A Brief Introduction
to Relativistic Quantum Mechanics

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1 Introduction

In Physics 215AB, you learned non-relativistic quantum mechanics, e.g., Schrödinger equation,

\[
E = \frac{p^2}{2m} + V,
\]

\[
E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad p \rightarrow -i\hbar \nabla,
\]

\[
i\hbar \frac{\partial}{\partial t} \Psi = \frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi. \tag{1}
\]

Now we would like to extend quantum mechanics to the relativistic domain. The natural thing at first is to search for a relativistic single-particle wave equation to replace the Schrödinger equation. It turns out that the form of the relativistic equation depends on the spin of the particle,

- spin-0: Klein-Gordon equation
- spin-1/2: Dirac equation
- spin-1: Proca equation
- etc

It is useful to study these one-particle equations and their solutions for certain problems. However, at certain point these one-particle relativistic quantum theory encounter fatal inconsistencies and break down. Essentially, this is because while energy is conserved in special relativity but mass is not. Particles with mass can be created and destroyed in real physical processes. For example, pair annihilation \( e^+ e^- \rightarrow 2\gamma \), muon decay \( \mu^- \rightarrow e^+ \bar{\nu}_e \nu_\mu \). They cannot be described by single-particle theory.

At that stage we are forced to abandon single-particle relativistic wave equations and go to a many-particle theory in which particles can be created and destroyed, that is, quantum field theory, which is the subject of the course.
2 Summary of Special Relativity

An event occurs at a single point in space-time and is defined by its coordinates $x^\mu, \mu = 0, 1, 2, 3$, 
\[ x^0 = ct, \quad x^1 = x, \quad x^2 = y, \quad x^3 = z, \] (2)
in any given frame.

The interval between 2 events $x^\mu$ and $\bar{x}^\mu$ is called $s$,
\[ s^2 = c^2(t - \bar{t})^2 - (x - \bar{x})^2 - (y - \bar{y})^2 - (z - \bar{z})^2 \]
\[ = (x^0 - \bar{x}^0)^2 - (x^1 - \bar{x}^1)^2 - (x^2 - \bar{x}^2)^2 - (x^3 - \bar{x}^3)^2. \] (3)

We define the metric
\[ g_{\mu\nu} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix}, \tag{4} \]
then we can write
\[ s^2 = \sum_{\mu,\nu} g_{\mu\nu}(x^\mu - \bar{x}^\mu)(x^\nu - \bar{x}^\nu) = g_{\mu\nu}\Delta x^\mu \Delta x^\nu, \] (5)
where we have used the Einstein convention: repeated indices (1 upper + 1 lower) are summed except when otherwise indicated.

Lorentz transformations

The postulates of Special Relativity tell us that the speed of light is the same in any inertial frame. $s^2$ is invariant under transformations from one inertial frame to any other. Such transformations are called Lorentz transformations. We will only need to discuss the homogeneous Lorentz transformations (under which the origin is not shifted) here,
\[ x'^\mu = \Lambda^\mu_\nu x^\nu. \] (6)

\[ g_{\mu\nu}x'^\mu x'^\nu = g_{\mu\nu}x^\mu x^\nu \]
\[ = g_{\mu\nu}\Lambda^\mu_\rho \Lambda^\nu_\sigma x^\rho x^\sigma \]
\[ \Rightarrow g_{\rho\sigma} = g_{\mu\nu}\Lambda^\mu_\rho \Lambda^\nu_\sigma. \] (7)

It’s convenient to use a matrix notation,
\[ x^\mu : \begin{pmatrix}
x^0 \\
x^1 \\
x^2 \\
x^3
\end{pmatrix} = \mathbf{x}. \] (8)
\[ s^2 = x^T g x, \]
\[ x' = \Lambda x \]
\[ \Rightarrow g = \Lambda^T g \Lambda \] (9)

Take the determinant,
\[ \det g = \det \Lambda^T \det g \det \Lambda, \] (10)
so \( \det \Lambda = \pm 1 \) (+1: proper Lorentz transformations, −1: improper Lorentz transformations).

Example: Rotations (proper):
\[ x'^0 = x^0 \]
\[ x'^1 = x^1 \cos \theta + x^2 \sin \theta \]
\[ x'^2 = -x^1 \sin \theta + x^2 \cos \theta \]
\[ x'^3 = x^3 \] (11)
\[ \Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta & \sin \theta & 0 \\ 0 & -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \] (12)

Example: Boosts (proper):
\[ t' = \gamma (t - \frac{v}{c^2} x^1) \] or \( x'^0 = \gamma x^0 - \gamma \beta x^1 \)
\[ x'^1 = \gamma (x^1 - vt) = \gamma x^1 - \gamma \beta x^0 \]
\[ x'^2 = x^2 \]
\[ x'^3 = x^3 \] (13)

where
\[ \beta = \frac{v}{c}, \quad \gamma = \frac{1}{\sqrt{1 - \beta^2}}. \] (14)

It’s convenient to define a quantity rapidity \( \eta \) such that \( \cosh \eta = \gamma, \ \sinh \eta = \gamma \beta \), then
\[ \Lambda = \begin{pmatrix} \cosh \eta & -\sinh \eta & 0 & 0 \\ -\sinh \eta & \cosh \eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \] (15)

One can easily check that \( \det \Lambda = \cosh^2 \eta - \sinh^2 \eta = 1. \)

**Four-vectors, tensors**

A contravariant vector is a set of 4 quantities which transforms like \( x^\mu \) under a
Lorentz transformation,
\[ V^\mu = \begin{pmatrix} V^0 \\ V^1 \\ V^2 \\ V^3 \end{pmatrix}, \quad V'^\mu = \Lambda^\mu_\nu V^\nu. \] (16)

A covariant vector is a set of 4 quantities which transforms as
\[ A'_\mu = A_\nu (\Lambda^{-1})^\nu_\mu, \quad \Lambda^{-1} = g \Lambda^T g. \] (17)

An upper index is called a contravariant index and a lower index is called a covariant index. Indices can be raised or lowered with the metric tensor \( g_{\mu \nu} \) and its inverse \( g^{\mu \nu} \).

