8 Relativistic Quantum Mechanics

Generalization of q.m. to describe relativistic particles is non-trivial

→ difficulty is intrinsic (conceptual) problem: creation and destruction of particles is not accounted for in "standard" q.m.

We will consider a single particle.

Start with scalar or spinless particle: e.g., π
K-meson

→ Klein-Gordon equation

In contrast: spin-½ particles: e.g., electron
positron

→ Dirac equation

Recall: mesons composed of two quarks (quark and anti-quark) → integer spin

baryons composed of three quarks (q, q′, q″) → half-integer spin

both feel strong force

Meson - theory of nuclear force goes back to Yukawa (in 1935):

$$m_{\pi^0} = 135\ \mathrm{MeV}/c^2 \quad (\text{also } \pi^+ \text{ and } \pi^-)$$

→ for comparison:
electron mass $0.511\ \mathrm{MeV}/c^2$

Aside: Short-lived hydrogenic atoms such as $\pi^+ e^-$ can form.

Meson observed in 1950 as product of high-energy collision: high-energy collision

⇓

high velocity

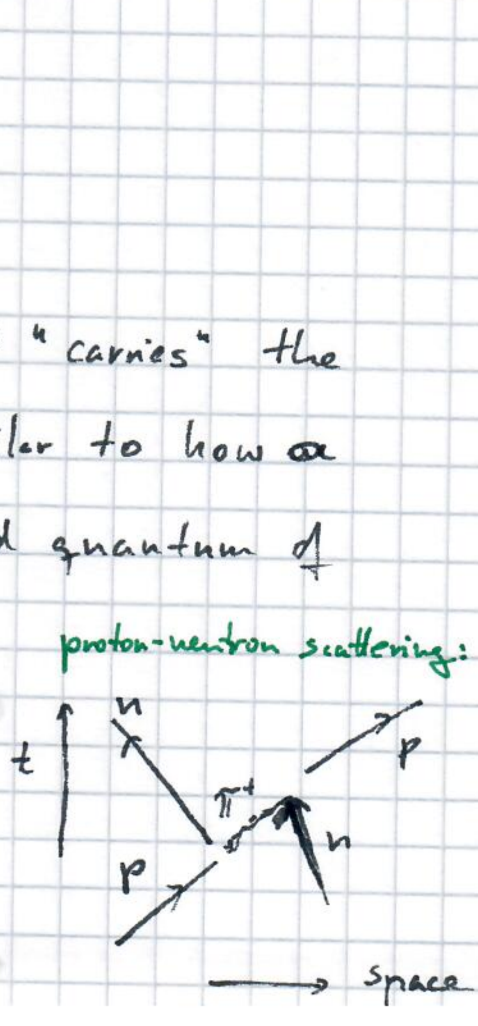
⇓

relativistic treatment

π - meson: field quantum that "carries" the "nuclear force" (similar to how a photon is the field quantum of the em force).

proton-neutron scattering:

proton emits a π^+ meson and becomes a neutron.
neutron absorbs the π^+ and becomes a proton.



Let's start off with a non-relativistic free particle:

Energy-momentum relation: $E = \frac{\vec{p}^{\,2}}{2m}$ (frame S)
(non-relativistic)
(free particle)

Quantum mechanically:

$E \rightarrow$ related to rate of change of the phase of the wave fct. in time

$\vec{p} \rightarrow$ related to rate of change of the phase of the wave fct. in space

$$\Psi(\vec{x},t) \propto e^{i(\vec{p}\cdot\vec{x} - Et/\hbar)}$$

$\hookrightarrow$ obeys time-dep. S.E.: $i\hbar \frac{\partial \Psi(\vec{x},t)}{\partial t} = \frac{1}{2m}\left(-i\hbar\vec{\nabla}\right)^2 \Psi(\vec{x},t)$

non-relativistic wave equation

Correspondence principle: $E \rightarrow i\hbar\frac{\partial}{\partial t}$

$\vec{p} \rightarrow -i\hbar\vec{\nabla}$

To treat interactions : $E \to E - e\,\Phi(\vec{x},t)$

$$\vec{p} \to \vec{p} - \frac{e}{c}\vec{A}(\vec{x},t)$$

accounts for coupling of a charged particle to an em field

(recall : e = charge of particle

Φ = scalar potential

$\vec{A}$ = vector potential)

Problem: S.E. changes its structure under transformation from one inertial frame to another :

⤳ time $\hat{=}$ first derivative

⟶ space $\hat{=}$ second derivative

(not compatible w/ covariance)

We want a relativistic wave equation that will give the correct relativistic energy-momentum relation

$$\boxed{E = \sqrt{\vec{p}^{\,2}c^2 + m^2c^4}}$$

special relativity

m: rest mass

Try "direct" application of correspondence principle:

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{x},t) = \underbrace{\sqrt{-\hbar^2 c^2 \vec{\nabla}^2 + m^2 c^4}}_{mc^2\sqrt{-\frac{\hbar^2}{m^2c^2}\vec{\nabla}^2 + 1}}\ \Psi(\vec{x},t)$$

$$\boxed{\frac{\hbar}{mc} = \lambda_c \quad \text{Compton wave length}}$$

what does the r.h.s. mean?

how to deal with operator under square root?

→ if we don't know how to deal with operator, we Taylor expand...

$$\sqrt{} \approx \underbrace{mc^2}_{\text{rest energy}} + \underbrace{\frac{\hat{\vec{p}}^2}{2m}}_{\text{"usual" kin. energy}} - \underbrace{\frac{1}{8m}\frac{\hat{\vec{p}}^4}{m^2c^2}}_{\text{relativistic correction}} + \dots$$

So: $$i\hbar\frac{\partial\Psi}{\partial t} = \underbrace{\left(mc^2 - \frac{\hbar^2\vec{\nabla}^2}{2m} - \frac{\hbar^4}{8m^3c^2}\vec{\nabla}^4 + \dots\right)}_{\text{infinitely high derivatives}}\Psi$$

→ non-local eq.

Space - time derivatives do not appear "symmetically"

Abandon this approach and find a local equation instead :

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

$$\Leftrightarrow \frac{E^2}{c^2} - \vec{p}^2 = m^2 c^4$$

$$\left(\frac{E}{c}, -p_x, -p_y, -p_z\right) \begin{pmatrix} E/c \\ p_x \\ p_y \\ p_z \end{pmatrix} = m^2 c^4$$

$$p^\mu p_\mu = m^2 c^4 \quad ; \quad p^\mu = \left(\frac{E}{c}, \vec{p}\right)$$

$$a^\mu a_\mu = (a^0)^2 - \vec{a}^2$$

contravariant four-vector $a^\mu = (a^0, \vec{a})$

covariant four-vector $a_\mu = (a^0, -\vec{a})$

$$a_\mu = \eta_{\mu\nu} a^\nu \quad \text{with} \quad \eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

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

(going to wave eq.) $\xrightarrow{}$ correspondence principle

$$\left(i\hbar \frac{\partial}{\partial t}\right)^2 \Psi(\vec{x},t) = \left[c^2(-i\hbar\vec{\nabla})^2 + m^2c^4\right]\Psi(\vec{x},t)$$

or $$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Psi(\vec{x},t) = \vec{\nabla}^2\Psi(\vec{x},t) - \frac{m^2c^2}{\hbar^2}\Psi(\vec{x},t)$$

$$\boxed{\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \vec{\nabla}^2 + \frac{1}{d_c^2}\right]\Psi(\vec{x},t)}$$

second derivative in space and time

(space and time are treated on equal footing)

Klein-Gordon equation for free particle

("Classical wave equation w/ extra d_c^{-2} term")

The equation is second order in time:

To know Ψ at $t+\Delta t$, we need to know Ψ and $\partial\Psi/\partial t$ at time t.

This can be thought of as an extra degree of freedom (corresponds to specifying the charge of a particle: there's a particle and there's an anti-particle).

→ $\boxed{\text{Klein-Gordon equation describes particle and anti-particle at the same time.}}$

Now: $x^\mu = (ct, \vec{x})$ $\hat{=}$ space-time position 4-vector

$$\frac{\partial}{\partial x^\mu} = \left(\frac{\partial}{\partial(ct)}, \vec{\nabla}\right) \quad \hat{=} \text{ four-gradient}$$

$$= \partial_\mu$$

↳ covariant vector operator despite the positive sign in front of the space-like part

A key point of Lorentz transformations is that inner products of four vectors are invariant. That is $a^\mu b_\mu$ will have the same value in any reference frame.

Recall: Lorentz transformation:

$$t' = \gamma\left(t - \frac{vx}{c^2}\right)$$

$$x' = \gamma(x - vt)$$

$$y' = y$$

$$z' = z$$

$$\gamma = \left(1 - \frac{v^2}{c^2}\right)^{-1/2}$$

Klein - Gordon equation:

$$\underbrace{\partial_\mu \partial^\mu}_{\partial^2} + m^2 c^2 \hbar^{-2}) \Psi(\vec{x}, t) = 0$$

the covariance of the equation can now be seen readily.

Since $\partial_\mu \partial^\mu$ takes the same form in any inertial frame, we have:

$$\underbrace{\Psi'(\vec{x}', t')}_{\substack{\text{wave fct. of} \\ \text{free spinless} \\ \text{particle in new} \\ \text{frame}}} = \underbrace{\Psi(\vec{x}, t)}_{\substack{\text{wave fct. of free} \\ \text{spinless particle} \\ \text{in old frame}}}$$

Let's try to find free-particle solution to KG equation:

Try $\boxed{\Psi(\vec{x}, t) = N e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}}$

N ↑ normalization constant

Plug into KG eq.: $\left[\frac{1}{c^2}\left(-\frac{iE}{\hbar}\right)^2 - \left(\frac{i\vec{p}}{\hbar}\right)^2 + \left(\frac{mc}{\hbar}\right)^2\right]\Psi(\vec{x}, t) = 0$

If $E^2 = c^2 \vec{p}^2 + m^2 c^4$, our ansatz works.

We find two energy eigenvalues:

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

$$\boxed{E = -\sqrt{c^2 p^2 + m^2 c^4} = -E_p}$$

The free-particle KG equation has positive and negative energy solutions!

$\rightsquigarrow$ this is a direct consequence of the $\partial^2/\partial t^2$ in the KG equation

For particle at rest ($\vec{p} = 0$): $E = \pm mc^2$

"+ solution": particle w/ restmass mc^2.

"− solution": particle w/ restmass $-mc^2$.

Let's increase $\vec{p}$: "+ solution": energy goes up.

"− solution": energy goes down.

↳ this seems strange...

To understand this, let's take the KG eq. and multiply from left with Ψ^*:

$$\Psi^* \underbrace{\left[\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \vec{\nabla}^2 + \left(\frac{mc}{\hbar}\right)^2 \right]}_{\text{"operator"}} \Psi = 0 \quad (*)$$

$\rightsquigarrow$ real

Since "operator" is real, Ψ^* solves KG equation provided Ψ does.

So:

$$\Psi \left[\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \vec{\nabla}^2 + \left(\frac{mc}{\hbar}\right)^2 \right] \Psi^* = 0 \quad (*')$$

Subtract $(*')$ from $(*)$:

$$\Psi^* (\ldots) \Psi - \Psi (\quad) \Psi^* = 0$$ $\rightsquigarrow$ $\frac{m^2c^2}{\hbar^2}$ terms vanish

Rewrite:

I'm multiplying by this

$$\frac{\partial}{\partial t} \Big[\underbrace{- \frac{\hbar}{2mi\, c^2} \left(\Psi^* \frac{\partial}{\partial t} \Psi - \Psi \frac{\partial}{\partial t} \Psi^* \right)}_{\substack{\rho(\vec{x},t) \\ \text{density} \\ (j^0(\vec{x},t))}} \Big] + \vec{\nabla} \cdot \Big[\underbrace{\frac{\hbar}{2mi} \left(\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^* \right)}_{\text{current } \vec{j}(\vec{x},t)} \Big] = 0$$

We have found the following continuity equation:

$$\boxed{\frac{\partial}{\partial t}\rho(\vec{x},t) + \vec{\nabla}\cdot\vec{j}(\vec{x},t) = 0}$$

We find: $\frac{\partial}{\partial t}\underbrace{\int \rho(\vec{x},t)\, d^3\vec{x}}_{\text{conserved quantity}} = 0$

So far, so good... Now take free-particle solution and calculate $\rho(\vec{x},t)$.

$$\Psi(\vec{x},t) = N e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}$$

$$\Rightarrow \rho(\vec{x},t) = -\frac{\hbar}{2mic^2}\left(\Psi^*\frac{\partial}{\partial t}\Psi - \Psi\frac{\partial}{\partial t}\Psi^*\right)$$

$$= \frac{E}{mc^2}$$

plug in positive and negative energy solutions $\rightarrow$ $= \pm\frac{E_p}{mc^2}$

$\rightsquigarrow$ ρ is negative if E is negative!

Specifically: for particle at rest w/ energy $-mc^2 \Rightarrow \rho = -1$ (negative)

"ρ is not the standard $\underbrace{}_{\text{probability}}$ density"

Let's add electromagnetic interactions:

$$E \rightarrow E - e\,\Phi(\vec{x},t)$$
$$\vec{p} \rightarrow \vec{p} - \frac{e}{c}\vec{A}(\vec{x},t)$$

again: correspondence principle

KG equation becomes:

$$\frac{1}{c^2}\left[i\hbar\frac{\partial}{\partial t} - e\,\Phi(\vec{x},t)\right]^2 \Psi(\vec{x},t) - \left[\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}(\vec{x},t)\right)^2 + m^2c^2\right]\Psi(\vec{x},t) = 0$$

Let Φ and $\vec{A}$ real and take complex conjugate:

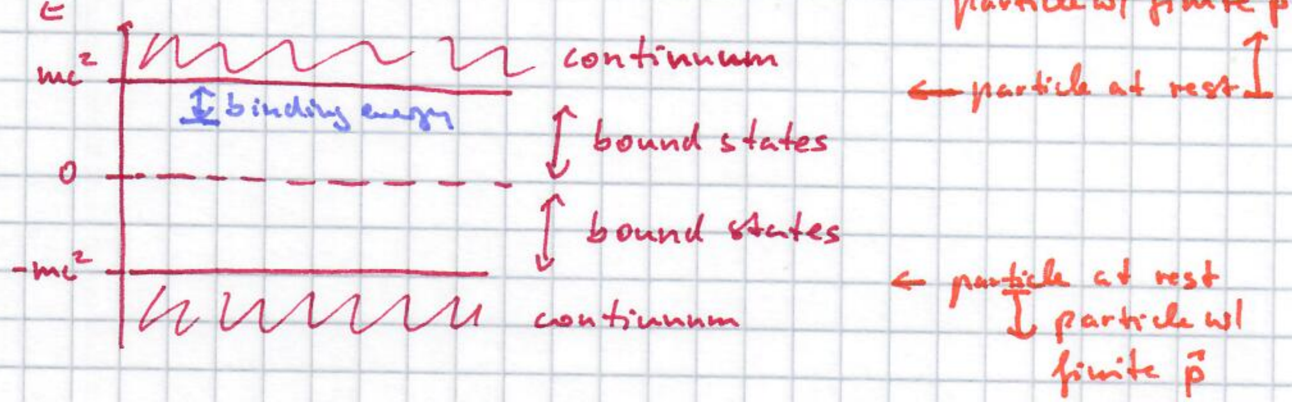
$$\frac{1}{c^2}\underbrace{\left[-i\hbar\frac{\partial}{\partial t} - e\,\Phi(\vec{x},t)\right]^2}_{\text{same as } \left[i\hbar\frac{\partial}{\partial t} + e\,\Phi(\vec{x},t)\right]^2} \Psi^*(\vec{x},t) - \left[\underbrace{\left(i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}(\vec{x},t)\right)^2}_{\text{same as } \left(-i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}(\vec{x},t)\right)^2} + m^2c^2\right]\Psi(\vec{x},t) = 0$$

$$\Rightarrow \frac{1}{c^2}\left[i\hbar\frac{\partial}{\partial t} + e\,\Phi(\vec{x},t)\right]^2 \Psi^*(\vec{x},t) - \left[\left(-i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}(\vec{x},t)\right)^2 + m^2c^2\right]\Psi(\vec{x},t) = 0$$

This is the Klein-Gordon equation but w/ opposite charge.

