.414\, mc^2$$

$$cp = \frac{mv}{\sqrt{1-\frac{v^2}{c^2}}}c = \sqrt{2}mcv = mc^2$$

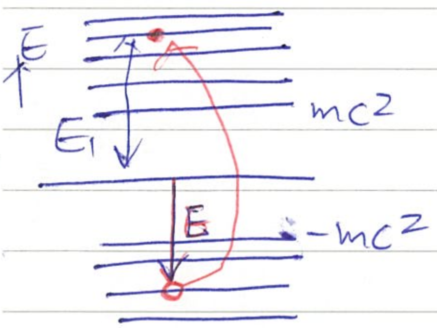
$$\therefore T = \frac{2mc^2}{(\sqrt{2}+1)mc^2} = \frac{2}{\sqrt{2}+1} = 2(\sqrt{2}-1) = 0.83$$

$\neq 0$ This clearly is in conflict with the intuition and is known as the "Klein paradox"

The Klein paradox bothered physicists in the earliest days of the Dirac theory.

∵ Dirac realized that this is tied up with the issue that the Dirac eq is still plagued with negative energy solutions.

<u>Negative energy</u> & <u>positrons</u>



He overcame this (paradox) by assuming all negative energy states are filled up.

Then, what happens when one negative energy electron is excited to positive energy?

Dirac argued that <u>the hole</u> that is left due to this transition has <u>positive charge</u>, since the whole world changes energy by $E_1 - E = E_1 + |E|$.
∴ Creating this transition, we need extra energy (extra to the energy of creating a positive energy electron E_1!) $|E|$ and extra charge $|e|$ for creating the hole.

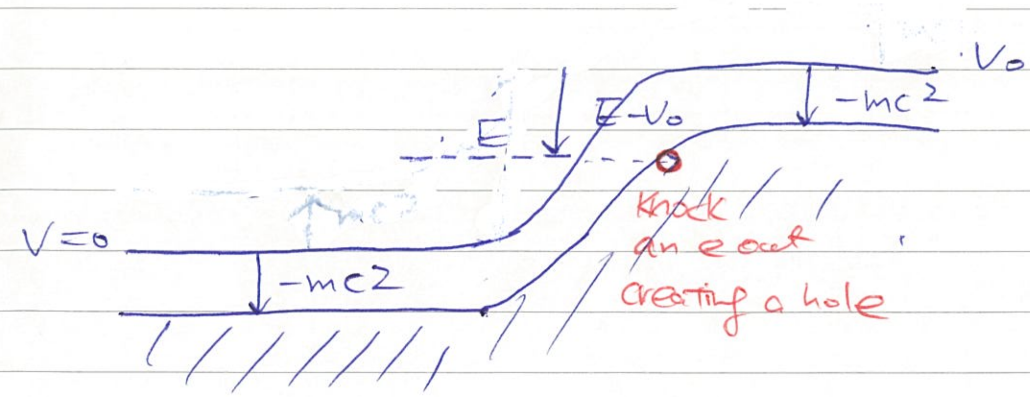
Dirac argued that this hole should be a particle, later confirmed by Anderson as "positron", which is the anti-particle of the electron in the sense that when they meet, the electron will transit back to the hole and is annihilated!

(emitting photons at the same time!)

<u>Modern analysis of the Klein paradox</u>

Using Dirac's hole theory, the Klein tunneling expt can be understood as follows:

one first fills all $E - V_0 < -mc^2$ by electrons



For $E_p - V_0 < -mc^2$, it is possible for the incident electron tunnels through the step and knocks out an electron in the filled electron sea, $E - V_0 < -mc^2$.

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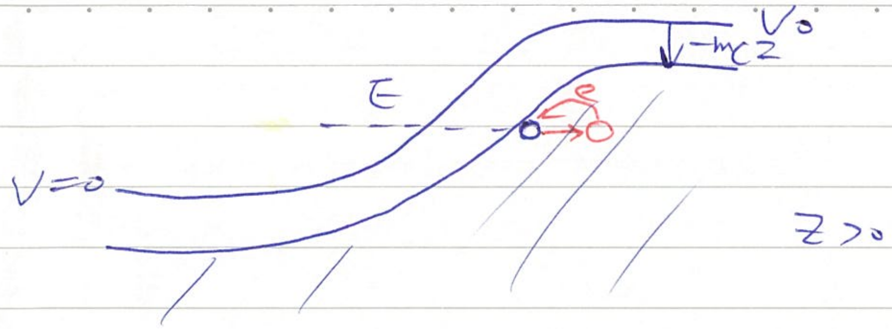

The hole can move toward $Z>0$; equivalent

e^- moves to the left $Z<0$!

$\therefore$ e^- moves from $Z>0$ towards $Z=0$

Hence, (J_z) transmission has to be <0 !