Examples: Energy and momentum form a contravariant 4-vector,
\[ p^\mu = \left( \frac{E}{c}, p_x, p_y, p_z \right). \] (18)

4- gradient,
\[ \frac{\partial}{\partial x^\mu} = \begin{pmatrix} \frac{1}{c} \frac{\partial}{\partial t} \\ \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \equiv \partial_\mu \] (19)
is a covariant vector,
\[ \frac{\partial}{\partial x'^\mu} = \frac{\partial x^\nu}{\partial x'^\mu} \frac{\partial}{\partial x^\nu} = (\Lambda^{-1})^\nu_\mu \frac{\partial}{\partial x^\nu}. \] (20)

One can generalize the concept to tensors,
\[ T'^{\mu_1 \nu_1 \cdots}_{\rho_1 \sigma_1 \cdots} = \Lambda^{\mu_1}_\mu \Lambda^{\nu_1}_\nu \cdots (\Lambda^{-1})^\rho_1_\rho \cdots (\Lambda^{-1})^\sigma_1_{\sigma} \cdots T^{\mu_2 \nu_2 \cdots}_{\rho_2 \sigma_2 \cdots}. \] (21)

Maxwell’s equations in Lorentz covariant from (Heaviside-Lorentz convention)
\[ \nabla \cdot E = \rho \] (22)
\[ \nabla \cdot B = 0 \] (23)
\[ \nabla \times E + \frac{1}{c} \frac{\partial B}{\partial t} = 0 \] (24)
\[ \nabla \times B - \frac{1}{c} \frac{\partial E}{\partial t} = \frac{1}{c} J \] (25)

From the second equation we can define a vector potential \( A \) such that
\[ B = \nabla \times A \] (26)
Substituting it into the third equation, we have

\[ \nabla \times \left( E + \frac{1}{c} \frac{\partial A}{\partial t} \right) = 0, \]  

(27)

then we can define a potential \( \phi \), such that

\[ E = -\nabla \phi - \frac{1}{c} \frac{\partial A}{\partial t}. \]  

(28)

Gauge invariance: \( E, B \) are not changed under the following transformation,

\[ A \rightarrow A - \nabla \chi, \]  
\[ \phi \rightarrow \phi + \frac{1}{c} \frac{\partial}{\partial t} \chi. \]  

(29)

\((c\rho, J)\) form a 4-vector \( J^\mu \). Charge conservation can be written in the Lorentz covariant form, \( \partial_\mu J^\mu = 0 \),

\((\phi, A)\) from a 4-vector \( A^\mu \) \((A^\mu = (\phi, -A))\), from which one can derive an antisymmetric electromagnetic field tensor,

\[ F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu \]  

(note: \( \partial^i = -\partial_i = -\frac{\partial}{\partial x^i}, i = 1, 2, 3 \)).  

(30)

\( F^{\mu\nu} = \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{pmatrix}, \quad F_\mu^{\nu} = \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & -B_z & B_y \\ -E_y & B_z & 0 & -B_x \\ -E_z & -B_y & B_x & 0 \end{pmatrix} \)  

(31)

Maxwell’s equations in the covariant form:

\[ \partial_\mu F^{\mu\nu} = \frac{1}{c} J^\nu \]  

(32)

\[ \partial_\mu \tilde{F}^{\mu\nu} = \partial_\mu F_{\lambda\nu} + \partial_\lambda F_{\nu\mu} + \partial_\nu F_{\mu\lambda} = 0 \]  

(33)

where

\[ \tilde{F}^{\mu\nu} \equiv \frac{1}{2} \varepsilon^{\mu\nu\lambda\rho} F_{\lambda\rho}, \]  

(34)

c^{0123} and its even permutation = +1, its odd permutation = -1.

Gauge invariance: \( A^\mu \rightarrow A^\mu + \partial^\mu \chi \). One can check \( F^{\mu\nu} \) is invariant under this transformation.
3 Klein-Gordon Equation

In non-relativistic mechanics, the energy for a free particle is

\[ E = \frac{p^2}{2m}. \]  

(35)

To get quantum mechanics, we make the following substitutions:

\[ E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad p \rightarrow -i\hbar \nabla, \]  

(36)

and the Schrödinger equation for a free particle is

\[ -\frac{\hbar^2}{2m} \nabla^2 \Psi = i\hbar \frac{\partial \Psi}{\partial t}. \]  

(37)

In relativistic mechanics, the energy of a free particle is

\[ E = \sqrt{p^2 c^2 + m^2 c^4}. \]  

(38)

Making the same substitution we obtain

\[ \sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4} \Psi = i\hbar \frac{\partial \Psi}{\partial t}. \]  

(39)

It’s difficult to interpret the operator on the left hand side, so instead we try

\[ E^2 = p^2 c^2 + m^2 c^4 \]  

(40)

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

(41)

or

\[ \frac{1}{c^2} \left( \frac{\partial}{\partial t} \right)^2 \Psi - \nabla^2 \Psi \equiv \Box \Psi = -\frac{m^2 c^2}{\hbar^2} \Psi, \]  

(42)

where

\[ \Box = \frac{1}{c^2} \left( \frac{\partial}{\partial t} \right)^2 - \nabla^2 = \partial_\mu \partial^\mu. \]  

(43)

Plane-wave solutions are readily found by inspection,

\[ \Psi = \frac{1}{\sqrt{V}} \exp \left( \frac{i}{\hbar} \mathbf{p} \cdot \mathbf{x} \right) \exp \left( -\frac{i}{\hbar} E t \right), \]  

(44)

where \( E^2 = p^2 c^2 + m^2 c^4 \) and thus \( E = \pm \sqrt{p^2 c^2 + m^2 c^4} \). Note that there is a negative energy solution as well as a positive energy solution for each value of \( \mathbf{p} \). Naïvely one should just discard the negative energy solution. For a free particle in a positive energy state, there is no mechanism for it to make a transition to
the negative energy state. However, if there is some external potential, the Klein-Gordon equation is then altered by the usual replacements,

\[ E \rightarrow E - e\phi, \quad p \rightarrow p - \frac{e}{c}A, \]  

\[ (i\hbar\partial_t - e\phi)^2\Psi = c^2(-i\hbar\nabla - \frac{e}{c}A)^2\Psi + m^2c^4\Psi. \]  

The solution \(\Psi\) can always be expressed as a superposition of free particle solutions, provided that the latter form a complete set. They form a complete set only if the negative energy components are retained, so they cannot be simply discarded.