So: If $\Psi(\vec{x},t)$ is a solution to the KG eq. for a certain sign of charge, then $\Psi^*(\vec{x},t)$ is a solution to the KG eq. w/ the opposite sign of the charge and the same mass.

In this sense, the relativistic theory for a spin-0 particle predicts the existence of an oppositely charged particle w/ the same mass as the original particle.



$$\Psi(\vec{x}, t) = N e^{i(\vec{p}\cdot\vec{x} - E_p t)/\hbar}$$

⤳ positive energy solution (momentum $\vec{p}$)

$$\Psi(\vec{x}, t) = N e^{i(\vec{p}\cdot\vec{x} + E_p t)/\hbar}$$

⤳ negative energy solution (momentum $\vec{p}$)

Take complex conjugate of negative energy solution:

$$\Psi^*(\vec{x},t) = N e^{-i(\vec{p}\cdot\vec{x} + E_p t)/\hbar}$$

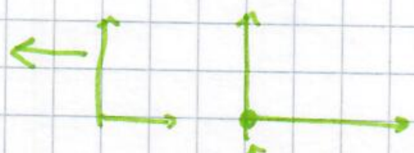
$$= N e^{i((-\vec{p})\cdot\vec{x} - E_p t)/\hbar}$$

this looks like a positive energy solution but with opposite momentum (opposite electric charge)

An aside:

Start w/ a free particle at rest (positive energy solution):

$$\Psi(\vec{x},t) = e^{-imc^2 t/\hbar} \quad ; \; mc^2 \text{ rest energy}$$



frame moving with velocity $-\vec{v}$ relative to particle at rest

particle at rest

→ in the moving frame, the particle appears to have a velocity $\vec{v}$, a momentum $\vec{p}$, and an energy E_p

$$\vec{p} = \gamma m \vec{v}$$

$$E_p = \gamma m c^2$$

$$\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$$

From $\vec{p} = \gamma m \vec{v}$: $\vec{v} = \frac{\vec{p}}{\gamma m} = \frac{\vec{p}c^2}{\gamma m c^2} = \frac{\vec{p}c^2}{E_p}$ (needed later)

Wave fct. in new frame: $\Psi'(\vec{x}',t') = \underbrace{e^{i(\vec{p}\cdot\vec{x}' - E_p t')/\hbar}}_{\begin{subarray}{l} = \Psi(\vec{x},t) \\ = e^{-imc^2 t/\hbar}\end{subarray}}$

It follows: $\rho(\vec{x}',t') = \frac{E_p}{mc^2} = \gamma$

a unit volume in the rest frame (recall $\rho = 1$ in rest frame) appears smaller by a factor of γ in the moving frame

$$\rho = -\frac{\hbar}{2mic^2}\left(\Psi^* \frac{\partial}{\partial t}\Psi - \Psi \frac{\partial}{\partial t}\Psi^*\right)$$

$$\vec{j}(\vec{x}',t') = \frac{\vec{p}}{m} = \frac{\vec{p}c^2}{mc^2}\,\frac{E_p}{E_p} = \frac{\vec{p}c^2}{E_p}\,\rho(\vec{x}',t')$$

$$\vec{j} = \frac{\hbar}{2mi}\left(\Psi^* \nabla \Psi - \Psi \nabla \Psi^*\right)$$

in rest frame: $\vec{j} = 0$

$$= \vec{v}\,\rho(\vec{x}',t')$$

current $\equiv$ relativistic velocity $\times$ density

Additional insight can be gained by rewriting KG equation in a more Schrödinger equation-like form.

For simplicity, work w/ free-particle KG eq. (Φ and $\vec{A}$ can be easily accounted for):

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \vec{\nabla}^2 + \left(\frac{mc}{\hbar}\right)^2\right]\Psi(\vec{x},t) = 0$$

Goal: Obtain first-order equation in time. → need two equations

Define:

$$\phi = \frac{1}{2}\left[\Psi(\vec{x},t) + \frac{i\hbar}{mc^2}\frac{\partial}{\partial t}\Psi(\vec{x},t)\right]$$

$$\chi = \frac{1}{2}\left[\Psi(\vec{x},t) - \frac{i\hbar}{mc^2}\frac{\partial}{\partial t}\Psi(\vec{x},t)\right]$$

see also homework

After some work:

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\phi\\ \chi\end{pmatrix} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\underbrace{\begin{pmatrix}1 & 1\\ -1 & -1\end{pmatrix}}\begin{pmatrix}\phi\\ \chi\end{pmatrix} + mc^2\underbrace{\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}_{\tau_3}\begin{pmatrix}\phi\\ \chi\end{pmatrix}$$

these are not spin component but charge components (the internal degree of freedom represented by these components is the charge of the particle)

$$\underbrace{\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}_{\tau_3} + i\underbrace{\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}}_{\tau_2}$$

any 2×2 matrix can be written in terms of Pauli matrices and identity matrix

"Hamiltonian": $-\frac{\hbar^2}{2m}\vec{\nabla}^2\begin{pmatrix}1 & 1\\ -1 & -1\end{pmatrix}+mc^2\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

Particles and anti-particles are coupled!

The probability density $\rho(\vec{x},t)$ can be shown to be given by

$$\rho(\vec{x},t) = (\phi^*, \chi^*)\ \tau_3 \begin{pmatrix}\phi\\ \chi\end{pmatrix}$$

$$= |\phi(\vec{x},t)|^2 - |\chi(\vec{x},t)|^2$$

ρ : probability charge density.

ϕ : wave fct. of "positive" particle.

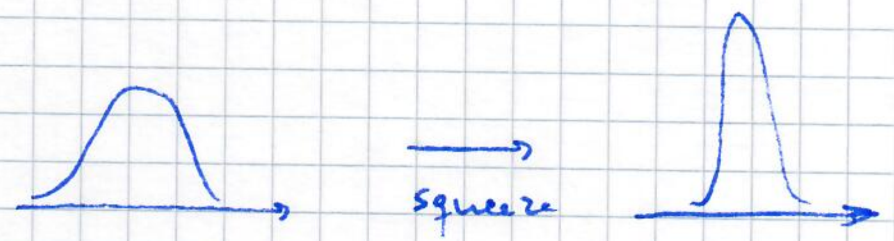
χ : wave fct. of "negative" particle.

$$\Upsilon(\vec{x},t) = \begin{pmatrix}\phi(\vec{x},t)\\ \chi(\vec{x},t)\end{pmatrix}$$

Another occasion where we see coupling of particles and anti-particles is the creation of a very localized wave packet.

If we attempt to create an extremely localized particle wave packet, it turns out that we will necessarily create anti-particles.

-> the theory with positive energy solutions alone is not capable of describing particles localized to within more than a Compton wave length $\lambda_c = \frac{\hbar}{mc}$.



wave packet of particles

wave packet of particles and anti-particles

We have been interpreting $\rho(\vec{x},t)$ as "charge" density.

This raises the question: what about neutral particles?

We will consider two examples:

(1) K^0, $\bar{K}^0$

$\uparrow$ particle $\downarrow$ strangeness 1

$\nwarrow$ anti-particle $\downarrow$ strangeness -1

since K^0 and $\bar{K}^0$ have different strangeness, they are distinguishable

aside: $K^0 \hat{=} d\bar{s}$

$\bar{K}^0 \hat{=} \bar{d} s$

(in contrast: $K^+ = u\bar{s}$

$K^- = \bar{u} s$)

u : charge $\frac{2}{3}$ $\quad$ c : $\frac{2}{3}$

d : charge $-\frac{1}{3}$ $\quad$ b : $-\frac{1}{3}$

s : charge $-\frac{1}{3}$ $\quad$ t : $\frac{2}{3}$

another aside:

strangeness conserved in strong and em interaction; not necessarily in weak interaction

So: We can define a "charge" (i.e., strangeness) that is one for particle and minus one for anti-particle.

$\hookrightarrow$ charge, strangeness, ... are just labels

(2) particle = anti-particle (i.e., particle is its own anti-particle)

→ this means that the particle and the anti-particle are <u>not</u> distinguishable

Example: π^0 meson

Recall: If Ψ satisfies the KG eq., then Ψ^* also satisfies the KG equation.

↓

usually KG eq. w/ opposite charge – but here we don't have an opposite charge

⇝ it follows: For a particle that is its own anti-particle, Ψ has to be real.

As a consequence, one finds that $\rho(\vec{x},t)$ is zero.

Example: Klein-Gordon equation for Coulomb potential $V(|\vec{x}|) = -\frac{Ze_0^2}{r}$ $\quad (|\vec{x}| = r)$

One finds the following positive energy solution:

$$E = \frac{mc^2}{\left[1 + (Z\alpha)^2 \left[n - \ell - \frac{1}{2} + \sqrt{(\ell+\frac{1}{2})^2 - (Z\alpha)^2}\right]^{-2}\right]^{\frac{1}{2}}}$$

$$\approx mc^2 \left[1 - \frac{(Z\alpha)^2}{2n^2} - \underbrace{\frac{1}{2n^4}\left(-\frac{3}{4} + \frac{n}{\ell+\frac{1}{2}}\right)(Z\alpha)^4 + \dots}_{} \right]$$

Taylor-expanding (assuming small $Z\alpha$)

rest energy $= mc^2$

fine structure term: removes degeneracy in n and ℓ (lowers the energy)

this term is what we would get by solving the SE: note: the interactions lower the energy ⇝ ~~binding~~ energy is smaller than mc^2

Finestructure constant $\alpha = \frac{e_0^2}{\hbar c} \approx \frac{1}{137}$

the larger Z, the larger the relativistic effects.

Handwaving Bohr model explanation: $v/c = \frac{Z\alpha}{n}$

Here, we have: $\Phi(\vec{x},t) = \Phi(\vec{x}) \rightsquigarrow e\Phi(\vec{x}) = -\frac{Ze_0^2}{r}$

$\vec{A} = 0$

Since we have a stationary potential, we can write

$$\Psi(\vec{x},t) = \psi(\vec{x})\, e^{-iEt/\hbar}$$ (let's assume $\vec{p} = 0$)

$$\Rightarrow \rho(\vec{x},t) = \frac{1}{2mc^2}\left[\Psi^*\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\Psi + \Psi\left(-i\hbar\frac{\partial}{\partial t} - e\Phi\right)\Psi^*\right]$$

there is a minus sign

$$= \frac{1}{mc^2}\left(E - e\Phi\right)|\psi(\vec{x})|^2$$

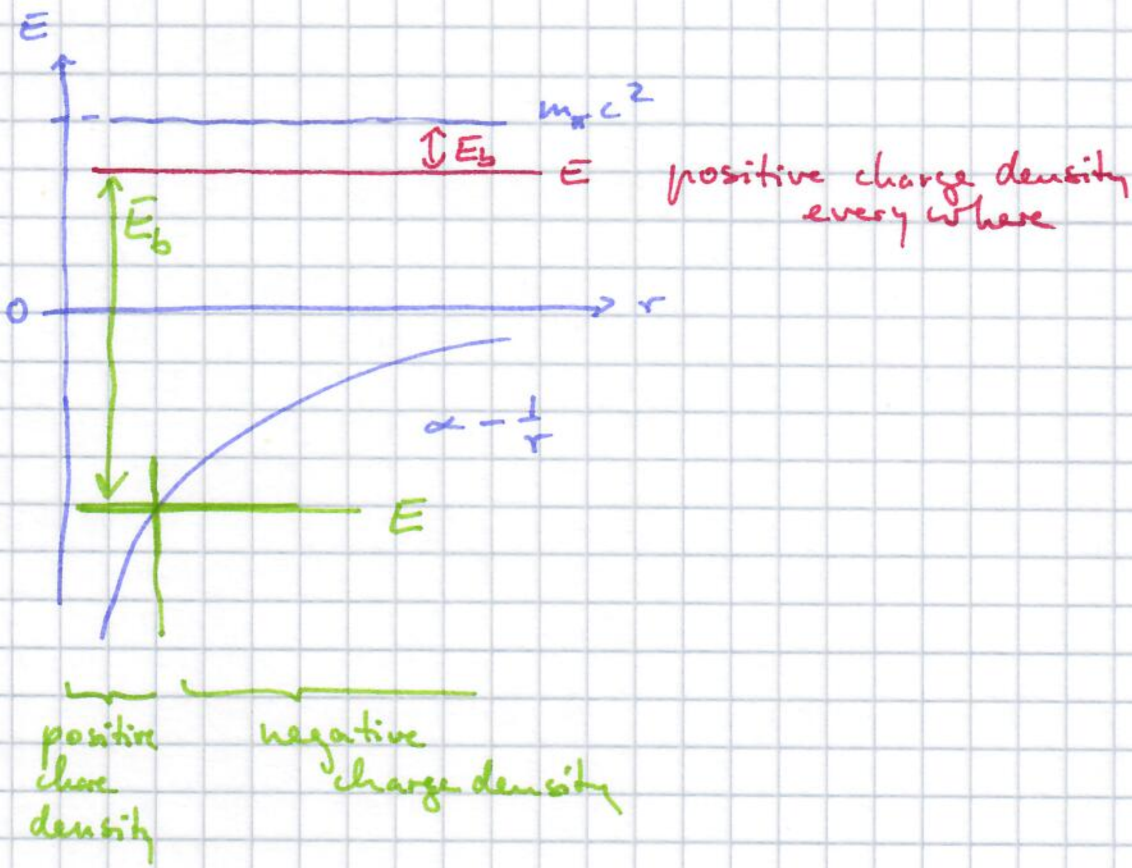
$$e\Phi = -\frac{Ze_0^2}{r}$$

$$E = m_\pi c^2 - E_b \quad \text{with } E_b \geq 0$$

$$= \frac{1}{mc^2}\left(m_\pi c^2 - E_b - \left(-\frac{Ze_0^2}{r}\right)\right)|\psi(\vec{x})|^2$$

So: $\rho(\vec{x})$ is positive if $m_\pi c^2 - E_b > -\frac{Ze_0^2}{r}$

$\rho(\vec{x})$ is negative if $m_\pi c^2 - E_b < -\frac{Ze_0^2}{r}$



For the $l=0$ solution: 1s state does not exist for $Z\alpha > \frac{1}{2}$

→ this implies that E never becomes negative

→ always have positive charge density

Let's make sense of $Z\alpha < \frac{1}{2}$ requirement.

$$Z\alpha < \frac{1}{2} \rightsquigarrow Z\frac{e_0^2}{\hbar c} < \frac{1}{2} \rightsquigarrow Z\frac{e_0^2}{\hbar/m_\pi c} < \frac{1}{2} m_\pi c^2$$

So: $Z\alpha < \frac{1}{2}$ corresponds to $\frac{Ze_0^2}{\lambda_c} < \frac{1}{2} m_\pi c^2$

if the Coulomb potential is deeper than $-\frac{1}{2} m_\pi c^2$ (which happens at $r = \lambda_c$), then the solution fails: this is telling us that the Coulomb potential is breaking down at this length scale.