Therefore, unlike the choice made by Klein, one has

$$(J_z)_{\text{transmission}} = \frac{2c^2\bar{p}}{E_p - V_0 + mc^2}|D|^2 < 0$$

With $c\bar{p} = +\sqrt{(E_p-V_0)^2 - m^2c^4}$

$$\therefore (J_z)_{\text{transmission}} = -2c\sqrt{\frac{V_0-E_p+mc^2}{V_0-E_p-mc^2}}\,|D|^2 < 0$$

cf. (K1)

$$\Rightarrow R = \left[\frac{1+\sqrt{\dfrac{(V_0-E_p+mc^2)(E_p+mc^2)}{(V_0-E_p-mc^2)(E_p+mc^2)}}}{1-\sqrt{\dfrac{(V_0-E_p+mc^2)(E_p+mc^2)}{(V_0-E_p-mc^2)(E_p+mc^2)}}}\right]^2$$

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Now, in the limit $V_0 \to \infty$, one gets

$$R \to \left[\frac{1+\frac{cp}{(\varepsilon_p - mc^2)}}{1-\frac{cp}{\varepsilon_p - mc^2}}\right]^2 = \frac{\varepsilon + cp}{\varepsilon - cp} > 1$$

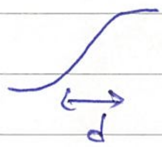
$R>1$ is due to the e^- being knocked out of the filled sea and joining the electron that is reflected to $z<0$!

For the example $\frac{v}{c} = \sqrt{\frac{1}{2}}$, we get

$$R = \frac{\sqrt{2}+1}{\sqrt{2}-1} = 5.8 > 1$$

$$T = 1 - R < 0$$

Note that for realistic potential steps, they must arise from $V=0$ to $V=V_0$ within certain lengthscale d



For the above picture of knocking e^- out to be valid, one requires $d \ll \frac{\hbar}{mc}$ (Compton length) in order that the step can be treated as a sharp step.

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For realistic steps, $d \ll \frac{\hbar}{m_e c}$ is usually hard to be achieved! In that case, the electron needs to tunnel through a barrier to knock out an electron in the filled sea. Since the wavefunction will decay when tunneling through the barrier, the reflection coefficient (R) is thus heavily reduced!

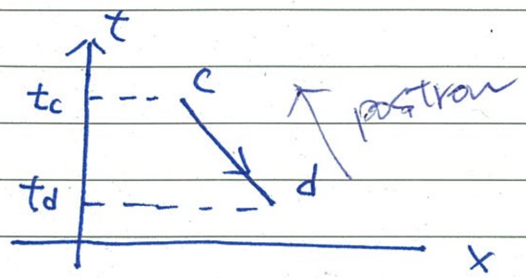
Even though the hole theory resolves the Klein paradox successfully and positrons were later observed in expts, it only works for Fermions and the search for a self-consistent quantum field theory had not been stopped. These progresses belong to the course of quantum field theory, we will just stop here. For more details about the Dirac eq., see Relativistic Q.M. by Bjorken & Drell

* For alternative interpretations of negative energy solutions, see Shankar's book for Feynman's interpretation!

Feynman's picture of positron

— positron = negative energy solution travel back in time $e^{-\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-Et)}$

<u>example:</u>



$\rightarrow e^{\frac{i}{\hbar}(-E)(-t)}$

(1) $t < t_d$, Nothing

(2) $t = t_d$, Negative energy $-|E|$ & charge $-|e|$ are destroyed

World energy goes up by $|E|$. Charge goes by $|e|$ relative to the past. A position is born.

(3) $t = t_c$, Negative Energy is created, charge $-|e|$ is created, this wipes out the position

(4) $t > t_c$ Nothing.

<u>Feynman propagator</u> $S_F(\vec{r}-\vec{r}')$ (1942 by Stückelberg indeptly by Feynman 1948)

$$\left(i\frac{\partial}{\partial t}-\hat{H}\right)G = i\delta(t-t')\,\delta^3(\vec{r}-\vec{r}') \quad \text{— ①}$$

One solution:

$$G(rt;r't') = \theta(t-t')\, U(rt,r't')$$

$$U(rt;r't') = \sum_n \psi_n(r)\psi_n^*(r')\, e^{\frac{-i}{\hbar}E_n(t-t')}$$

Here $\sum_n = \sum_{E_n>0} + \sum_{E_n<0}$

$\because$ $(i\partial_t - \hat{H})G = \sum_n \psi_n(r)\psi_n^*(r')\; i\delta(t-t')$

$$= i\delta(t-t')\,\delta^3(\vec{r}-\vec{r}')$$

$\uparrow$ only if $\sum_n = \sum_{n+} + \sum_{n-}$!