Recall the probability density and current in Schrödinger equation. If we multiply the Schrödinger equation by \(\Psi^*\) on the left and multiply the conjugate of the Schrödinger equation by \(\Psi\), and then take the difference, we obtain

\[-\frac{\hbar^2}{2m}(\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*) = i\hbar(\Psi^*\dot{\Psi} + \Psi\dot{\Psi}^*)\]  

\[\Rightarrow -\frac{\hbar^2}{2m}\nabla(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) = i\hbar\frac{\partial}{\partial t}(\Psi^*\Psi) \tag{47}\]

Using \(\rho_s = \Psi^*\Psi, \quad j_s = \frac{\hbar}{2ma}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*),\) we then obtain the equation of continuity,

\[\frac{\partial \rho_s}{\partial t} + \nabla \cdot j_s = 0 \tag{48}\]

Now we can carry out the same procedure for the free-particle Klein-Gordon equation:

\[\Psi^*\Box\Psi = -\frac{m^2c^2}{\hbar}\Psi^*\Psi\]

\[\Psi\Box\Psi^* = -\frac{m^2c^2}{\hbar}\Psi\Psi^* \tag{49}\]

Taking the difference, we obtain

\[\Psi^*\Box\Psi - \Psi\Box\Psi^* = \partial_\mu(\Psi^*\partial^\mu\Psi - \Psi\partial^\mu\Psi^*) = 0. \tag{50}\]

This suggests that we can define a probability 4-current,

\[j^\mu = \alpha(\Psi\partial^\mu\Psi - \Psi\partial^\mu\Psi^*), \quad \text{where } \alpha \text{ is a constant} \tag{51}\]

and it’s conserved, \(\partial_\mu j^\mu = 0, \quad j^\mu = (j^0, \mathbf{j}).\) To make \(\mathbf{j}\) agree with \(\mathbf{j}_s,\) \(\alpha\) is chosen to be \(\alpha = -\frac{\hbar}{2mc}.\) So,

\[\rho = \frac{j^0}{c} = \frac{i\hbar}{2mc^2}\left(\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right). \tag{52}\]

\(\rho\) does reduce to \(\rho_s = \Psi^*\Psi\) in the non-relativistic limit. However, \(\rho\) is not positive-definite and hence can not describe a probability density for a single particle.

Pauli and Weisskopf in 1934 showed that Klein-Gordon equation describes a spin-0 (scalar) field. \(\rho\) and \(\mathbf{j}\) are interpreted as charge and current density of the particles in the field.


4 Dirac Equation

To solve the negative probability density problem of the Klein-Gordon equation, people were looking for an equation which is first order in $\partial/\partial t$. Such an equation is found by Dirac.

It is difficult to take the square root of $-\hbar^2 c^2 \nabla^2 + m^2 c^4$ for a single wave function. One can take the inspiration from E&M: Maxwell’s equations are first-order but combining them gives the second order wave equations.

Imagining that $\psi$ consists of $N$ components $\psi_l$,

$$\frac{1}{c} \frac{\partial \psi}{\partial t} + \sum_{k=1}^{3} \sum_{n=1}^{N} \alpha_{lk} \frac{\partial \psi_n}{\partial x^k} + \frac{imc}{\hbar} \sum_{n=1}^{N} \beta_{ln} \psi_n = 0,$$

where $l = 1, 2, \ldots, N$, and $x^k = x, y, z$, $k = 1, 2, 3$.

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix},$$

and $\alpha^k, \beta$ are $N \times N$ matrices. Using the matrix notation, we can write the equations as

$$\frac{1}{c} \frac{\partial \psi}{\partial t} + \alpha \cdot \nabla \psi + \frac{imc}{\hbar} \beta \psi = 0,$$

where $\alpha = \alpha^1 \hat{x} + \alpha^2 \hat{y} + \alpha^3 \hat{z}$. $N$ components of $\psi$ describe a new degree of freedom just as the components of the Maxwell field describe the polarization of the light quantum. In this case, the new degree of freedom is the spin of the particle and $\psi$ is called a spinor.

We would like to have positive-definite and conserved probability, $\rho = \psi^\dagger \psi$, where $\psi^\dagger$ is the hermitian conjugate of $\psi$ (so is a row matrix). Taking the hermitian conjugate of Eq. (55),

$$\frac{1}{c} \frac{\partial \psi^\dagger}{\partial t} + \nabla \psi^\dagger \cdot \alpha^\dagger - \frac{imc}{\hbar} \psi^\dagger \beta^\dagger = 0.$$

Multiplying the above equation by $\psi$ and then adding it to $\psi^\dagger \times$ (55), we obtain

$$\frac{1}{c} \left( \psi^\dagger \frac{\partial \psi}{\partial t} + \frac{\partial \psi^\dagger}{\partial t} \psi \right) + \nabla \psi^\dagger \cdot \alpha^\dagger \psi + \psi^\dagger \alpha \cdot \nabla \psi + \frac{imc}{\hbar} (\psi^\dagger \beta \psi - \psi^\dagger \beta^\dagger \psi) = 0.$$  

The continuity equation

$$\frac{\partial}{\partial t} (\psi^\dagger \psi) + \nabla \cdot j = 0$$
can be obtained if $\alpha^\dagger = \alpha$, $\beta^\dagger = \beta$, then

$$\frac{1}{c} \frac{\partial}{\partial t} (\psi^\dagger \psi) + \nabla \cdot (\psi^\dagger \alpha \psi) = 0 \quad (59)$$

with

$$j = c \psi^\dagger \alpha \psi. \quad (60)$$

From Eq. (55) we can obtain the Hamiltonian,

$$H \psi = i \hbar \frac{\partial \psi}{\partial t} = \left( c \nabla \cdot \frac{\hbar}{i} \nabla + \beta mc^2 \right) \psi. \quad (61)$$

One can see that $H$ is hermitian if $\alpha$, $\beta$ are hermitian.