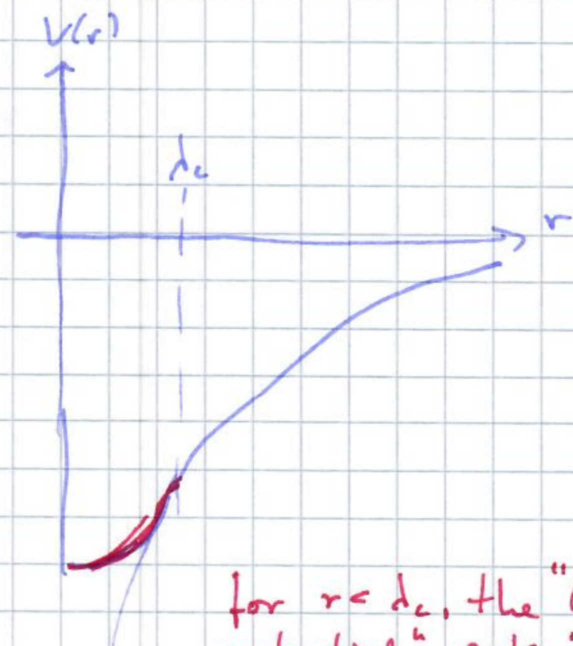
$\lambda_c \sim 1.4 \cdot 10^{-15}$ m

potential should be weaker than $\frac{1}{2} m_\pi c^2$

p-state has less amplitude near origin

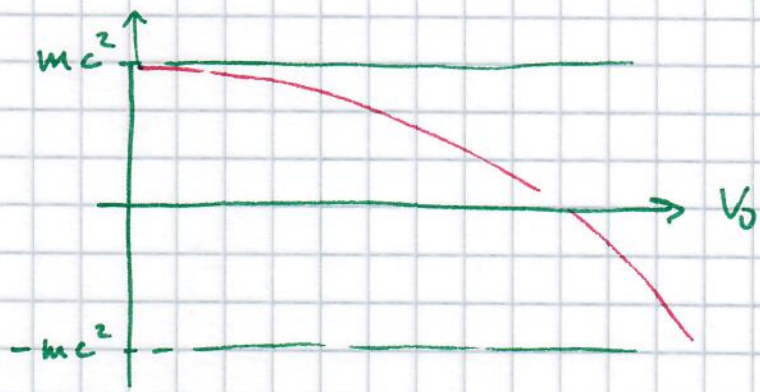
=> solution exists for larger $Z\alpha$

More realistic picture:



for $r < \lambda_c$, the "Coulomb potential" gets "rounded" due to the fact that the "nuclear force" needs to be accounted force.

Note: For a square well potential with depth V_0, the s-wave ($\ell = 0$) state can go to negative energy.



handwaving explanation: the potential is "wider" than the Coulomb potential and "naturally" rounded near $r = 0$.

An interlude:

4-vectors:

Some motivation:

$$\left.\begin{aligned} (ct)^2 - (x^2+y^2+z^2) &= 0 \\ (ct')^2 - (x'^2+y'^2+z'^2) &= 0 \end{aligned}\right\}$$ wave front equation in two different frames

$$\left.\begin{aligned} m &= \left(\frac{E}{c}\right)^2 - (p_x^2 + p_y^2 + p_z^2) \\ m &= \left(\frac{E'}{c}\right)^2 - (p_x'^2 + p_y'^2 + p_z'^2) \end{aligned}\right\}$$ energy-momentum relation in two different frames

We are seeing the invariance of a quantity that kind of looks like a "weird" scalar product.

One vector has $(a^0, \vec{a})$ components.

The other vector has $(a^0, -\vec{a})$ components.

Here $\vec{a}$ is a "normal" three-component vector.

We define contravariant four-vector $a^\mu = (a^0, \vec{a})$.

We define covariant four-vector $a_\mu = (a^0, -\vec{a})$.

$$a^\mu = (a^0, \vec{a}) = (a^0, a^1, a^2, a^3) \; ; \; a_\mu = (a^0, -a^1, -a^2, -a^3) = (a_0, a_1, a_2, a_3)$$

Let $\eta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$

$$a_\mu = \eta_{\mu\nu}\, a^\nu$$

↑
repeated
indices are
being summed over

$$a^\mu = \eta^{\mu\nu}\, a_\nu \qquad \eta^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

contravariant covariant

The four-momentum p^μ is defined as $\left(\frac{E}{c}, \vec{p}\right)$.

We want to show that $p^\mu = i\hbar \frac{\partial}{\partial x_\mu}$.

To show this, we use the "rules" $E \to i\hbar \frac{\partial}{\partial t}$ and $p_x \to -i\hbar \frac{\partial}{\partial x}$, etc.

Thus, $p^\mu = \left(i\hbar \frac{\partial}{\partial(tc)}, -i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y}, -i\hbar \frac{\partial}{\partial z} \right)$

$$= i\hbar \left(\frac{\partial}{\partial(tc)}, -\frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z} \right)$$

$$= i\hbar \left(\frac{\partial}{\partial(tc)}, \frac{\partial}{\partial(-x)}, \frac{\partial}{\partial(-y)}, \frac{\partial}{\partial(-z)} \right)$$

$$= i\hbar \frac{\partial}{\partial x_\mu}$$

Similarly, we want to show that $p_\mu = i\hbar \frac{\partial}{\partial x^\mu}$:

$$p_\mu = \left(i\hbar \frac{\partial}{\partial (tc)}, -\left(-i\hbar \frac{\partial}{\partial x}\right), -\left(-i\hbar \frac{\partial}{\partial y}\right), -\left(-i\hbar \frac{\partial}{\partial z}\right) \right)$$

$$= i\hbar \left(\frac{\partial}{\partial (tc)}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) = i\hbar \frac{\partial}{\partial x^\mu}$$

proceed as before

We also define:

$$\partial_\mu = \left(\frac{\partial}{\partial (ct)}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial y} \right)$$

$$= \frac{\partial}{\partial x^\mu}$$

see above

Similarly:

$$\partial^\mu = \left(\frac{\partial}{\partial (ct)}, \frac{\partial}{\partial (-x)}, \frac{\partial}{\partial (-y)}, \frac{\partial}{\partial (-z)} \right)$$

$$= \frac{\partial}{\partial x_\mu}$$

Then $\partial_\mu \partial^\mu = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \vec{\nabla}^2$

We can introduce another 4-vector (to deal with interactions):

$$\Phi, \vec{A} \quad : \quad \text{scalar, vector potential}$$

$$A^\mu = (\Phi, \vec{A})$$

$$A_\mu = (\Phi, -\vec{A})$$

Define: $D_\mu = \partial_\mu + \frac{ie}{c\hbar} A_\mu$

$$\vec{p} \rightarrow \underbrace{\underbrace{\vec{p} - \frac{e}{c}\vec{A}}_{i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}}}_{i\hbar\left(\vec{\nabla} + i\frac{e}{c\hbar}\vec{A}\right)}$$

also $E \longrightarrow \underbrace{E - e\Phi}_{E + i\hbar \frac{ie}{\hbar}\Phi}$

$$i\hbar\left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi\right)$$

$$i\hbar c\left(\frac{\partial}{\partial(ct)} + \frac{ie}{c\hbar}\Phi\right)$$

8.2 Dirac Equation

$\hookrightarrow$ relativistic spin-$\frac{1}{2}$ particle

Start w/ free particle!

Make a guess:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{x},t) = \Big(c\,\underbrace{\vec{\alpha} \cdot \hat{\vec{p}}}_{\alpha_x \hat{p}_x + \alpha_y \hat{p}_y + \alpha_z \hat{p}_z} + \beta mc^2 \Big) \Psi(\vec{x},t)$$

$\hat{\vec{p}} = -i\hbar\vec{\nabla}$

some as of yet unknown 3-component "vector"

some as of yet unknown "constant"

Recall: When we rewrote the KG eq. in terms of

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{x},t) = \hat{H}\, \Psi(\vec{x},t),$$

we found that Ψ has two components (we called them ϕ and χ) and that $\hat{H}$ is a 2×2 Hamiltonian.

Thus, we expect that we will get at least a 2×2 Hamiltonian (spin degree of freedom could enlarge this).

Require:

(i) Components of Ψ must satisfy KG equation so that plane waves fulfill the relativistic energy-momentum relation

$$E^2 = p^2c^2 + m^2c^4.$$

(ii) We want to get the continuity equation back, with

$$\frac{\partial}{\partial t} \int \rho(\vec{x},t)\, d^3\vec{x}$$

a conserved quantity.

(iii) We want a Lorentz covariant equation, i.e., we want it to have the same form in all inertial reference frames.

→ these are all reasonable requirements but they will not lead to a rigorous proof of the Dirac equation. Yet, they help us rationalize the result (= final Dirac equation).

Let's start with requirement (i):

We "postulated": $i\hbar \frac{\partial}{\partial t}\Psi(\vec{x},t) = \left(c\,\vec{\alpha}\cdot\hat{\vec{p}} + \beta mc^2\right)\Psi(\vec{x},t)$

To get KG equation, apply $\frac{\partial}{\partial t}$:

$$i\hbar \frac{\partial^2}{\partial t^2} \Psi(\vec{x},t) = (c\vec{\alpha}\cdot\vec{p} + \beta mc^2) \underbrace{\frac{\partial}{\partial t}\Psi(\vec{x},t)}_{\frac{1}{i\hbar}(c\vec{\alpha}\cdot\vec{p}+\beta mc^2)\Psi}$$

according to what we started with

$$\Rightarrow -\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Psi(\vec{x},t) - \left(-i\vec{\alpha}\cdot\vec{\nabla} + \frac{\beta mc}{\hbar}\right)\left(-i\vec{\alpha}\cdot\vec{\nabla} + \frac{\beta mc}{\hbar}\right)\Psi(\vec{x},t) = 0$$

Rearrange:

$$\frac{1}{c^2}\frac{\partial^2\Psi(\vec{x},t)}{\partial t^2} - (\vec{\alpha}\cdot\vec{\nabla})(\vec{\alpha}\cdot\vec{\nabla})\Psi(\vec{x},t) - i\vec{\alpha}\cdot\vec{\nabla}\frac{\beta mc}{\hbar}\Psi(\vec{x},t)$$

$$-i\beta\frac{mc}{\hbar}\vec{\alpha}\cdot\vec{\nabla}\Psi(\vec{x},t) + \left(\frac{mc}{\hbar}\right)^2 \beta\beta\,\Psi(\vec{x},t) = 0$$

$$\alpha_x\alpha_x = \alpha_y\alpha_y = \alpha_z\alpha_z = 1$$

$$\alpha_x\alpha_y + \alpha_y\alpha_x = 0$$
$$\alpha_y\alpha_z + \alpha_z\alpha_y = 0$$
$$\alpha_z\alpha_x + \alpha_x\alpha_z = 0$$

$$\alpha_x\beta + \beta\alpha_x = 0$$

$$\alpha_y\beta + \beta\alpha_y = 0$$

$$\alpha_z\beta + \beta\alpha_z = 0$$

$$\beta\beta = 1$$

Note: Anticipating that α_x, α_y, α_z, and β are not simply scalars but matrices, we were careful about the order $\rightsquigarrow$ e.g.: $\alpha_x\beta \neq \beta\alpha_x$

(we allowed for this inequality)

Let's look at what requirement (ii) gives us:

Write $\Psi(\vec{x}, t)$ as $\begin{pmatrix} \Psi_1(\vec{x}, t) \\ \Psi_2(\vec{x}, t) \\ \Psi_3(\vec{x}, t) \\ \vdots \\ \Psi_N(\vec{x}, t) \end{pmatrix}$

with adjoint Ψ^+.

To obtain continuity equation, multiply Dirac equation from left with Ψ^+.

Take complex conjugate of Dirac equation and substract.

After a bit of work:

$$\frac{\partial}{\partial t}(\Psi^+ \Psi) = -c\left[(\Psi^+ \vec{\alpha}) \cdot (\vec{\nabla} \Psi) + (\vec{\nabla} \Psi^+) \cdot \vec{\alpha}^* \Psi\right]$$

$$+ \frac{imc^2}{\hbar^2}(\Psi^+ \beta \Psi - \Psi^+ \beta^* \Psi)$$

For this to look like the continuity equation:

$$\frac{\partial}{\partial t} \rho(\vec{x}, t) + \vec{\nabla} \cdot \vec{j} = 0 ,$$

we need $\beta^* = \beta$

4x4 matrizes fulfill all the requirements:

$$\alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\alpha_y = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

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

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

Time-dependent Dirac equation for free particle:

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

4 components

Solution to free-particle Dirac equation:

Start with particle at rest.

$$i\hbar \frac{\partial \Psi(\vec{x},t)}{\partial t} = (\underbrace{\vec{\alpha}\cdot\hat{\vec{p}}}_{\substack{\text{does not}\\ \text{contribute}\\ \text{for particle}\\ \text{at rest}}} + \beta mc^2)\,\Psi(\vec{x},t)$$

⇝ all four spinors are decoupled

$$\left.\begin{aligned} * \quad \Psi_1(\vec{x},t) &= e^{-imc^2t/\hbar}\begin{pmatrix}1\\0\\0\\0\end{pmatrix} \\ * \quad \Psi_2(\vec{x},t) &= e^{-imc^2t/\hbar}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}\end{aligned}\right\}\ \text{positive energy solution}$$

$$\left.\begin{aligned} * \quad \Psi_3(\vec{x},t) &= e^{imc^2t/\hbar}\begin{pmatrix}0\\0\\1\\0\end{pmatrix} \\ * \quad \Psi_4(\vec{x},t) &= e^{imc^2t/\hbar}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\end{aligned}\right\}\ \text{negative energy solution}$$

Define
$$\Sigma_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

We find readily:
$$\left.\begin{aligned} \Sigma_z \Psi_1 &= +\Psi_1 &&\rightsquigarrow \text{spin-up} \\ \Sigma_z \Psi_2 &= -\Psi_2 &&\rightsquigarrow \text{spin-down} \\ \Sigma_z \Psi_3 &= +\Psi_3 &&\rightsquigarrow \text{spin-up} \\ \Sigma_z \Psi_4 &= -\Psi_4 &&\rightsquigarrow \text{spin-down} \end{aligned}\right\} \text{tentative assignment}$$

Next, let us consider a particle with momentum (not at rest).