However, $\because$ $\sum_{n_-} \psi_n(r)\psi_n^*(r')\, e^{\frac{-i}{\hbar}E_n(t-t')} \equiv U_-$

satisfies $(i\partial_t - \hat{H})U_- = 0$

$\therefore$ We can form $S_F = G - U_-$ and S_F still satisfies ① ! Now

$$S_F = \theta(t-t')\left(\sum_{n+} + \sum_{n-}\right) - \left(\underbrace{\theta(t-t') + \theta(t'-t)}_{1}\right)\sum_{n-}$$

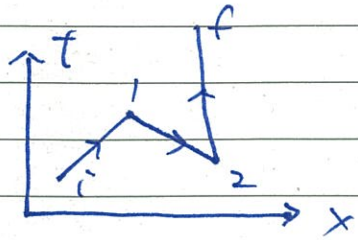
$$= \theta(t-t')\sum_{n+} - \theta(t'-t)\sum_{n-}$$

$\Downarrow$ propagate backward in time

Therefore $\psi_f(t) = S_F(t,t')\psi_i(t')$

$$+ \sum S_F(t,t'')V(t'')S_F(t'',t')\psi_i(t') + \cdots$$

Contains terms such as:



e^+e^- is created at 2

e^+ and original e^- annihilate at 1 !

Formally, the Feynman propagator can be obtained by choosing the Contours:

non-relativistic: $(i\partial_t - \hat{H})G = i\delta(\vec{r}-\vec{r}')\delta(t-t')$

$$\Rightarrow \quad G = \frac{i}{\underset{\overset{\shortparallel}{E}}{\omega} - \frac{p^2}{2m} + i\epsilon}$$

$$G \propto \frac{e^{ik|r-r'|}}{4\pi|r-r'|} \qquad E = \frac{k^2}{2m} \quad \text{if } \epsilon \to 0^+$$

Simple pole at $\frac{p^2}{2m} - i\epsilon$

Relativistic: $(i\partial_t - \underset{\uparrow \atop c\vec{\alpha}\cdot\vec{p} + \beta mc^2}{\hat{H}})G = i\delta(\vec{r}-\vec{r}')\delta(t-t')$

$$G = \frac{i}{\omega I - c\vec{\alpha}\cdot\vec{p} - \beta mc^2}$$

$$\sim \frac{\omega I + c\vec{\alpha}\cdot\vec{p} + \beta mc^2}{\omega^2 - \sqrt{c^2p^2 + (mc^2)^2}^{\,2}} = \frac{(\cdots)}{\omega^2 - E_k^2} \to \frac{(\cdots)}{\omega^2 - E_k^2 + i\epsilon}$$

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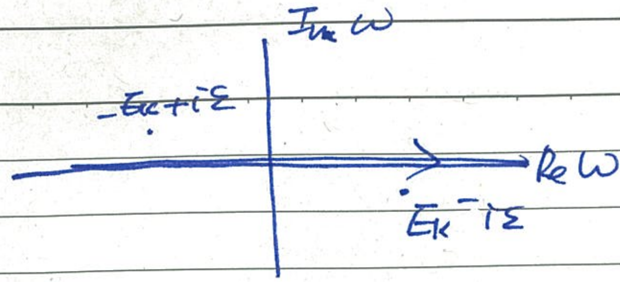
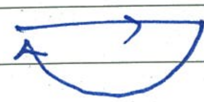


$\because\ e^{i\vec{p}\cdot\vec{r}-i\omega t}$

$\therefore\ t>0$  pick up positive energy

$t<0$  " negative energy

* The Dirac equation can be consider as the 1st quantized version of relativistic Q.M.

Unlike the Schrödinger eq. (which is also the 1st quantized version of non-relativistic Q.M.), here it must ~~go to~~ 2nd quantized form as we have seen that the propagator automatically generates e^+e^- pair, it seems that to deal with many particles feature is unavoidable!

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$\leftrightarrow \vec{A}$ (vector potential) $\vec{A}^{+} = \vec{A}$ FS

In the 2nd quantized form, one writes

$$\psi(\vec{r},t) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{2E_k}} \sum_{\alpha=1,2} \Big\{ b_\alpha(k)\, u^\alpha(k)\, e^{-ik\cdot r}$$

$$+ d_\alpha(k)\, v^\alpha(k)\, e^{ik\cdot r} \Big\}$$

if one tries to use d_α

One ends up with

$$H = \int \frac{d^3k}{(2\pi)^3} \sum_\alpha E_k\, b_\alpha^+ b_\alpha - E_k\, d_\alpha^+ d_\alpha$$

for both $[b_\alpha, b_\alpha^+] = 1$ and $\{b_\alpha, b_\alpha^+\} = 1$

Obviously, the Boson case will result in a Hamiltonian with arbitrary negative energy!

However, for Fermions (this is the reason why the Dirac eq. describe Spin 1/2 Fermions)

$$d_\alpha^+ d_\alpha = - d_\alpha d_\alpha^+ + 1$$

Note that Const $= -\sum_k E_k$ represents Dirac's filled negative solutions!

$$\therefore H = \text{Const} + \int \frac{d^3k}{(2\pi)^3} \sum_\alpha E_\alpha\, b_\alpha^+ b_\alpha + E_\alpha\, d_\alpha d_\alpha^+$$

The important character of $\{\,,\}$ is that

if one defines $d_\alpha = \tilde{d}_\alpha^{+} \Rightarrow d_\alpha^{+} = \tilde{d}_\alpha$

all anti-commutators are obeyed!

In this way, one can interpretate $\tilde{d}_\alpha^{+}$ as creating a positron!