To derive properties of $\alpha$, $\beta$, we multiply Eq. (55) by the conjugate operator,

$$\left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \alpha^i \alpha^j \partial_i \partial_j + \frac{m^2 c^2}{\hbar^2} \beta^2 - \frac{i mc}{\hbar} (\beta \alpha^i + \alpha^i \beta) \partial_i \right] \psi = 0 \quad (62)$$

We can rewrite $\alpha^i \alpha^j \partial_i \partial_j$ as $\frac{1}{2} (\alpha^i \alpha^j + \alpha^j \alpha^i) \partial_i \partial_j$. Since it’s a relativistic system, the second order equation should coincide with the Klein-Gordon equation. Therefore, we must have

$$\alpha^i \alpha^j + \alpha^j \alpha^i = 2 \delta^{ij} \mathbb{I} \quad (63)$$
$$\beta \alpha^i + \alpha^i \beta = 0 \quad (64)$$
$$\beta^2 = \mathbb{I} \quad (65)$$

Because

$$\beta \alpha^i = -\alpha^i \beta = (-\mathbb{I}) \alpha^i \beta, \quad (66)$$

if we take the determinant of the above equation,

$$\det \beta \det \alpha^i = (-1)^N \det \alpha^i \det \beta, \quad (67)$$

we find that $N$ must be even. Next, we can rewrite the relation as

$$(\alpha^i)^{-1} \beta \alpha^i = -\beta \quad \text{(no summation)}. \quad (68)$$

Taking the trace,

$$\text{Tr} \left[ (\alpha^i)^{-1} \beta \alpha^i \right] = \text{Tr} \left[ (\alpha^i \alpha^i)^{-1} \beta \right] = \text{Tr}[\beta] = \text{Tr}[-\beta], \quad (69)$$

we obtain $\text{Tr}[\beta] = 0$. Similarly, one can derive $\text{Tr}[\alpha^i] = 0$. 


Covariant form of the Dirac equation

Define

\[ \gamma^0 = \beta, \]
\[ \gamma^j = \beta \alpha^j, \quad j = 1, 2, 3 \]
\[ \gamma^\mu = (\gamma^0, \gamma^1, \gamma^2, \gamma^3), \quad \gamma_\mu = g_{\mu\nu}\gamma^\nu \]

(70)

Multiply Eq. (55) by \( i\beta \),

\[ i\beta \times \left( \frac{1}{c} \frac{\partial}{\partial t} + \alpha \cdot \nabla + \frac{imc}{\hbar} \beta \right) \psi = 0 \]

\[ \Rightarrow \left( i\gamma^0 \frac{\partial}{\partial x^0} + i\gamma^j \frac{\partial}{\partial x^j} - \frac{mc}{\hbar} \right) \psi = \left( i\gamma^\mu \partial_\mu - \frac{mc}{\hbar} \right) \psi = 0 \]

(71)

Using the short-hand notation: \( \gamma^\mu \partial_\mu \equiv \partial, \gamma^\mu A_\mu \equiv A, \)

\[ \left( i \partial - \frac{mc}{\hbar} \right) \psi = 0 \]

(72)

From the properties of the \( \alpha^j \) and \( \beta \) matrices, we can derive

\[ \gamma^{0\dagger} = \gamma^0, \quad \text{(hermitian)} \]
\[ \gamma^{j\dagger} = (\beta \alpha^j)^\dagger = \alpha^{j\dagger} \beta^\dagger = \alpha^j \beta = -\beta \alpha^j = -\gamma^j, \quad \text{(anti-hermitian)} \]
\[ \gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0, \]
\[ \gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu} I. \quad \text{(Clifford algebra).} \]

(73-76)

Conjugate of the Dirac equation is given by

\[ -i\partial_\mu \psi^\dagger \gamma^{\mu\dagger} - \frac{mc}{\hbar} \psi^\dagger = 0 \]

\[ \Rightarrow -i\partial_\mu \psi^\dagger \gamma^0 \gamma^\mu \gamma^0 - \frac{mc}{\hbar} \psi^\dagger = 0 \]

(77)

We will define the Dirac adjoint spinor \( \bar{\psi} \) by \( \bar{\psi} \equiv \psi^\dagger \gamma^0 \). Then

\[ i\partial_\mu \bar{\psi} \gamma^\mu + \frac{mc}{\hbar} \bar{\psi} = 0. \]

(78)

The four-current is

\[ \frac{j^\mu}{c} = \bar{\psi} \gamma^\mu \psi = \left( \rho, \frac{j}{c} \right), \quad \partial_\mu j^\mu = 0. \]

(79)
Properties of the $\gamma^\mu$ matrices

We may form new matrices by multiplying $\gamma$ matrices together. Because different $\gamma$ matrices anticommute, we only need to consider products of different $\gamma$’s and the order is not important. We can combine them in $2^4 - 1$ ways. Plus the identity we have 16 different matrices,

\[
I \\
\gamma^0, i\gamma^1, i\gamma^2, i\gamma^3 \\
\gamma^0\gamma^1, \gamma^0\gamma^2, \gamma^0\gamma^3, i\gamma^2\gamma^3, i\gamma^3\gamma^1, i\gamma^1\gamma^2 \\
i\gamma^0\gamma^2\gamma^3, i\gamma^0\gamma^3\gamma^1, i\gamma^0\gamma^1\gamma^2, \gamma^1\gamma^2\gamma^3 \\
i\gamma^0\gamma^1\gamma^2\gamma^3 \equiv \gamma_5 (= \gamma^5).
\]

(80)

Denoting them by $\Gamma_l, l = 1, 2, \cdots, 16$, we can derive the following relations.

(a) $\Gamma_l\Gamma_m = a_{lm}\Gamma_n$, $a_{lm} = \pm 1$ or $\pm i$.

(b) $\Gamma_l\Gamma_m = I$ if and only if $l = m$.

(c) $\Gamma_l\Gamma_m = \pm \Gamma_m\Gamma_l$.

(d) If $\Gamma_l \neq I$, there always exists a $\Gamma_k$, such that $\Gamma_k\Gamma_l\Gamma_k = -\Gamma_l$.

(e) $\text{Tr}(\Gamma_l) = 0$ for $\Gamma_l \neq I$.