Let us make an ansatz of the form:

$$\Psi(\vec{x},t) = e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar} \underbrace{u(\vec{p})}_{\substack{\text{four-component} \\ \text{spinor (independent} \\ \text{of } \vec{x} \text{ and } t)}}$$

positive energy solution

$$\Psi(\vec{x},t) = e^{-i(-E_p t - \vec{p}\cdot\vec{x})/\hbar} u(\vec{p})$$

negative energy solution

Note: $\hat{\vec{p}}\, u(\vec{p}) = -i\hbar\vec{\nabla} u(\vec{p}) = 0.$

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

Plug $\Psi = e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}\, u$ into the Dirac equation

no longer operator!

$$E_p\, e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}\, u(\vec{p}) = \left[c\,\vec{\alpha}\cdot\left(\cancel{\hbar}\frac{\vec{p}}{\cancel{\hbar}}\right) + \beta m c^2 \right]$$

$$\times\, e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}\, u(\vec{p})$$

So, we need $\vec{\alpha}\cdot\vec{p}$:

$$\vec{\alpha}\cdot\vec{p} = \underbrace{\begin{pmatrix} 0 & 0 & p_z & p_- \\ 0 & 0 & p_+ & -p_z \\ p_z & p_- & 0 & 0 \\ p_+ & -p_z & 0 & 0 \end{pmatrix}}_{\text{non-diagonal!}}$$

where
$$\left.\begin{aligned} p_+ &= p_x + i p_y \\ p_- &= p_x - i p_y \end{aligned}\right\}\ \text{definition}$$

So:
$$\begin{pmatrix} mc^2 & 0 & cp_z & cp_- \\ 0 & mc^2 & cp_+ & -cp_z \\ cp_z & cp_- & -mc^2 & 0 \\ cp_+ & -cp_z & 0 & -mc^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = E_p \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}$$

multiple non-zero entries!

We can "almost" read off:
$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = N \begin{pmatrix} 1 \\ 0 \\ cp_z/(E_p + mc^2) \\ cp_+/(E_p + mc^2) \end{pmatrix}$$

normalization constant

Check if our guess works:

Multiplying the l.h.s. out, we have

$$N \begin{pmatrix} mc^2 + \frac{c^2p^2}{E_p + mc^2} \\ 0 \\ cp_z - \frac{mc^3 p_z}{E_p + mc^2} \\ cp_+ - \frac{mc^3 p_+}{E_p + mc^2} \end{pmatrix}$$

$$= N \begin{pmatrix} E_p \\ 0 \\ \frac{E_p \; cp_z}{E_p + mc^2} \\ \frac{E_p \, cp_+}{E_p + mc^2} \end{pmatrix}$$

$$= E_p \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}$$ ⟶ great: the "guess" we made works (we found one free-particle solution)

The second positive energy solution is: $\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = N \begin{pmatrix} 0 \\ 1 \\ cp_- / (E_p + mc^2) \\ -cp_z / (E_p + mc^2) \end{pmatrix}$

Can be checked analogously to what we did above.

Negative energy solution:

$$\Psi(\vec{x}, t) = e^{-i(-E_p t - \vec{p}\cdot\vec{x})t/\hbar}\, u(\vec{p})$$

Plug into time-dependent Dirac equation:

$$-E_p\, u(\vec{p}) = \left[c\,\vec{\alpha}\cdot\vec{p} + \beta mc^2 \right] u(\vec{p})$$

Again, write out $\vec{\alpha}\cdot\vec{p}$ and write $u(\vec{p}) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}$

Try: $$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = N \begin{pmatrix} -cp_z/(E_p+mc^2) \\ -cp_+/(E_p+mc^2) \\ 1 \\ 0 \end{pmatrix}$$

and $$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = N \begin{pmatrix} -cp_-/(E_p+mc^2) \\ cp_z/(E_p+mc^2) \\ 0 \\ 1 \end{pmatrix}$$

In all cases: $N = \sqrt{\dfrac{E_p + mc^2}{2E_p}}$

obtained from $u_1 u_1^* + u_2 u_2^* + u_3 u_3^* + u_4 u_4^*$

$$= \frac{c^2 p_- p_+ + c^2 p_z^2}{(E_p+mc^2)^2} + 1 = (E_p+mc^2)^{-2}\left[c^2\vec{p}^{\,2} + (E_p+mc^2)^2\right] = \frac{2E_p}{E_p+mc^2}$$

In summary:

positive energy solution

$$\Psi_1(\vec{x},t) = N \begin{pmatrix} 1 \\ 0 \\ cp_z\,[E_p+mc^2]^{-1} \\ cp_+\,[E_p+mc^2]^{-1} \end{pmatrix} e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

$$\Psi_2(\vec{x},t) = N \begin{pmatrix} 0 \\ 1 \\ cp_-\,[E_p+mc^2]^{-1} \\ -cp_z\,[E_p+mc^2]^{-1} \end{pmatrix} e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

negative energy solution

$$\Psi_3(\vec{x},t) = N \begin{pmatrix} -cp_z\,[E_p+mc^2]^{-1} \\ -cp_+\,[E_p+mc^2]^{-1} \\ 1 \\ 0 \end{pmatrix} e^{-i(-E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

$$\Psi_4(\vec{x},t) = N \begin{pmatrix} -cp_-\,[E_p+mc^2]^{-1} \\ cp_z\,[E_p+mc^2]^{-1} \\ 0 \\ 1 \end{pmatrix} e^{-i(-E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

$$N = \sqrt{\frac{E_p+mc^2}{2E_p}}$$

Note: for $\vec{p} = 0$, we find $N = 1$; in addition, p_-, p_+, and $p_z = 0$ => we get the particle at rest solutions back.

We had found that the $\Psi_j(\vec{x},t)$ with $j=1,\ldots,4$ are eigenstates of Σ_z when $\vec{p}=0$.

The $\vec{p}\neq 0$ solutions are, in general, not eigenstates of Σ_z, i.e., the "boost" leads to a mixing of the different spin components.

However, if we take $p_+ = p_- = 0$ and finite p_z, then we have

$$\left.\begin{aligned} \Sigma_z \Psi_1 &= +\Psi_1 \\ \Sigma_z \Psi_2 &= -\Psi_2 \\ \Sigma_z \Psi_3 &= +\Psi_3 \\ \Sigma_z \Psi_4 &= -\Psi_4 \end{aligned}\right\} \begin{aligned} &p_z \text{ finite,} \\ &p_+ = p_- = 0 \end{aligned}$$

(just as we had for $\vec{p}=0$). Hence, we can still tentatively identify the Ψ_1 and Ψ_3 solutions as spin-up and the Ψ_2 and Ψ_4 solutions as spin-down.

Can we find another good label?

Let us look at the expectation value of $c\Sigma\cdot\hat{\vec{p}}$

$$c\,\Sigma\cdot\underset{\substack{\uparrow\\ \text{operator}}}{\hat{\vec{p}}}\;\Psi_j(\vec{x},t) = c\,\Sigma\cdot\underset{\substack{\uparrow\\ \text{scalar}}}{\vec{p}}\;\Psi_j(\vec{x},t)$$

$$c\,\Sigma\cdot\vec{p} = c\begin{pmatrix} p_z & p_- & 0 & 0 \\ p_+ & -p_z & 0 & 0 \\ 0 & 0 & p_z & p_- \\ 0 & 0 & p_+ & -p_z \end{pmatrix}$$

Calculate $c\,\Sigma\cdot\vec{p}\;\Psi_j$:

$$c\,\Sigma\cdot\vec{p}\;\Psi_j = c\begin{pmatrix} p_z u_1 + p_- u_2 \\ p_+ u_1 - p_z u_2 \\ p_z u_3 + p_- u_4 \\ p_+ u_3 - p_z u_4 \end{pmatrix} e^{-i(Et-\vec{p}\cdot\vec{x})/\hbar}$$

$$\Rightarrow \Psi_j^+\, c\,\Sigma\cdot\hat{\vec{p}}\;\Psi_j = c\Big[p_z|u_1|^2 + p_- u_1^* u_2 + p_+ u_2^* u_1 - p_z|u_2|^2 + p_z|u_3|^2 + p_- u_3^* u_4 + p_+ u_4^* u_3 - p_z|u_4|^2\Big]$$

for $j=1$:

$$= \Big[c\,p_z + 0 + 0 - 0 + \frac{c^3|p_z|^2 p_z}{(E_p+mc^2)^2} + \frac{p_- p_z^* p_+ c^3}{(E_p+mc^2)^2} + \underbrace{\frac{p_+ p_- p_z c^3}{(E_p+mc^2)^2}} - \underbrace{\frac{p_z p_+ p_- c^3}{(E_p+mc^2)^2}}\Big]|N|^2$$

let $p_x, p_y,$ p_z be real

$$= \left(c p_z + \underbrace{\frac{c p_z \; c^2 \bar{p}^2}{(E_p + mc^2)^2}}_{\frac{(E_p - mc^2)\, c p_z}{E_p + mc^2}} \right) |N|^2$$

$$= \left(c p_z \; \frac{E_p + mc^2 + E_p - mc^2}{E_p + mc^2} \right) |N|^2$$

$$= c p_z \; \underbrace{\frac{2 E_p}{E_p + mc^2} \; |N|^2}_{=1}$$

$$= c p_z$$

for $j = 2$:

$$= \Big[0 + 0 + 0 - c p_z + p_z p_+ p_- c^3 (E_p + mc^2)^{-2}$$

$$+ p_- p_+ p_z c^3 (E_p + mc^2)^{-2} - p_+ p_z p_- c^3 (E_p + mc^2)^{-2}$$

$$- c p_z \, p_z^2 (E_p + mc^2)^{-2} \Big] |N|^2$$

$$= - c p_z$$

for $j = 3$:

$$= \Big[p_z^3 c^3 (E_p + mc^2)^2 + p_- p_+ p_z c^3 (E_p + mc^2)^{-2}$$

$$+ p_+ p_- p_z c^3 (E_p + mc^2)^2 - p_z p_+ p_- c^3 (E_p + mc^2)^2$$

$$+ c p_z \Big] |N|^2 = + c p_z$$

for $j = 4$: $= \Big[p_z \underline{p_+ p_- c^3} (E_p + mc^2)^{-2} - p_- \underline{p_+ p_z c^3} (E_p + mc^2)^{-2}$

$- p_+ p_z p_- c^3 (E_p + mc^2)^{-2} - p_z^3 (E_p + mc^2)^{-2}$

$+ 0 + 0 + 0 - c p_z \Big] |N|^2$

$= - c p_z$

operator

helicity = R (right handed)

$$\Rightarrow \boxed{ \Psi_j^+ \frac{c\, \Sigma \cdot \hat{p}}{c p_z} \Psi_j = \begin{cases} +1 & \text{for } j = 1 \,\&\, 3 \\ -1 & \text{for } j = 2 \,\&\, 4 \end{cases} }$$

scalar

helicity = L (left-handed)

New, updated summary:

positive/negative energy solution

$$\Psi_j(\vec{x}, t) = N\, u^{(+/-)}_{\text{helicity}}(\vec{p})\, e^{-i(Et - \vec{p} \cdot \vec{x})/\hbar}$$

where $j = 1$: $u^{(+)}_R(\vec{p})$

$j = 2$: $u^{(+)}_L(\vec{p})$

$j = 3$: $u^{(-)}_R(\vec{p})$

$j = 4$: $u^{(-)}_L(\vec{p})$

$$N = \sqrt{\frac{E_p + mc^2}{2E_p}}$$

$j=1$: $$u_R^{(+)}(\vec{p}) = \begin{pmatrix} 1 \\ 0 \\ cp_z (E_p + mc^2)^{-1} \\ cp_+ (E_p + mc^2)^{-1} \end{pmatrix}$$

$j=2$: $$u_L^{(+)}(\vec{p}) = \begin{pmatrix} 0 \\ 1 \\ cp_- (E_p + mc^2)^{-1} \\ -cp_z (E_p + mc^2)^{-1} \end{pmatrix}$$

$j=3$: $$u_R^{(-)}(\vec{p}) = \begin{pmatrix} -cp_z (E_p + mc^2)^{-1} \\ -cp_+ (E_p + mc^2)^{-1} \\ 1 \\ 0 \end{pmatrix}$$

$j=4$: $$u_L^{(-)}(\vec{p}) = \begin{pmatrix} -cp_- (E_p + mc^2)^{-1} \\ cp_z (E_p + mc^2)^{-1} \\ 0 \\ 1 \end{pmatrix}$$

We can find $u^{(+/-)}_{\text{helicity}}(\vec{p})$ by acting with "generator" on $u^{(+/-)}_{\text{helicity}}(\vec{p}=0)$.

Specifically: $$\boxed{u^{(+/-)}_{\text{helicity}}(\vec{p}) = N\left(\underline{1} - \beta \frac{c\,\vec{\alpha}\cdot\vec{p}}{E_p + mc^2}\right) u^{(+/-)}_{\text{helicity}}(\vec{p}=0)}$$

here: $\underline{1} = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \end{pmatrix}$; $\beta = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & -1 & \\ 0 & & & -1 \end{pmatrix}$

So far, we have considered the free-particle Dirac equation:

$$i\hbar \frac{\partial \Psi(\vec{x},t)}{\partial t} = \left(c\vec{\alpha}\cdot\hat{\vec{p}} + \beta mc^2 \right) \Psi(\vec{x},t)$$

To introduce electromagnetic interactions, we resort (again) to the correspondence principle:

$$\vec{p} \rightarrow \vec{p} - \frac{e}{c}\vec{A}$$

$$E \rightarrow E - e\Phi$$

$$\Rightarrow \quad i\hbar \frac{\partial \Psi(\vec{x},t)}{\partial t} = \left[c\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}\right) + \left(e\Phi + \beta mc^2\right)\right] \Psi(\vec{x},t)$$

It is convenient to write $\Psi(\vec{x},t)$ as $\begin{pmatrix} u(\vec{x},t) \\ v(\vec{x},t) \end{pmatrix}$.