Proof:

\[
\text{Tr}(\Gamma_l) = \text{Tr}(\Gamma_k\Gamma_l\Gamma_k) = \text{Tr}(\Gamma_I\Gamma_k\Gamma_k) = \text{Tr}(\Gamma_I)
\]

(f) $\Gamma_l$ are linearly independent: $\sum_{k=1}^{16} x_k\Gamma_k = 0$ only if $x_k = 0, k = 1, 2, \cdots, 16$.

Proof:

\[
\left(\sum_{k=1}^{16} x_k\Gamma_k\right)\Gamma_m = x_m I + \sum_{k\neq m} x_k\Gamma_k\Gamma_m = x_m I + \sum_{k\neq m} x_k a_{km}\Gamma_n = 0 (\Gamma_n \neq I)
\]

. Taking the trace, $x_m\text{Tr}(I) = -\sum_{k\neq m} x_k a_{km}\text{Tr}(\Gamma_n) = 0 \Rightarrow x_m = 0$ for any $m$. This implies that $\Gamma_k$’s cannot be represented by matrices smaller than $4 \times 4$. In fact, the smallest representations of $\Gamma_k$’s are $4 \times 4$ matrices. (Note that this 4 is not the dimension of the space-time. the equality is accidental.)

(g) Corollary: any $4 \times 4$ matrix $X$ can be written uniquely as a linear combination of the $\Gamma_k$’s.

\[
X = \sum_{k=1}^{16} x_k\Gamma_k \\
\text{Tr}(X\Gamma_m) = x_m\text{Tr}(\Gamma_m\Gamma_m) + \sum_{k \neq m} x_k\text{Tr}(\Gamma_k\Gamma_m) = x_m\text{Tr}(I) = 4x_m \\
x_m = \frac{1}{4}\text{Tr}(x\Gamma_m)
\]
(h) Stronger corollary: \( \Gamma_l \Gamma_m = a_{lm} \Gamma_n \) where \( \Gamma_n \) is a different \( \Gamma_n \) for each \( m \), given a fixed \( l \).

Proof: If it were not true and one can find two different \( \Gamma_m, \Gamma_{m'} \) such that \( \Gamma_l \Gamma_m = a_{lm} \Gamma_n, \Gamma_l \Gamma_{m'} = a_{lm'} \Gamma_n \), then we have

\[
\Gamma_m = a_{lm} \Gamma_l \Gamma_n, \Gamma_{m'} = a_{lm'} \Gamma_l \Gamma_n \Rightarrow \Gamma_m = \frac{a_{lm}}{a_{lm'}} \Gamma_{m'},
\]

which contradicts that \( \gamma_k \)'s are linearly independent.

(i) Any matrix \( X \) that commutes with \( \gamma^\mu \) (for all \( \mu \)) is a multiple of the identity.

Proof: Assume \( X \) is not a multiple of the identity. If \( X \) commutes with all \( \gamma^\mu \) then it commutes with all \( \Gamma_i \)'s, i.e., \( X = \Gamma_i X \Gamma_i \). We can express \( X \) in terms of the \( G \) matrices,

\[
X = x_m \Gamma_m + \sum_{k \neq m} x_k \Gamma_k, \quad \Gamma_m \neq I.
\]

There exists a \( \Gamma_i \) such that \( \Gamma_i \Gamma_m \Gamma_i = -\Gamma_m \). By the hypothesis that \( X \) commutes with this \( \Gamma_i \), we have

\[
X = x_m \Gamma_m + \sum_{k \neq m} x_k \Gamma_k = \Gamma_i X \Gamma_i.
\]

\[
= x_m \Gamma_i \Gamma_m \Gamma_i + \sum_{k \neq m} x_k \Gamma_i \Gamma_k \Gamma_i
\]

\[
= -x_m \Gamma_m + \sum_{k \neq m} \pm x_k \Gamma_k.
\]

Since the expansion is unique, we must have \( x_m = -x_m \). \( \Gamma_m \) was arbitrary except that \( \Gamma_m \neq I \). This implies that all \( x_m = 0 \) for \( \Gamma_m \neq I \) and hence \( X = aI \).

(j) Pauli’s fundamental theorem: Given two sets of \( 4 \times 4 \) matrices \( \gamma^\mu \) and \( \gamma'^\mu \) which both satisfy \( \{ \gamma^\mu, \gamma^\nu \} = 2g^{\mu \nu} I \), there exists a nonsingular matrix \( S \) such that

\[
\gamma'^\mu = S \gamma^\mu S^{-1}.
\]

Proof: \( F \) is an arbitrary \( 4 \times 4 \) matrix, set \( \Gamma_i \) is constructed from \( \gamma^\mu \) and \( \Gamma'_i \) is constructed from \( \gamma'^\mu \). Let

\[
S = \sum_{i=1}^{16} \Gamma'_i F \Gamma_i.
\]

\[
\Gamma_i \Gamma_j = a_{ij} \Gamma_k
\]

\[
\Gamma_i \Gamma_j \Gamma_i \Gamma_j = a_{ij}^2 \Gamma_k = a_{ij}^2
\]

\[
\Gamma_i \Gamma_j \Gamma_j \Gamma_i = \Gamma_j \Gamma_i = a_{ij} \Gamma_i \Gamma_j = a_{ij} \Gamma_k
\]

\[
\Gamma'_i \Gamma'_j = a_{ij} \Gamma'_k
\]

\[
\Gamma'_i \Gamma'_j = a_{ij} \Gamma'_k
\]

12
For any \( i \),
\[
\Gamma_i S \Gamma_i = \sum_j \Gamma_j \gamma_j F \Gamma_j \Gamma_i = \sum_j a_{ij}^4 \Gamma_k F \Gamma_k = \sum_j \Gamma_k F \Gamma_k = S, \quad (a_{ij}^4 = 1).
\]

It remains only to prove that \( S \) is nonsingular.
\[
S' = \sum_{i=1}^{16} \Gamma_i G \Gamma_i', \quad \text{for } G \text{ arbitrary.}
\]

By the same argument, we have \( S' = \Gamma_i S' \Gamma_i' \).
\[
S'S = \Gamma_i S' \Gamma_i' \Gamma_i S = \Gamma_i S' \Gamma_i.
\]

\( S'S \) commutes with \( \Gamma_i \) for any \( i \) so \( S'S = aI \). We can choose \( a \neq 0 \) because \( F, G \) are arbitrary, then \( S \) is nonsingular. Also, \( S \) is unique up to a constant. Otherwise if we had \( S_1 \gamma^\mu S_1^{-1} = S_2 \gamma^\mu S_2^{-1} \), then \( S_2^{-1} S_1 \gamma^\mu = \gamma^\mu S_2^{-1} S_1 \Rightarrow S_2^{-1} S_1 = aI \).

**Specific representations of the \( \gamma^\mu \) matrices**

Recall \( H = (-c\alpha(i\hbar \nabla + \beta mc^2)) \). In the non-relativistic limit, \( mc^2 \) term dominates the total energy, so it’s convenient to represent \( \beta = \gamma^0 \) by a diagonal matrix. Recall \( \text{Tr} \beta = 0 \) and \( \beta^2 = I \), so we choose
\[
\beta = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \quad \text{where } I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.
\]

\( \alpha^k \)'s anticommute with \( \beta \) and are hermitian,
\[
\alpha^k = \begin{pmatrix} 0 & A^k \\ (A^k)^\dagger & 0 \end{pmatrix},
\]
\[A^k: 2 \times 2 \text{ matrices, anticommute with each other. These properties are satisfied by the Pauli matrices, so we have}
\]
\[
\alpha^k = \begin{pmatrix} 0 & \sigma^k \\ \sigma^k & 0 \end{pmatrix}, \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

From these we obtain
\[
\gamma^0 = \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \gamma^i = \beta \alpha^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}, \quad \gamma_5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}.
\]

This is the “Pauli-Dirac” representation of the \( \gamma^\mu \) matrices. It’s most useful for system with small kinetic energy, e.g., atomic physics.

Let’s consider the simplest possible problem: free particle at rest. \( \psi \) is a 4-component wave-function with each component satisfying the Klein-Gordon equation,
\[
\psi = \chi e^{i(p_0 x - Et)}, \quad (85)
\]

\[13\]
where $\chi$ is a 4-component spinor and $E^2 = p^2 c^2 + m^2 c^4$.

Free particle at rest: $p = 0$, $\psi$ is independent of $x$,

$$H\psi = (-i\hbar c \mathbf{\alpha} \cdot \nabla + mc^2 \gamma^0)\psi = mc^2 \gamma^0 \psi = E\psi. \quad (86)$$

In Pauli-Dirac representation, $\gamma^0 = \text{diag}(1, 1, -1, -1)$, the 4 fundamental solutions are

$$\chi_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = mc^2,$$

$$\chi_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad E = mc^2,$$

$$\chi_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad E = -mc^2,$$

$$\chi_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E = -mc^2.$$

As we shall see, Dirac wavefunction describes a particle of spin-1/2. $\chi_1, \chi_2$ represent spin-up and spin-down respectively with $E = mc^2$. $\chi_3, \chi_4$ represent spin-up and spin-down respectively with $E = -mc^2$. As in Klein-Gordon equation, we have negative solutions and they cannot be discarded.

For ultra-relativistic problems (most of this course), the “Weyl” representation is more convenient.

$$\psi_{\text{PD}} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}, \quad \psi_A = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad \psi_B = \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix}. \quad (87)$$

In terms of $\psi_A$ and $\psi_B$, the Dirac equation is

$$i \frac{\partial}{\partial x^0} \psi_A + i \mathbf{\sigma} \cdot \nabla \psi_B = \frac{mc}{\hbar} \psi_A,$$

$$-i \frac{\partial}{\partial x^0} \psi_B - i \mathbf{\sigma} \cdot \nabla \psi_A = \frac{mc}{\hbar} \psi_B. \quad (88)$$

Let’s define

$$\psi_A = \frac{1}{\sqrt{2}} (\phi_1 + \phi_2), \quad \psi_B = \frac{1}{\sqrt{2}} (\phi_2 - \phi_1). \quad (89)$$
and rewrite the Dirac equation in terms of $\phi_1$ and $\phi_2$,

\[
\begin{align*}
    i \frac{\partial}{\partial x^0} \phi_1 - i \sigma \cdot \nabla \phi_1 & = \frac{mc}{\hbar} \phi_2, \\
    i \frac{\partial}{\partial x^0} \phi_2 + i \sigma \cdot \nabla \phi_2 & = \frac{mc}{\hbar} \phi_1.
\end{align*}
\]  

(90)

On can see that $\phi_1$ and $\phi_2$ are coupled only via the mass term. In ultra-relativistic limit (or for nearly massless particle such as neutrinos), rest mass is negligible, then $\phi_1$ and $\phi_2$ decouple,

\[
\begin{align*}
    i \frac{\partial}{\partial x^0} \phi_1 - i \sigma \cdot \nabla \phi_1 & = 0, \\
    i \frac{\partial}{\partial x^0} \phi_2 + i \sigma \cdot \nabla \phi_2 & = 0.
\end{align*}
\]  

(91)

The 4-component wavefunction in the Weyl representation is written as

\[
    \psi_{\text{Weyl}} = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}.
\]  

(92)

Let’s imagine that a massless spin-1/2 neutrino is described by $\phi_1$, a plane wave state of a definite momentum $p$ with energy $E = |p|c$,

\[
\phi_1 \propto e^{i(p \cdot x - Et)}. 
\]  

(93)

\[
\begin{align*}
    i \frac{\partial}{\partial x^0} \phi_1 & = \frac{1}{c} \frac{\partial}{\partial t} \phi_1 = \frac{E}{\hbar c} \phi_1, \\
    i \sigma \cdot \nabla \phi_1 & = -\frac{1}{\hbar} \sigma \cdot p \phi_1 \\
    \Rightarrow E \phi_1 & = |p|c \phi_1 = -c \sigma \cdot p \phi_1 \quad \text{or} \quad \sigma \cdot p |p| \phi_1 = -\phi_1.
\end{align*}
\]  

(94)

The operator $h = \sigma \cdot p / |p|$ is called the “helicity.” Physically it refers to the component of spin in the direction of motion. $\phi_1$ describes a neutrino with helicity $-1$ (“left-handed”). Similarly,

\[
\frac{\sigma \cdot p}{|p|} \phi_2 = \phi_2, \quad (h = +1, \ \text{“right-handed”}).
\]  

(95)

The $\gamma^\mu$’s in the Weyl representation are

\[
\gamma^0 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix}.
\]  

(96)

Exercise: Find the $S$ matrix which transform between the Pauli-Dirac representation and the Weyl representation and verify that the $g\alpha^\mu$ matrices in the Weyl representation are correct.
5 Lorentz Covariance of the Dirac Equation

We will set $\hbar = c = 1$ from now on.