After some work (see also HW 11), one finds:

$$\boxed{i\hbar \frac{\partial}{\partial t} u(\vec{x},t) \approx \left[\frac{1}{2m}\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 - \frac{\hbar e}{2mc}\vec{\sigma}\cdot\vec{B} + e\Phi + mc^2 \right] u(\vec{x},t)}$$

The magnetic moment associated with the spin is predicted to be $\frac{e\hbar}{2mc}$

this is the so-called Pauli equation

obeyed by a charged particle with spin-$\frac{1}{2}$ in an em field.

$$\frac{e\hbar}{2mc}\vec{\sigma} = \frac{e}{mc}\vec{S}$$

$$= \frac{e\hbar}{2mc}\, 2\, \frac{\vec{S}}{\hbar}$$

Bohr magneton

$g = 2$ (Lande factor)

if vacuum fluctuations were included, the g factor would be slightly larger than 2

$$\vec{M}_{spin} = g\,\frac{e}{2mc}\,\vec{S}$$

Since e is negative for the electron, $\vec{M}_{spin}$ points in the opposite direction as $\vec{S}$

The spin of the electron has twice as large of a magnetic moment associated with it, per unit angular momentum, as the orbital angular momentum:

$$\vec{M}_{tot} = \frac{e}{2mc}\left(\vec{L} + 2\,\vec{S}\right)$$

Solution to free-particle Dirac equation:

Start with particle at rest.

$$i\hbar \frac{\partial \Psi(\vec{x},t)}{\partial t} = (\underbrace{\vec{\alpha}\cdot\hat{\vec{p}}}_{\text{does not contribute for particle at rest}} + \beta mc^2)\,\Psi(\vec{x},t)$$

⇝ all four spinors are decoupled

$$\left.\begin{array}{l} * \;\; \Psi_1(\vec{x},t) = e^{-imc^2t/\hbar}\begin{pmatrix}1\\0\\0\\0\end{pmatrix} \\[2em] * \;\; \Psi_2(\vec{x},t) = e^{-imc^2t/\hbar}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}\end{array}\right\}\text{positive energy solution}$$

$$\left.\begin{array}{l} * \;\; \Psi_3(\vec{x},t) = e^{imc^2t/\hbar}\begin{pmatrix}0\\0\\1\\0\end{pmatrix} \\[2em] * \;\; \Psi_4(\vec{x},t) = e^{imc^2t/\hbar}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\end{array}\right\}\text{negative energy solution}$$

Define
$$\Sigma_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

We find readily:
$$\left.\begin{array}{lll} \Sigma_z \Psi_1 = +\Psi_1 & \rightsquigarrow & \text{spin-up} \\ \Sigma_z \Psi_2 = -\Psi_2 & \rightsquigarrow & \text{spin-down} \\ \Sigma_z \Psi_3 = +\Psi_3 & \rightsquigarrow & \text{spin-up} \\ \Sigma_z \Psi_4 = -\Psi_4 & \rightsquigarrow & \text{spin-down} \end{array}\right\} \text{tentative assignment}$$

Next, let us consider a particle with momentum (not at rest).

Let us make an ansatz of the form:

$$\Psi(\vec{x}, t) = e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar} \underbrace{u(\vec{p})}_{}$$

positive energy solution

four-component spinor (independent of $\vec{x}$ and t)

$$\Psi(\vec{x}, t) = e^{-i(-E_p t - \vec{p}\cdot\vec{x})/\hbar} u(\vec{p})$$

negative energy solution

Note: $\hat{\vec{p}}\, u(\vec{p}) = -i\hbar\vec{\nabla} u(\vec{p}) = 0$.

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

Plug $\Psi = e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}\, u$ into the Dirac equation

no longer operator!

$$E_p\, e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}\, u(\vec{p}) = \left[c\,\vec{\alpha}\cdot\left(\cancel{\hbar}\hbar\frac{\vec{p}}{\hbar}\right) + \beta m c^2 \right]$$

$$\times\, e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}\, u(\vec{p})$$

So, we need $\vec{\alpha}\cdot\vec{p}$:

$$\vec{\alpha}\cdot\vec{p} = \underbrace{\begin{pmatrix} 0 & 0 & p_z & p_- \\ 0 & 0 & p_+ & -p_z \\ p_z & p_- & 0 & 0 \\ p_+ & -p_z & 0 & 0 \end{pmatrix}}_{\text{non-diagonal!}}$$

where
$$\left.\begin{aligned} p_+ &= p_x + i p_y \\ p_- &= p_x - i p_y \end{aligned}\right\} \text{definition}$$

So:
$$\begin{pmatrix} mc^2 & 0 & cp_z & cp_- \\ 0 & mc^2 & cp_+ & -cp_z \\ cp_z & cp_- & -mc^2 & 0 \\ cp_+ & -cp_z & 0 & -mc^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = E_p \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}$$

multiple non-zero entries!

We can "almost" read off:
$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = N \begin{pmatrix} 1 \\ 0 \\ cp_z/(E_p + mc^2) \\ cp_+/(E_p + mc^2) \end{pmatrix}$$

normalization constant

Check if our guess works:

Multiplying the l.h.s. out, we have

$$N \begin{pmatrix} mc^2 + \frac{c^2p^2}{E_p+mc^2} \\ 0 \\ cp_z - \frac{mc^3 p_z}{E_p+mc^2} \\ cp_+ - \frac{mc^3 p_+}{E_p+mc^2} \end{pmatrix}$$

$$= N \begin{pmatrix} E_p \\ 0 \\ \frac{E_p \, cp_z}{E_p+mc^2} \\ \frac{E_p \, cp_+}{E_p+mc^2} \end{pmatrix}$$

$$= E_p \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}$$ ⟶ great: the "guess" we made works (we found one free-particle solution)

The second positive energy solution is: $\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = N \begin{pmatrix} 0 \\ 1 \\ cp_-/(E_p+mc^2) \\ -cp_z/(E_p+mc^2) \end{pmatrix}$

Can be checked analogously to what we did above.

Negative energy solution:

$$\Psi(\vec{x}, t) = e^{-i(-E_p t - \vec{p}\cdot\vec{x})t/\hbar}\, u(\vec{p})$$

Plug into time-dependent Dirac equation:

$$-E_p\, u(\vec{p}) = \left[c\,\vec{\alpha}\cdot\vec{p} + \beta mc^2 \right] u(\vec{p})$$

Again, write out $\vec{\alpha}\cdot\vec{p}$ and write $u(\vec{p}) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}$

Try:
$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = N \begin{pmatrix} -cp_z/(E_p+mc^2) \\ -cp_+/(E_p+mc^2) \\ 1 \\ 0 \end{pmatrix}$$

and
$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = N \begin{pmatrix} -cp_-/(E_p+mc^2) \\ cp_z/(E_p+mc^2) \\ 0 \\ 1 \end{pmatrix}$$

In all cases: $N = \sqrt{\dfrac{E_p + mc^2}{2E_p}}$

obtained from $u_1 u_1^* + u_2 u_2^* + u_3 u_3^* + u_4 u_4^*$

$$= \frac{c^2 p_- p_+ + c^2 p_z^2}{(E_p + mc^2)^2} + 1 = (E_p + mc^2)^{-2}\left[c^2\vec{p}^{\,2} + (E_p + mc^2)^2\right] = \frac{2E_p}{E_p + mc^2}$$

In summary:

positive energy solution

$$\Psi_1(\vec{x},t) = N \begin{pmatrix} 1 \\ 0 \\ cp_z\,[E_p+mc^2]^{-1} \\ cp_+\,[E_p+mc^2]^{-1} \end{pmatrix} e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

$$\Psi_2(\vec{x},t) = N \begin{pmatrix} 0 \\ 1 \\ cp_-\,[E_p+mc^2]^{-1} \\ -cp_z\,[E_p+mc^2]^{-1} \end{pmatrix} e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

negative energy solution

$$\Psi_3(\vec{x},t) = N \begin{pmatrix} -cp_z\,[E_p+mc^2]^{-1} \\ -cp_+\,[E_p+mc^2]^{-1} \\ 1 \\ 0 \end{pmatrix} e^{-i(-E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

$$\Psi_4(\vec{x},t) = N \begin{pmatrix} -cp_-\,[E_p+mc^2]^{-1} \\ cp_z\,[E_p+mc^2]^{-1} \\ 0 \\ 1 \end{pmatrix} e^{-i(-E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

$$N = \sqrt{\frac{E_p + mc^2}{2E_p}}$$

Note: for $\vec{p} = 0$, we find $N = 1$; in addition, p_-, p_+, and $p_z = 0$ => we get the particle at rest solutions back.

We had found that the $\Psi_j(\vec{x},t)$ with $j=1,\dots,4$ are eigenstates of Σ_z when $\vec{p}=0$.

The $\vec{p}\neq 0$ solutions are, in general, not eigenstates of Σ_z, i.e., the "boost" leads to a mixing of the different spin components.

However, if we take $p_+ = p_- = 0$ and finite p_z, then we have

$$\left.\begin{aligned}\Sigma_z\,\Psi_1 &= +\Psi_1\\ \Sigma_z\,\Psi_2 &= -\Psi_2\\ \Sigma_z\,\Psi_3 &= +\Psi_3\\ \Sigma_z\,\Psi_4 &= -\Psi_4\end{aligned}\right\}\quad \begin{array}{l}p_z \text{ finite,}\\ p_+ = p_- = 0\end{array}$$

(just as we had for $\vec{p}=0$). Hence, we can still tentatively identify the Ψ_1 and Ψ_3 solutions as spin-up and the Ψ_2 and Ψ_4 solutions as spin-down.

Can we find another good label?

Let us look at the expectation value of $c\Sigma\cdot\hat{\vec{p}}$

$$c\,\Sigma\cdot\underset{\substack{\uparrow\\ \text{operator}}}{\hat{\vec{p}}}\;\Psi_j(\vec{x},t) = c\,\Sigma\cdot\underset{\substack{\uparrow\\ \text{scalar}}}{\vec{p}}\;\Psi_j(\vec{x},t)$$

$$c\,\Sigma\cdot\vec{p} = c\begin{pmatrix} p_z & p_- & 0 & 0 \\ p_+ & -p_z & 0 & 0 \\ 0 & 0 & p_z & p_- \\ 0 & 0 & p_+ & -p_z \end{pmatrix}$$

Calulate $c\,\Sigma\cdot\vec{p}\;\Psi_j$:

$$c\,\Sigma\cdot\vec{p}\;\Psi_j = c\begin{pmatrix} p_z u_1 + p_- u_2 \\ p_+ u_1 - p_z u_2 \\ p_z u_3 + p_- u_4 \\ p_+ u_3 - p_z u_4 \end{pmatrix} e^{-i(Et-\vec{p}\cdot\vec{x})/\hbar}$$

$$\Rightarrow \Psi_j^\dagger\, c\,\Sigma\cdot\hat{\vec{p}}\;\Psi_j = c\Big[\, p_z|u_1|^2 + p_- u_1^* u_2 +$$
$$p_+ u_2^* u_1 - p_z|u_2|^2 +$$
$$p_z|u_3|^2 + p_- u_3^* u_4 +$$
$$p_+ u_4^* u_3 - p_z|u_4|^2 \,\Big]$$

for $j=1$:
$$= \Big[\, c\,p_z + 0 + 0 - 0 + \frac{c^3|p_z|^2 p_z}{(E_p+mc^2)^2} + \frac{p_- p_z^* p_+ c^3}{(E_p+mc^2)^2}$$
$$+ \underbrace{\frac{p_+ p_- p_z c^3}{(E_p+mc^2)^2}}_{} - \underbrace{\frac{p_z p_+ p_- c^3}{(E_p+mc^2)^2}}_{}\,\Big]|N|^2$$

let $p_x, p_y,$ p_z be real

$$= \left(c p_z + \underbrace{\frac{c p_z \; c^2 \vec{p}^{\,2}}{(E_p + mc^2)^2}}_{\frac{(E_p - mc^2)\, c p_z}{E_p + mc^2}} \right) |N|^2$$

$$= \left(c p_z \; \frac{E_p + mc^2 + E_p - mc^2}{E_p + mc^2} \right) |N|^2$$

$$= c p_z \; \underbrace{\frac{2 E_p}{E_p + mc^2} \; |N|^2}_{=1}$$

$$= \; c p_z$$

for $j = 2$: $$= \Big[0 + 0 + 0 - c p_z + \underline{p_z p_+ p_- c^3 (E_p + mc^2)^{-2}}$$

$$+ p_- p_+ p_z c^3 (E_p + mc^2)^{-2} - p_+ \underline{p_z p_- c^3 (E_p + mc^2)^{-2}}$$

$$- c p_z \; p_z^2 \, (E_p + mc^2)^{-2} \Big] \, |N|^2$$

$$= - c p_z$$

for $j = 3$: $$= \Big[p_z^3 c^3 (E_p + mc^2)^2 + p_- p_+ p_z c^3 (E_p + mc^2)^{-2}$$

$$+ p_+ p_- \underline{p_z c^3 (E_p + mc^2)^2} - p_z \underline{p_+ p_- c^3 (E_p + mc^2)^{-2}}$$

$$+ c p_z \Big] \, |N|^2 = + c p_z$$

for $j = 4$:

$$= \Big[p_z \underline{p_+ p_- c^3} (E_p + mc^2)^{-2} - p_- \underline{p_+ p_z} c^3 (E_p + mc^2)^{-2}$$

$$- p_+ p_z p_- c^3 (E_p + mc^2)^{-2} - p_z^3 (E_p + mc^2)^{-2}$$

$$+ 0 + 0 + 0 - c p_z \Big] |N|^2$$

$$= - c p_z$$

operator

helicity = R (right handed)

$$\Rightarrow \boxed{\Psi_j^\dagger \frac{c\, \Sigma \cdot \hat{p}}{c p_z} \Psi_j = \begin{cases} +1 & \text{for } j = 1 \,\&\, 3 \\ -1 & \text{for } j = 2 \,\&\, 4 \end{cases}}$$

scalar

helicity = L (left-handed)

New, updated summary:

positive/negative energy solution

$$\Psi_j(\vec{x}, t) = N \, u^{(+/-)}_{\text{helicity}}(\vec{p}) \, e^{-i(Et - \vec{p}\cdot\vec{x})/\hbar}$$

where

$j = 1$: $u_R^{(+)}(\vec{p})$

$j = 2$: $u_L^{(+)}(\vec{p})$

$j = 3$: $u_R^{(-)}(\vec{p})$

$j = 4$: $u_L^{(-)}(\vec{p})$

$$N = \sqrt{\frac{E_p + mc^2}{2E_p}}$$

$j=1$: $$u_R^{(+)}(\vec{p}) = \begin{pmatrix} 1 \\ 0 \\ cp_z(E_p+mc^2)^{-1} \\ cp_+(E_p+mc^2)^{-1} \end{pmatrix}$$

$j=2$: $$u_L^{(+)}(\vec{p}) = \begin{pmatrix} 0 \\ 1 \\ cp_-(E_p+mc^2)^{-1} \\ -cp_z(E_p+mc^2)^{-1} \end{pmatrix}$$

$j=3$: $$u_R^{(-)}(\vec{p}) = \begin{pmatrix} -cp_z(E_p+mc^2)^{-1} \\ -cp_+(E_p+mc^2)^{-1} \\ 1 \\ 0 \end{pmatrix}$$

$j=4$: $$u_L^{(-)}(\vec{p}) = \begin{pmatrix} -cp_-(E_p+mc^2)^{-1} \\ cp_z(E_p+mc^2)^{-1} \\ 0 \\ 1 \end{pmatrix}$$

We can find $u_{\text{helicity}}^{(+/-)}(\vec{p})$ by acting with "generator" on $u_{\text{helicity}}^{(+/-)}(\vec{p}=0)$.

Specifically: $$\boxed{u_{\text{helicity}}^{(+/-)}(\vec{p}) = N\left(\underline{1} - \beta\,\frac{c\,\vec{\alpha}\cdot\vec{p}}{E_p+mc^2}\right) u_{\text{helicity}}^{(+/-)}(\vec{p}=0)}$$

here: $\underline{1} = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \end{pmatrix}$; $\beta = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & -1 & \\ 0 & & & -1 \end{pmatrix}$

So far, we have considered the free-particle Dirac equation:

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

To introduce electromagnetic interactions, we resort (again) to the correspondence principle:

$$\vec{p} \rightarrow \vec{p} - \frac{e}{c}\vec{A}$$

$$E \rightarrow E - e\Phi$$

$$\Rightarrow \quad i\hbar \frac{\partial \Psi(\vec{x},t)}{\partial t} = \left[c\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}\right) + (e\Phi + \beta mc^2)\right]\Psi(\vec{x},t)$$

It is convenient to write $\Psi(\vec{x},t)$ as $\begin{pmatrix} u(\vec{x},t) \\ v(\vec{x},t) \end{pmatrix}$.

After some work (see also HW 11), one finds:

$$\boxed{i\hbar \frac{\partial}{\partial t} u(\vec{x},t) \approx \left[\frac{1}{2m}\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 - \frac{\hbar e}{2mc}\vec{\sigma}\cdot\vec{B} + e\Phi + mc^2\right]u(\vec{x},t)}$$

The magnetic moment associated with the spin is predicted to be $\frac{e\hbar}{2mc}$

this is the so-called Pauli equation

obeyed by a charged particle with spin-½ in an em field.

$$\frac{e\hbar}{2mc}\vec{\sigma} = \frac{e}{mc}\vec{S}$$

$$= \frac{e\hbar}{2mc}\, 2\,\frac{\vec{S}}{\hbar}$$

Bohr magneton

$g = 2$ (Lande factor)

if vacuum fluctuations were included, the g factor would be slightly larger than 2

$$\vec{M}_{spin} = g\,\frac{e}{2mc}\,\vec{S}$$

Since e is negative for the electron, $\vec{M}_{spin}$ points in the opposite direction as $\vec{S}$

The spin of the electron has twice as large of a magnetic moment associated with is, per unit angular momentum, as the orbital angular momentum:

$$\vec{M}_{tot} = \frac{e}{2mc}\left(\vec{L} + 2\vec{S}\right)$$

Goal: Decoupling of upper and lower components of Dirac equation with interactions.

Let $\Psi(\vec{x},t) = \begin{pmatrix} u(\vec{x},t) \\ v(\vec{x},t) \end{pmatrix}$

Then:

$$i\hbar \frac{\partial}{\partial t} u = \overbrace{c\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\vec{\sigma}}^{2mc^2\hat{B}\ \text{(this defines } \hat{B}\text{)}}\, v + (e\Phi + mc^2)\, u \quad ①$$

$$i\hbar \frac{\partial}{\partial t} v = c\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\vec{\sigma}\, u + (e\Phi - mc^2)\, v \quad ②$$

Rewrite ②:

$$c\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\vec{\sigma}\, u + \left(e\Phi - mc^2 - i\hbar\frac{\partial}{\partial t}\right) v = 0$$

Add $2mc^2 v$ to both sides and divide by $2mc^2$:

switching sign in bracket

$$v = \underbrace{\frac{1}{2mc}\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\vec{\sigma}}_{\hat{B}\ \text{(see above)}}\, u - \underbrace{\frac{1}{2mc^2}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)}_{\hat{C}\ \text{(this defines } \hat{C}\text{)}} v \quad ②'$$

Importantly: ① and ②' are equivalent to Dirac eq.!

②' reads: $v = \hat{B}\,u - \hat{C}\,v$

Now, we will start making some approximations.

1^{st} - order: $v \approx \hat{B} u$

2^{nd} - order: $v = \hat{B} u - \hat{C} v \approx \hat{B} u - \hat{C} \underbrace{(\hat{B} u)}_{\text{first-order expression}}$

$$\text{So: } v = (\hat{B} - \hat{C}\hat{B}) u \quad (3)$$

$\rightsquigarrow v$ expressed in terms of u only

Rewrite (1):

$$i\hbar \frac{\partial}{\partial t} u = 2mc^2 \hat{B} v + (e\Phi + mc^2) u$$

replace by (3)

$$\approx 2mc^2 \hat{B} (\hat{B} - \hat{C}\hat{B}) u + (e\Phi + mc^2) u$$

So, we have an approximate(!) equation for u (we decoupled v):

$$i\hbar \frac{\partial}{\partial t} u = 2mc^2 (\hat{B}\hat{B} - \hat{B}\hat{C}\hat{B}) u + (e\Phi + mc^2) u$$

need to analyze $\hat{B}\hat{B}u$

need to analyze $\hat{B}\hat{C}\hat{B}u$

$$2mc^2\ \hat{\beta}\ \hat{B}\ u = \frac{1}{2m}\Big[\underbrace{(-i\hbar\vec{\nabla} - \tfrac{e}{c}\vec{A})}_{\hat{\vec{a}}}\cdot\vec{\sigma}\Big]\Big[(-i\hbar\vec{\nabla} - \tfrac{e}{c}\vec{A})\cdot\vec{\sigma}\Big]u$$

plugging in def. of $\hat{B}$

$$= \frac{1}{2m}(\hat{\vec{a}}\cdot\vec{\sigma})(\hat{\vec{a}}\cdot\vec{\sigma})\,u$$

$$= \frac{1}{2m}\Big(\hat{\vec{a}}\cdot\hat{\vec{a}} + i\,\vec{\sigma}\cdot\underbrace{(\hat{\vec{a}}\times\hat{\vec{a}})}\Big)u$$

$$(-i\hbar\vec{\nabla} - \tfrac{e}{c}\vec{A})\times(-i\hbar\vec{\nabla} - \tfrac{e}{c}\vec{A})$$

$$= (-i\hbar\vec{\nabla})\times(-i\hbar\vec{\nabla}) + \frac{i\hbar e}{c}(\vec{\nabla}\times\vec{A} + \vec{A}\times\vec{\nabla})$$

$$+ \frac{e^2}{c^2}\underbrace{\vec{A}\times\vec{A}}_{=0}$$

now: $(\vec{\nabla}\times\vec{A} + \vec{A}\times\vec{\nabla})u$

chain rule $= (\vec{\nabla}u)\times\vec{A} + \underbrace{(\vec{\nabla}\times\vec{A})}_{\vec{B}}u + \vec{A}\times(\vec{\nabla}u)$

cancel

$$= \vec{B}\,u$$

$$= \frac{1}{2m}\Big(\hat{\vec{a}}\cdot\hat{\vec{a}} - \frac{\hbar e}{c}\vec{\sigma}\cdot\vec{B} - \hbar^2\vec{\nabla}^2\Big)u$$

$$\vec{a}\cdot\vec{a} = \left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)$$

$$= -\hbar^2\vec{\nabla}^2 + \frac{e}{c}\vec{A}^2 + i\hbar\frac{e}{c}\left(\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}\right)$$

$$\left(\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}\right)u = \left(\vec{\nabla}\cdot\vec{A}\right)u + \vec{A}\cdot\vec{\nabla}u + \vec{A}\cdot\vec{\nabla}u$$

$$= \left(\vec{\nabla}\cdot\vec{A}\right)u + 2\vec{A}\cdot\left(\vec{\nabla}u\right)$$

So: $$2mc^2\,\hat{B}\,\hat{B}\,u = \frac{1}{2m}\left(-\hbar^2\vec{\nabla}^2 - \frac{\hbar e}{c}\vec{\sigma}\cdot\vec{B} + \left(\vec{\nabla}\cdot\vec{A}\right) + 2\vec{A}\cdot\vec{\nabla}\right)u$$

we already interpreted this term earlier

We also need the $-2mc^2\,\hat{B}\,\hat{C}\,\hat{B}\,u$ term.

After a fair bit of work we find, specializing to an electron in a Coulomb field, that the equation for u gives us relativistic correction to kinetic energy, $\vec{L}\cdot\vec{S}$ coupling term, and Darwin term.

Goal: Decoupling of upper and lower components of Dirac equation with interactions.

Let $\Psi(\vec{x},t) = \begin{pmatrix} u(\vec{x},t) \\ v(\vec{x},t) \end{pmatrix}$

Then:

$$i\hbar \frac{\partial}{\partial t} u = \overbrace{c\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\vec{\sigma}}^{2mc^2\hat{B} \text{ (this defines } \hat{B})} v + \left(e\Phi + mc^2\right) u \quad (1)$$

$$i\hbar \frac{\partial}{\partial t} v = c\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\vec{\sigma}\, u + \left(e\Phi - mc^2\right) v \quad (2)$$

Rewrite (2):

$$c\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\vec{\sigma}\, u + \left(e\Phi - mc^2 - i\hbar\frac{\partial}{\partial t}\right) v = 0$$

Add $2mc^2 v$ to both sides and divide by $2mc^2$:

switching sign in bracket

$$v = \underbrace{\frac{1}{2mc}\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\cdot\vec{\sigma}}_{\hat{B} \text{ (see above)}}\, u - \underbrace{\frac{1}{2mc^2}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)}_{\hat{C} \text{ (this defines } \hat{C})} v \quad (2')$$

Importantly: (1) and (2') are equivalent to Dirac eq.!

(2') reads: $v = \hat{B}u - \hat{C}v$

Now, we will start making some approximations.

A small add-on:

Let us analyze (2') a little bit more. What do we call first-order? and what second-order?

(2') $$v(\vec{x},t) = \frac{1}{2c}\left(-\frac{i\hbar\vec{\nabla}}{m} - \frac{e}{cm}\vec{A}\right)\cdot\vec{\sigma}\, u - \frac{1}{2mc^2}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\phi\right) v$$

let us assume time-independent case.

Then: $i\hbar\frac{\partial}{\partial t} \to E$

Write $E = mc^2 + E'$

$|E'|$ is small compared to mc^2

Second term:

$$-\frac{1}{2mc^2}\left(E' + \underbrace{mc^2 - mc^2}_{\text{cancel}} - e\Phi\right) v$$

now: $\left|\frac{E' - e\Phi}{2mc^2}\right| \ll 1$

(recall $|E'| \ll mc^2$)

what about first term?

$$\left|\frac{1}{2c}\left(\frac{\vec{p}}{m} - \frac{e}{cm}\vec{A}\right)\cdot\vec{\sigma}\, u\right| \simeq \left|\frac{v}{c}\, u\right|$$

velocity

So: Our equation (2') has ~~the~~ following structure

$$v(\vec{x},t) = \hat{B}\, u(\vec{x},t) - \hat{C}\, v(\vec{x},t)$$

$$|\hat{B} u| \sim \left|\frac{v}{c} u\right| \qquad |\hat{C} v| \ll |v|$$

velocity (not component)

This is telling us that $|v|$ is much smaller than $|u|$ → because of this, we can drop the $|\hat{C} v|$ term since $|\hat{C} v| \ll |v|$

→ We have established a "hirarchy"!

1^{st} - order: $v \approx \hat{B} u$

2^{nd} - order: $v = \hat{B} u - \hat{C} v \approx \hat{B} u - \hat{C} \underbrace{(\hat{B} u)}_{\text{first-order expression}}$

approximately

So: $v \approx (\hat{B} - \hat{C}\hat{B}) u$ (3)

$\rightsquigarrow$ v expressed in terms of u only

Rewrite (1):

$$i\hbar \frac{\partial}{\partial t} u = 2mc^2 \hat{B} \underbrace{v}_{\text{replace by (3)}} + (e\Phi + mc^2) u$$

$$\approx 2mc^2 \hat{B} (\hat{B} - \hat{C}\hat{B}) u + (e\Phi + mc^2) u$$

So, we have an approximate(!) equation for u (we decoupled v):

$$i\hbar \frac{\partial}{\partial t} u = 2mc^2 (\hat{B}\hat{B} - \hat{B}\hat{C}\hat{B}) u + (e\Phi + mc^2) u$$

need to analyze $\hat{B}\hat{B} u$

need to analyze $\hat{B}\hat{C}\hat{B} u$

$$2mc^2\, \hat{B}\, \hat{B}\, u = \frac{1}{2m}\Big[\underbrace{\big(-i\hbar\vec{\nabla} - \tfrac{e}{c}\vec{A}\big)}_{\hat{\vec{a}}}\cdot\vec{\sigma}\Big]\Big[\big(-i\hbar\vec{\nabla} - \tfrac{e}{c}\vec{A}\big)\cdot\vec{\sigma}\Big]u$$

plugging in
def. of $\hat{B}$

$$= \frac{1}{2m}\,(\hat{\vec{a}}\cdot\vec{\sigma})(\hat{\vec{a}}\cdot\vec{\sigma})\,u$$

$$= \frac{1}{2m}\Big(\hat{\vec{a}}\cdot\hat{\vec{a}} + i\,\vec{\sigma}\cdot\underbrace{(\hat{\vec{a}}\times\hat{\vec{a}})}\Big)u$$

$$\big(-i\hbar\vec{\nabla} - \tfrac{e}{c}\vec{A}\big)\times\big(-i\hbar\vec{\nabla} - \tfrac{e}{c}\vec{A}\big)$$

$$= (-i\hbar\vec{\nabla})\times(-i\hbar\vec{\nabla}) + \frac{i\hbar e}{c}\big(\vec{\nabla}\times\vec{A} + \vec{A}\times\vec{\nabla}\big)$$

$$+ \frac{e^2}{c^2}\underbrace{\vec{A}\times\vec{A}}_{=0}$$

now: $(\vec{\nabla}\times\vec{A} + \vec{A}\times\vec{\nabla})\,u$

chain rule

$$= \underbrace{(\vec{\nabla}u)\times\vec{A}} + (\underbrace{\vec{\nabla}\times\vec{A}}_{\vec{B}})\,u + \underbrace{\vec{A}\times(\vec{\nabla}u)}$$

cancel

$$= \vec{B}\,u$$

magnetic field vector

$$\Rightarrow 2mc^2 \; \hat{B} \; \hat{B} \; u = \frac{1}{2m} \left(\hat{\vec{a}} \cdot \hat{\vec{a}} - \frac{\hbar e}{c} \vec{\sigma} \cdot \vec{B} \right) u$$

$$= \frac{1}{2m} \left[\left(-i\hbar \vec{\nabla} - \frac{e}{c} \vec{A} \right)^2 - \frac{\hbar e}{c} \vec{\sigma} \cdot \vec{B} \right] u$$