In E&M, we write down Maxwell’s equations in a given inertial frame, $x, t$, with the electric and magnetic fields $E, B$. Maxwell's equations are covariant with respect to Lorentz transformations, i.e., in a new Lorentz frame, $x', t'$, the equations have the same form, but the fields $E'(x', t'), B'(x', t')$ are different.

Similarly, Dirac equation is Lorentz covariant, but the wavefunction will change when we make a Lorentz transformation. Consider a frame $F$ with an observer $O$ and coordinates $x^\mu$. $O$ describes a particle by the wavefunction $\psi(x^\mu)$ which obeys

$$\left(i\gamma^\mu \frac{\partial}{\partial x^\mu} - m\right) \psi(x^\mu). \tag{97}$$

In another inertial frame $F'$ with an observer $O'$ and coordinates $x'^\nu$ given by

$$x'^\nu = \Lambda^\nu_\mu x^\mu, \tag{98}$$

$O'$ describes the same particle by $\psi'(x'^\nu)$ and $\psi'(x'^\nu)$ satisfies

$$\left(i\gamma^\nu \frac{\partial}{\partial x'^\nu} - m\right) \psi'(x'^\nu). \tag{99}$$

Lorentz covariance of the Dirac equation means that the $\gamma$ matrices are the same in both frames.

What is the transformation matrix $S$ which takes $\psi$ to $\psi'$ under the Lorentz transformation?

$$\psi'(\Lambda x) = S\psi(x). \tag{100}$$

Applying $S$ to Eq. (97),

$$iS\gamma^\mu S^{-1} \frac{\partial}{\partial x^\mu} S\psi(x^\mu) - mS\psi(x^\mu) = 0$$

$$\Rightarrow iS\gamma^\mu S^{-1} \frac{\partial}{\partial x'^\nu} \psi'(x'^\nu) - m\psi'(x'^\nu) = 0. \tag{101}$$

Using

$$\frac{\partial}{\partial x^\mu} = \frac{\partial}{\partial x'^\nu} \frac{\partial x'^\nu}{\partial x^\mu} = \Lambda^\nu_\mu \frac{\partial}{\partial x'^\nu}, \tag{102}$$

we obtain

$$iS\gamma^\mu S^{-1} \Lambda^\nu_\mu \frac{\partial}{\partial x'^\nu} \psi'(x'^\nu) - m\psi'(x'^\nu) = 0. \tag{103}$$

Comparing it with Eq. (99), we need

$$S\gamma^\mu S^{-1} \Lambda^\nu_\mu = \gamma^\nu \quad \text{or equivalently} \quad S\gamma^\mu S^{-1} = (\Lambda^{-1})^\mu_\nu \gamma^\nu. \tag{104}$$
We will write down the form of the $S$ matrix without proof. You are encouraged to read the derivation in Shulten’s notes Chapter 10, p.319-321 and verify it by yourself.

For an infinitesimal Lorentz transformation, $\Lambda^\mu_\nu = \delta^\mu_\nu + \epsilon^\mu_\nu$. Multiplied by $g^{\nu\lambda}$ it can be written as

$$\Lambda^{\mu\lambda} = g^{\mu\lambda} + \epsilon^{\mu\lambda}, \quad (105)$$

where $\epsilon^{\mu\lambda}$ is antisymmetric in $\mu$ and $\lambda$. Then the corresponding Lorentz transformation on the spinor wavefunction is given by

$$S(\epsilon^{\mu\nu}) = I - \frac{i}{4} \sigma_{\mu\nu} \epsilon^{\mu\nu}, \quad (106)$$

where

$$\sigma_{\mu\nu} = \frac{i}{2} (\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu) = \frac{i}{2} [\gamma_\mu, \gamma_\nu]. \quad (107)$$

For finite Lorentz transformation,

$$S = \exp \left( -\frac{i}{4} \sigma_{\mu\nu} \epsilon^{\mu\nu} \right). \quad (108)$$

Note that one can use either the active transformation (which transforms the object) or the passive transformation (which transforms the coordinates), but care should be taken to maintain consistency. We will mostly use passive transformations unless explicitly noted otherwise.

Example: Rotation about $z$-axis by $\theta$ angle (passive).

$$-\epsilon^{12} = +\epsilon^{21} = \theta, \quad (109)$$

$$\sigma_{12} = \frac{i}{2} [\gamma_1, \gamma_2] = i\gamma_1 \gamma_2$$

$$= i \begin{pmatrix} -i\sigma^3 & 0 \\ 0 & -i\sigma^3 \end{pmatrix}$$

$$= \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix} \equiv \Sigma_3 \quad (110)$$

$$S = \exp \left( +\frac{i}{2} \theta \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix} \right) = I \cos \frac{\theta}{2} + i \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix} \sin \frac{\theta}{2}. \quad (111)$$

We can see that $\psi$ transforms under rotations like an spin-1/2 object. For a rotation around a general direction $\hat{n}$,

$$S = I \cos \frac{\theta}{2} + i \hat{n} \cdot \Sigma \sin \frac{\theta}{2}. \quad (112)$$
Example: Boost in $\hat{x}$ direction (passive).

\[
e^{01} = -e^{10} = \eta, \tag{113}
\]

\[
\sigma_{01} = \frac{i}{2}[\gamma_0, \gamma_1] = i\gamma_0\gamma_1, \tag{114}
\]

\[
S = \exp\left(-\frac{i}{4}\sigma_{\mu\nu}e^{\mu\nu}\right) = \exp\left(-\frac{i}{2}\eta i\gamma_0\gamma_1\right)
\]

\[
= \exp\left(\frac{\eta}{2}\gamma_0\gamma_1\right) = \exp\left(-\frac{\eta}{2}\alpha^1\right)
\]

\[
= I \cosh \frac{\eta}{2} - \alpha^1 \sinh \frac{\eta}{2}, \tag{115}
\]