So: Without the $-2mc^2 \hat{B} \hat{C} \hat{B} u$ term, we have:

first-order result

$$\boxed{i\hbar \frac{\partial}{\partial t} u = \Bigg[\frac{1}{2m} \left(-i\hbar \vec{\nabla} - \frac{e}{c} \vec{A} \right)^2 - \underbrace{\frac{\hbar e}{2mc} \vec{\sigma} \cdot \vec{B}}_{\text{we had interpreted this term earlier}} + e\Phi + mc^2 \Bigg] u}$$

$$\underbrace{\text{let } e\Phi = -\frac{Ze^2}{r}}_{\text{we are specializing to Coulomb potential}} = V(r)$$

We still need to simplify $-2mc^2 \hat{B} \hat{C} \hat{B} u$ term:

Recall: $\hat{B} = \frac{1}{2mc} \left(-i\hbar \vec{\nabla} - \frac{e}{c} \vec{A} \right) \cdot \vec{\sigma}$

$$\hat{C} = \frac{1}{2mc^2} \Big(i\hbar \frac{\partial}{\partial t} - mc^2 - \underbrace{e\Phi}_{V(r)} \Big)$$

For simplicity, let us assume $\vec{A} = 0$ and let us assume that we are looking at the time-independent case:

$$-2mc^2 \hat{B} \hat{C} \hat{B} u \longrightarrow -2mc^2 \left(-i\hbar \vec{\nabla} \right) \cdot \vec{\sigma} \, \frac{1}{2mc^2} \left(E - mc^2 - V(r) \right)$$

$$\left(-i\hbar \vec{\nabla} \right) \cdot \vec{\sigma} \left(\frac{1}{2mc} \right)^2 u$$

$$= +\hbar^2 \frac{1}{4m^2c^2} \vec{\nabla}\cdot\vec{\sigma}\,(E - mc^2 - V(r))\,\vec{\nabla}\cdot\vec{\sigma}\; u$$

$$= \left[\hbar^2 \frac{E-mc^2}{4m^2c^2} \underbrace{(\vec{\nabla}\cdot\vec{\sigma})(\vec{\nabla}\cdot\vec{\sigma})}_{\nabla^2} - \frac{\hbar^2}{4m^2c^4} \underbrace{\vec{\nabla}\cdot\vec{\sigma}\; V(r)\; \vec{\nabla}\cdot\vec{\sigma}}\right] u$$

chain rule:

$$\left[(\vec{\nabla}V(r))\cdot\vec{\sigma}\right]\left[(\vec{\nabla}\cdot\vec{\sigma})u\right]$$
$$+ V(r)\,\vec{\nabla}\cdot\vec{\sigma}\;\vec{\nabla}\cdot\vec{\sigma}\,u$$
$$= (\vec{\nabla}V)\cdot\vec{\sigma}(\vec{\nabla}\cdot\vec{\sigma}u) + V\vec{\nabla}^2 u$$

$$= \frac{\hbar^2}{4m^2c^2}\left[E - mc^2 - V(r)\right]\vec{\nabla}^2 u - \frac{\hbar^2}{4m^2c^4}(\vec{\nabla}V\cdot\vec{\sigma})(\vec{\nabla}\cdot\vec{\sigma}u)$$

Now: $(\vec{\sigma}\cdot\vec{\nabla}V)(\vec{\sigma}\cdot\vec{\nabla}u)$

$$= \underbrace{\vec{\nabla}V\cdot\vec{\nabla}u}_{\frac{\partial V}{\partial r}\frac{\partial u}{\partial r}} + \underbrace{i\,\vec{\sigma}\cdot(\vec{\nabla}V\times\vec{\nabla}u)}_{-\frac{2}{\hbar^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{S}\cdot(\vec{r}\times\hat{\vec{p}}u)}$$

$$\vec{\sigma} = \frac{2\vec{S}}{\hbar} \qquad \underbrace{\vec{\nabla}V\times\vec{\nabla}u}_{\frac{\partial V}{\partial r}\,\cancel{\frac{\partial u}{\partial r}}\,\hat{r}\times\vec{\nabla}u}$$

$$-\frac{2}{\hbar^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{S}\cdot\underbrace{(\vec{r}\times\hat{\vec{p}}u)}_{\vec{L}u}$$

$$= \frac{\partial V}{\partial r}\frac{\partial u}{\partial r} - \frac{2}{\hbar^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{L}\cdot\vec{S}\,u$$

So: $-2mc^2 \hat{B}\hat{C}\hat{B}u$

$$= \frac{\hbar^2}{4m^2c^2}\Big[\underbrace{E - mc^2 - V(r)}_{\approx \frac{\hat{p}^2}{2m}}\Big]\vec{\nabla}^2 u$$

$$- \frac{\hbar^2}{4m^2c^2}\frac{\partial V}{\partial r}\frac{\partial u}{\partial r}$$

$$+ \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{L}\cdot\vec{S}\,u$$

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

$$+ \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{L}\cdot\vec{S}\,u$$

the treatment of the Darwin term is a bit intricate mathematically

$$+\frac{1}{2}\left[\left(-\frac{\hbar^2}{4m^2c^2}\frac{\partial V}{\partial r}\frac{\partial}{\partial r}\right) + \left(-\frac{\hbar^2}{4m^2c^2}\frac{\partial V}{\partial r}\frac{\partial}{\partial r}\right)^{+}\right]u$$

$$= \frac{\hbar^2}{8m^2c^2}\vec{\nabla}^2 V$$

$$\vec{\nabla}^2 V \to 4\pi Ze^2\delta(\vec{r})$$

$$= \frac{\pi\hbar^2}{2m^2c^2}\, Ze^2\delta(\vec{r})$$

$$\approx \left(-\frac{\hat{\vec{p}}^4}{8m^3c^2} + \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{L}\cdot\vec{S} + \frac{\pi\hbar^2}{2m^2c^2}Ze^2\delta(r)\right)u$$

Finally:

this term comes from expanding v to first order

$$i\hbar \frac{\partial}{\partial t} u = \Big[\frac{1}{2m} \left(-i\hbar \vec{\nabla} - \frac{e}{c} \vec{A}\right)^2 - \frac{\hbar e}{2mc} \vec{\sigma} \cdot \vec{B}$$

$V(r)$

$$+ e\Phi + mc^2$$

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

correction to kin. energy

$$+ \frac{1}{2m^2c^2} \frac{1}{r} \frac{\partial V}{\partial r} \vec{L} \cdot \vec{S}$$

$\vec{L} \cdot \vec{S}$ coupling term

$$+ \frac{\pi \hbar^2}{2m^2c^2} Ze^2 \delta(\vec{r}) \Big] u$$

Darwin term (correction to potential energy)

the green terms come from "expanding" v to 2nd order

Dirac Hamiltonian with central potential:

$$\hat{H}_{Dirac} = \begin{pmatrix} mc^2 + V(|\vec{x}|) & c\,\vec{\sigma}\cdot\hat{\vec{p}} \\ c\,\vec{\sigma}\cdot\hat{\vec{p}} & -mc^2 + V(|\vec{x}|) \end{pmatrix}$$

each of these blocks is a 2×2 matrix

Just as the Hamiltonian is $(2\times 2)\cdot 4$,
↳ 4 blocks of 2×2 matrices

we write the spinor $\Psi(\vec{x})$ in terms of $\psi_1(\vec{x})$ and $\psi_2(\vec{x})$ — each with two components: $\Psi(\vec{x}) = \begin{pmatrix} \psi_1(\vec{x}) \\ \psi_2(\vec{x}) \end{pmatrix}$

$$\psi_1(\vec{x}) = \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}$$

$$\psi_2(\vec{x}) = \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}$$

Since we have a spherically symmetric interaction potential, we can find simultaneous eigenstates of $\hat{H}_{Dirac}$, $\hat{J}^2$, and $\hat{J}_z$

$\hat{J}^2 \to$ q.n. j

$\hat{J}_z \to$ q.n. m_j

We expect:

$$\Psi \sim \begin{pmatrix} m_s = \frac{1}{2} \Rightarrow m_\ell = m_j - \frac{1}{2} \\ m_s = -\frac{1}{2} \Rightarrow m_\ell = m_j + \frac{1}{2} \\ m_s = \frac{1}{2} \Rightarrow m_\ell = m_j - \frac{1}{2} \\ m_s = -\frac{1}{2} \Rightarrow m_\ell = m_j + \frac{1}{2} \end{pmatrix}$$

From parity conservation: $\beta\, \Psi(-\vec{x}) = \pm\, \Psi(\vec{x})$

not just $\vec{x} \to -\vec{x}$; also need to make sure that spin is included (hence the "β multiplication")

$$\Rightarrow \overbrace{\psi_1(-\vec{x}) = +\psi_1(\vec{x})}^{\ell = \text{even}} \quad \text{and} \quad \overbrace{\psi_2(-\vec{x}) = -\psi_2(\vec{x})}^{\ell \text{ odd}} \quad \to \text{Case A}$$

or

$$\underbrace{\psi_1(-\vec{x}) = -\psi_1(\vec{x})}_{\ell \text{ odd}} \quad \text{and} \quad \underbrace{\psi_2(-\vec{x}) = +\psi_2(\vec{x})}_{\ell \text{ even}} \quad \to \text{Case B}$$

So: The idea is to couple ℓ and s ($\hat{L}$ and $\hat{S}$) to give good quantum numbers j and $m_j \to \mathcal{Y}^{jm}_{\ell}(\hat{x})$.

Chapter 3 : Review on spin angular functions $\mathcal{Y}_{\ell}^{j m_j}(\hat{x})$

Where does Eq. (3.8.64) come from?

↳ the equation is written on next page

Look at the "+ sign" equation:

$$\mathcal{Y}_{\ell}^{j=\ell+\frac{1}{2}, m_j} = \sqrt{\frac{\ell+m_j+\frac{1}{2}}{2\ell+1}}\, \underbrace{\underbrace{Y_{\ell}^{m_j-\frac{1}{2}}}_{m_\ell = m_j-\frac{1}{2}}(\theta,\phi)\underbrace{X_+}_{m_s=\frac{1}{2}}}_{m_j = m_\ell + m_s} + \sqrt{\frac{\ell-m_j+\frac{1}{2}}{2\ell+1}}\, \underbrace{\underbrace{Y_{\ell}^{m_j+\frac{1}{2}}}_{m_\ell = m_j+\frac{1}{2}}(\theta,\phi)\underbrace{X_-}_{m_s=-\frac{1}{2}}}_{m_j = m_\ell + m_s}$$

$\langle m_j-\frac{1}{2}, \frac{1}{2} | \underbrace{\ell+\frac{1}{2}}, m_j\rangle$

$\langle m_\ell, m_s | j, m_j\rangle$

Clebsch-Gordon coefficient

$\langle m_j+\frac{1}{2}, -\frac{1}{2} | j, m_j\rangle$

$\langle m_\ell, m_s | j, m_j\rangle$

Clebsch-Gordon coefficient

Look at the "− sign" equation:

$$\mathcal{Y}_{\ell}^{j=\ell-\frac{1}{2}, m_j} = -\sqrt{\frac{\ell-m_j+\frac{1}{2}}{2\ell+1}}\, \underbrace{\underbrace{Y_{\ell}^{m_j-\frac{1}{2}}}_{m_\ell = m_j-\frac{1}{2}}(\theta,\phi)\underbrace{X_+}_{m_s=+\frac{1}{2}}}_{m_j = m_\ell + m_s} + \sqrt{\frac{\ell+m_j+\frac{1}{2}}{2\ell+1}}\, \underbrace{\underbrace{Y_{\ell}^{m_j+\frac{1}{2}}}_{m_\ell = m_j+\frac{1}{2}}(\theta,\phi)\underbrace{X_-}_{m_s=-\frac{1}{2}}}_{m_j = m_\ell + m_s}$$

$\langle m_j-\frac{1}{2}, \frac{1}{2} | \overbrace{\ell-\frac{1}{2}}^{j}, m_j\rangle$

$\langle m_j+\frac{1}{2}, -\frac{1}{2} | j, m_j\rangle$

$$\mathcal{Y}_{l}^{j=l+\frac{1}{2},\,m_j} = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \sqrt{l+m_j+\frac{1}{2}}\; Y_l^{m_j-\frac{1}{2}}(\theta,\phi) \\ \sqrt{l-m+\frac{1}{2}}\; Y_l^{m_j+\frac{1}{2}}(\theta,\phi) \end{pmatrix}$$

(3.8.64)

(+ sign)

$\uparrow$

$j = l+\frac{1}{2}$

$\Rightarrow l = j - \frac{1}{2}$

$m_l = m_j - m_s$

$$\mathcal{Y}_{j-\frac{1}{2}}^{j,\,m_j} = \frac{1}{\sqrt{2j}} \begin{pmatrix} \sqrt{j+m_j}\; Y_{j-\frac{1}{2}}^{m_j-\frac{1}{2}}(\theta,\phi) \\ \sqrt{j-m_j}\; Y_{j-\frac{1}{2}}^{m_j+\frac{1}{2}}(\theta,\phi) \end{pmatrix} \begin{array}{l} \to m_s = \frac{1}{2} \\ \to m_s = -\frac{1}{2} \end{array}$$

$$\mathcal{Y}_{l}^{j=l-\frac{1}{2},\,m_j} = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} -\sqrt{l-m_j+\frac{1}{2}}\; Y_l^{m_j-\frac{1}{2}}(\theta,\phi) \\ \sqrt{l-m_j+\frac{1}{2}}\; Y_l^{m_j+\frac{1}{2}}(\theta,\phi) \end{pmatrix}$$

(3.8.64)

(− sign)

$\uparrow$

$j = l - \frac{1}{2}$

$\Rightarrow l = j + \frac{1}{2}$

$$\mathcal{Y}_{j+\frac{1}{2}}^{j,\,m_j} = \frac{1}{\sqrt{2(j+1)}} \begin{pmatrix} \sqrt{j+1-m_j}\; Y_{j+\frac{1}{2}}^{m_j-\frac{1}{2}}(\theta,\phi) \\ \sqrt{j+1-m_j}\; Y_{j+\frac{1}{2}}^{m_j+\frac{1}{2}}(\theta,\phi) \end{pmatrix} \begin{array}{l} \to m_s = \frac{1}{2} \\ \to m_s = -\frac{1}{2} \end{array}$$

$\mathcal{Y}$: two-component spin-angular functions

$\uparrow$

for the + sign expression and the − sign expression, the l values differ by one

Continued from page 8-54:

Choose:

Case A:

$$\Psi_A(\vec{x}) = \begin{pmatrix} u_A(r)\, \mathcal{Y}^{jm_j}_{j-\frac{1}{2}}(\hat{x}) \\ -i\, v_A(r)\, \mathcal{Y}^{jm_j}_{j+\frac{1}{2}}(\hat{x}) \end{pmatrix}$$

later convenience

Case B:

$$\Psi_B(\vec{x}) = \begin{pmatrix} u_B(r)\, \mathcal{Y}^{jm_j}_{j+\frac{1}{2}}(\hat{x}) \\ -i\, v_B(r)\, \mathcal{Y}^{jm_j}_{j-\frac{1}{2}}(\hat{x}) \end{pmatrix}$$

later convenience

Ψ_A: even parity if $j-\frac{1}{2}$ is even

odd parity if $j+\frac{1}{2}$ is odd

Ψ_B: odd parity if $j-\frac{1}{2}$ is even

even parity if $j+\frac{1}{2}$ is odd

After a bunch of work: For any central potential:

For choice A:

$$\left[E - mc^2 - V(r)\right] u_A(r) - \left(\hbar c\left(\frac{d}{dr} + \frac{\lambda+1}{r}\right)\right) v_A(r) = 0$$

$$\left[E + mc^2 - V(r)\right] v_A(r) - \left(\hbar c\left(\frac{d}{dr} - \frac{\lambda-1}{r}\right)\right) u_A(r) = 0$$

For choice B:

$$\left[E - mc^2 - V(r)\right] u_B(r) - \left(\hbar c\left(\frac{d}{dr} - \frac{\lambda-1}{r}\right)\right) v_B(r) = 0$$

$$\left[E + mc^2 - V(r)\right] v_B(r) - \left(\hbar c\left(\frac{d}{dr} + \frac{\lambda+1}{r}\right)\right) u_B(r) = 0$$

Here: $\lambda = j + \frac{1}{2}$.

We see: The radial equations for choice A are the same as the radial equation for choice B, provided the replacement $\lambda \to -\lambda$ is made.

$\Rightarrow$ We only have to solve the equations for choice A.

For one-electron atom: $V(r) = -\frac{Ze^2}{r}$

Use series expansion and look for bound states with energy $E < mc^2$.

After a bunch of work:

$$\boxed{E = mc^2 \left[1 + \frac{(Z\alpha)^2}{\left(n - (j+\frac{1}{2}) + \sqrt{(j+\frac{1}{2})^2 - (Z\alpha)^2}\right)^2} \right]^{-1/2}}$$

independent of l

$\rightarrow$ different l can give rise to the same j quantum number

require:

$j + \frac{1}{2} > Z\alpha$

$\frac{j+\frac{1}{2}}{\alpha} > Z$

$j = \frac{1}{2}$: $Z \leq 137$

Taylor expansion:

$$E \approx \underbrace{mc^2}_{\substack{\text{rest} \\ \text{energy}}} - \underbrace{\frac{1}{2} mc^2 \frac{(Z\alpha)^2}{n^2}}_{\text{"usual" energy for Coulomb pot.}} + \dots$$

"usual" energy for Coulomb pot.
(↪ as obtained by solving Schrödinger equation)

next term agrees w/ what we obtained when we treated three corrections perturbatively:

- correction to kinetic energy
- "corrective" spin-orbit coupling term
- correction to potential energy (Darwin term)

→ See end of Chapter problems 8.16 and 8.17

According to Dirac equation: $2P_{1/2}$ and $2S_{1/2}$ states have the same energy.

Experiment ⟶ small energy splitting

Energy splitting $\hat{=}$ Lamb shift

(quantum electrodynamics)

→ Lamb shift tends to be larger than hyperfine structure splitting

↳ due to nuclear spin and finite charge distribution of nucleus

Recall:

Schrödinger equation for H-atom yields:

(n, l, m_l, s, m_s) quantum numbers

$$\left.\begin{aligned} n &= 1, 2, 3, \ldots \\ l &= 0, 1, \ldots, n-1 \\ m_l &= -l, -l+1, \ldots, l \\ m_s &= \pm \tfrac{1}{2} \end{aligned}\right\} \begin{aligned} &E = E_n \\ &2n^2 \text{ degeneracy} \end{aligned}$$

Now: Dirac equation:

$$\left.\begin{aligned} n &= 1, 2, 3, \ldots \\ j &= \tfrac{1}{2}, \tfrac{3}{2}, \ldots, n - \tfrac{1}{2} \\ m_j &= -j, -j+1, \ldots, j \end{aligned}\right\} \quad E = E_{nj}$$

Ground state:

$-13.6\,eV$

$n=1, \ell=0, m_\ell=0, m_s=\pm\frac{1}{2}$

$\updownarrow 1.46\,cm^{-1}$

$n=1, \ell=0, j=\frac{1}{2}, m_j=\pm\frac{1}{2}$

SE
deg. 2
(including spin)

Dirac
deg. 2

$1\,cm^{-1} \mathrel{\hat{=}} 1.24 \cdot 10^{-4}\,eV$

$n=2$ manifold:

SE
deg. $2n^2=8$

$\ell=0, m_\ell=0, m_s=\pm\frac{1}{2}$

$\ell=1, m_\ell= 0, m_s=\pm\frac{1}{2}$
$\quad +1 \quad \pm\frac{1}{2}$
$\quad -1 \quad \pm\frac{1}{2}$

$\updownarrow 0.09\,cm^{-1}$

$2P_{3/2}$
deg. 4

$\updownarrow 0.46\,cm^{-1}$

$2S_{1/2}, 2P_{1/2}$
deg. 4

$2P_{3/2}$: $j=\frac{3}{2}$; $m_j=\pm\frac{3}{2}, \pm\frac{1}{2}$

$2S_{1/2}$: $j=\frac{1}{2}$; $m_j=\pm\frac{1}{2}$

$2P_{1/2}$: $j=\frac{1}{2}$; $m_j=\pm\frac{1}{2}$

Dirac Hamiltonian with central potential:

$$\hat{H}_{Dirac} = \begin{pmatrix} mc^2 + V(|\vec{x}|) & c\,\vec{\sigma}\cdot\hat{\vec{p}} \\ c\,\vec{\sigma}\cdot\hat{\vec{p}} & -mc^2 + V(|\vec{x}|) \end{pmatrix}$$

each of these blocks is a 2×2 matrix

Just as the Hamiltonian is $(2\times 2)\cdot 4$,

$\hookrightarrow$ 4 blocks of 2×2 matrices

we write the spinor $\Psi(\vec{x})$ in terms of $\psi_1(\vec{x})$ and $\psi_2(\vec{x})$ — each with two components: $\Psi(\vec{x}) = \begin{pmatrix} \psi_1(\vec{x}) \\ \psi_2(\vec{x}) \end{pmatrix}$

$\psi_1(\vec{x}) = \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}$

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Since we have a spherically symmetric interaction potential, we can find simultaneous eigenstates of $\hat{H}_{Dirac}$, $\underset{\downarrow \text{ q.n. } j}{\hat{J}^2}$, and $\underset{\downarrow \text{ q.n. } m_j}{\hat{J}_z}$

We expect:

$$\Psi \sim \begin{pmatrix} m_s = \frac{1}{2} \Rightarrow m_\ell = m_j - \frac{1}{2} \\ m_s = -\frac{1}{2} \Rightarrow m_\ell = m_j + \frac{1}{2} \\ m_s = \frac{1}{2} \Rightarrow m_\ell = m_j - \frac{1}{2} \\ m_s = -\frac{1}{2} \Rightarrow m_\ell = m_j + \frac{1}{2} \end{pmatrix}$$

From $\underbrace{\text{parity conservation}}$: $\beta\, \Psi(-\vec{x}) = \pm \Psi(\vec{x})$

not just $\vec{x} \to -\vec{x}$;
also need to make
sure that spin is
included (hence the
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$$\Rightarrow \overbrace{\psi_1(-\vec{x}) = +\psi_1(\vec{x})}^{\ell = \text{even}} \quad \text{and} \quad \overbrace{\psi_2(-\vec{x}) = -\psi_2(\vec{x})}^{\ell \text{ odd}} \quad \to \text{Case A}$$

or

$$\underbrace{\psi_1(-\vec{x}) = -\psi_1(\vec{x})}_{\ell \text{ odd}} \quad \text{and} \quad \underbrace{\psi_2(-\vec{x}) = +\psi_2(\vec{x})}_{\ell \text{ even}} \quad \to \text{Case B}$$

So: The idea is to couple ℓ and s ($\hat{L}$ and $\hat{S}$) to give good quantum numbers j and $m_j \to \mathcal{Y}_\ell^{jm}(\hat{x})$.

Choose: **Case A:**

$$\Psi_A(\vec{x}) = \begin{pmatrix} u_A(r)\, \mathcal{Y}^{jm_j}_{j-\frac{1}{2}}(\hat{x}) \\ -i\, v_A(r)\, \mathcal{Y}^{jm_j}_{j+\frac{1}{2}}(\hat{x}) \end{pmatrix}$$

later convenience

Case B:

$$\Psi_B(\vec{x}) = \begin{pmatrix} u_B(r)\, \mathcal{Y}^{jm_j}_{j+\frac{1}{2}}(\hat{x}) \\ -i\, v_B(r)\, \mathcal{Y}^{jm_j}_{j-\frac{1}{2}}(\hat{x}) \end{pmatrix}$$

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Ψ_B: odd parity if $j-\frac{1}{2}$ is even

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After a bunch of work: For any central potential:

For choice A:

$$\boxed{\begin{aligned} &\left[E - mc^2 - V(r)\right] u_A(r) - \left(\hbar c\left(\frac{d}{dr} + \frac{j+1}{r}\right)\right) v_A(r) = 0 \\ &\left[E + mc^2 - V(r)\right] v_A(r) - \left(\hbar c\left(\frac{d}{dr} - \frac{j-1}{r}\right)\right) u_A(r) = 0 \end{aligned}}$$

For choice B:

$$\left[E - mc^2 - V(r)\right] u_B(r) - \left(\hbar c\left(\frac{d}{dr} - \frac{j-1}{r}\right)\right) v_B(r) = 0$$

$$\left[E + mc^2 - V(r)\right] v_B(r) - \left(\hbar c\left(\frac{d}{dr} + \frac{j+1}{r}\right)\right) u_B(r) = 0$$

We see: The radial equations for choice A are the same as the radial equation for choice B, provided the replacement $\lambda \to -\lambda$ is made.

$\Rightarrow$ We only have to solve the equations for choice A.

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After a bunch of work:

$$\boxed{E = mc^2\left[1 + \frac{(Z\alpha)^2}{\left(n - (j+\frac{1}{2}) + \sqrt{(j+\frac{1}{2})^2 - (Z\alpha)^2}\right)^2}\right]^{-1/2}}$$

independent of l

$\to$ different l can give rise to the same j quantum number

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$\frac{j+\frac{1}{2}}{\alpha} > Z$

$j = \frac{1}{2}$: $Z \leq 137$

Taylor expansion:

$$E \approx \underbrace{mc^2}_{\text{rest energy}} - \underbrace{\frac{1}{2}\, mc^2 \, \frac{(Z\alpha)^2}{n^2}}_{\substack{\text{"usual" energy} \\ \text{for Coulomb pot.} \\ (\hookrightarrow \text{ as obtained by} \\ \text{solving Schrödinger} \\ \text{equation})}} + \ldots$$

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- "corrective" spin-orbit coupling term
- correction to potential energy (Darwin term)

→ See end of Chapter problems 8.16 and 8.17

According to Dirac equation: $2P_{1/2}$ and $2S_{1/2}$ states have the same energy.

Experiment ⟶ small energy splitting

Energy splitting $\hat{=}$ Lamb shift

(quantum electrodynamics)

→ Lamb shift tends to be larger than hyperfine structure splitting

↳ due to nuclear spin and finite charge distribution of nucleus

Recall:

Schrödinger equation for H-atom yields:

(n, l, m_l, s, m_s) quantum numbers

$$\left.\begin{array}{l} n = 1, 2, 3, \ldots \\ l = 0, 1, \ldots, n-1 \\ m_l = -l, -l+1, \ldots, l \\ m_s = \pm \frac{1}{2} \end{array}\right\} \begin{array}{l} E = E_n \\ 2n^2 \text{ degeneracy} \end{array}$$

Now: Dirac equation:

$$\left.\begin{array}{l} n = 1, 2, 3, \ldots \\ j = \frac{1}{2}, \frac{3}{2}, \ldots, n - \frac{1}{2} \\ m_j = -j, -j+1, \ldots, j \end{array}\right\} E = E_{nj}$$

Ground state:

$-13.6\,eV$

$n=1, l=0, m_l=0, m_s=\pm\frac{1}{2}$

$1.46\,cm^{-1}$

$n=1, l=0, j=\frac{1}{2}, m_j=\pm\frac{1}{2}$

SE
deg. 2
(including
spin)

Dirac
deg. 2

$1\,cm^{-1} \hat{=} 1.24\cdot 10^{-4}\,eV$

n=2 manifold:

SE
deg. $2n^2=8$

$l=0,\ m_l=0,\ m_s=\pm\frac{1}{2}$

$l=1,\ m_l=0,\ m_s=\pm\frac{1}{2}$
$\quad\quad\quad +1 \quad \pm\frac{1}{2}$
$\quad\quad\quad -1 \quad \pm\frac{1}{2}$

$0.09\,cm^{-1}$

$2P_{3/2}$
deg. 4

$0.46\,cm^{-1}$

$2S_{1/2}, 2P_{1/2}$
deg. 4

$2P_{3/2}:\ j=\frac{3}{2};\ m_j=\pm\frac{3}{2}, \pm\frac{1}{2}$

$2S_{1/2}:\ j=\frac{1}{2};\ m_j=\pm\frac{1}{2}$

$2P_{1/2}:\ j=\frac{1}{2};\ m_j=\pm\frac{1}{2}$