For a particle moving in the direction of $\hat{n}$ in the new frame, we need to boost the frame in the $-\hat{n}$ direction,

\[
S = I \cosh \frac{\eta}{2} + \alpha \cdot \hat{n} \sinh \frac{\eta}{2}. \tag{116}
\]

6 Free Particle Solutions to the Dirac Equation

The solutions to the Dirac equation for a free particle at rest are

\[
\psi_1 = \sqrt{\frac{2m}{V}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-imt}, \quad E = +m,
\]

\[
\psi_2 = \sqrt{\frac{2m}{V}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-imt}, \quad E = +m,
\]

\[
\psi_3 = \sqrt{\frac{2m}{V}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{imt}, \quad E = -m,
\]

\[
\psi_4 = \sqrt{\frac{2m}{V}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{imt}, \quad E = -m, \tag{117}
\]

where we have set $\hbar = c = 1$ and $V$ is the total volume. Note that I have chosen a particular normalization

\[
\int d^3x \psi^\dagger \psi = 2m \tag{118}
\]
for a particle at rest. This is more convenient when we learn field theory later, because $\psi^\dagger \psi$ is not invariant under boosts. Instead, it’s the zeroth component of a 4-vector, similar to $E$.

The solutions for a free particle moving at a constant velocity can be obtained by a Lorentz boost,

$$S = I \cosh \frac{\eta}{2} + \alpha \cdot \hat{n} \sinh \frac{\eta}{2}. \tag{119}$$

Using the Pauli-Dirac representation,

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix},$$

$$S = \begin{pmatrix} \cosh \frac{\eta}{2} & \hat{n} \cdot \sigma \sinh \frac{\eta}{2} \\ \sigma \cdot \hat{n} \sinh \frac{\eta}{2} & \cosh \frac{\eta}{2} \end{pmatrix}, \tag{120}$$

and the following relations,

$$\cosh \eta = \gamma' = \frac{E'}{m}, \quad \sinh \eta = \gamma' \beta',$$

$$\cosh \frac{\eta}{2} = \sqrt{1 + \cosh \eta} = \sqrt{1 + \gamma'} \frac{2}{\gamma'},$$

$$\sinh \frac{\eta}{2} = \sqrt{\cosh \frac{\eta - 1}{2}} = \sqrt{\cosh \frac{E' - m}{2m}}$$

$$-p'_\mu x'^\mu = p'_+ \cdot x' - E' t' = -p_\mu x^\mu = -mt, \tag{121}$$

where $p'_+ = |p'_+| \hat{n}$ is the 3-momentum of the positive energy state, we obtain

$$\psi'_1(x') = S \psi_1(x) = \sqrt{\frac{2m}{V}} \begin{pmatrix} \cosh \frac{\eta}{2} & 1 \\ \sigma \cdot \hat{n} \sinh \frac{\eta}{2} & 1 \end{pmatrix} e^{-imt}$$

$$= \frac{1}{\sqrt{V}} \sqrt{m + E'} \begin{pmatrix} 1 \\ \frac{E' - m}{E' + m} \sigma \cdot \hat{n} \end{pmatrix} e^{i(p'_+ \cdot x' - E't')},$$

$$= \frac{1}{\sqrt{V}} \sqrt{m + E'} \begin{pmatrix} 1 \\ \frac{E' - m}{E' + m} p'_+ \end{pmatrix} e^{i(p'_+ \cdot x' - E't')} \tag{122}$$

where we have used

$$\sqrt{\frac{E' - m}{E' + m}} = \frac{\sqrt{E'^2 - m^2}}{E' + m} = \frac{|p'_+|}{E' + m} \tag{123}$$

in the last line.
ψ′_2(x′) has the same form except that \(1\) is replaced by \(0\).

For the negative energy solutions \(E'_- = -E' = -\sqrt{|p'|^2 + m^2}\) and \(p'_- = v\hat{n}E'_- = -vE'\hat{n} = -p'_+\). So we have

\[
\psi'_3(x') = \frac{1}{\sqrt{V}} \sqrt{m + E'} \left( \begin{array}{c} \sigma p'_{E+m} \chi_{E+m, +} \\ 0 \end{array} \right) e^{i(p'_- \cdot x' + E't')},
\]

(124)

and \(\psi'_4(x')\) is obtained by the replacement \(\begin{array}{c} 1 \\ 0 \end{array} \rightarrow \begin{array}{c} 0 \\ 1 \end{array}\).

Now we can drop the primes and the ± subscripts,

\[
\psi_{1,2} = \frac{1}{\sqrt{V}} \sqrt{E + m} \left( \begin{array}{c} \chi^+_{E+m, +} \\ \sigma p_{E+m} \chi_{E+m, +} \end{array} \right) e^{i(p \cdot x - Et)} = \frac{1}{\sqrt{V}} u_{1,2} e^{i(p \cdot x - Et)},
\]

\[
\psi_{3,4} = \frac{1}{\sqrt{V}} \sqrt{E + m} \left( \begin{array}{c} -\sigma p_{E+m} \chi_{E+m, -} \\ \chi_{E+m, -} \end{array} \right) e^{i(p \cdot x + Et)} = \frac{1}{\sqrt{V}} u_{3,4} e^{i(p \cdot x + Et)},
\]

(125)

where

\[
\chi_+ = \begin{array}{c} 1 \\ 0 \end{array}, \quad \chi_- = \begin{array}{c} 0 \\ 1 \end{array}
\]

(126)

\((V\) is the proper volume in the frame where the particle is at rest.)

**Properties of spinors** \(u_1, \ldots, u_4\)

\[
u^*_r u_s = 0 \quad \text{for} \quad r \neq s.
\]

(127)

\[
u^*_1 u_1 = (E + m) \left( \begin{array}{c} \chi^+_{E+m} \\ \sigma p_{E+m} \chi_{E+m, +} \end{array} \right) e^{i(p \cdot x - Et)}
\]

\[
= (E + m) \chi^+_E + \frac{\sigma p(E + m)}{(E + m)^2} \chi_+.
\]

(128)

Using the following identity:

\[
(\sigma \cdot a)(\sigma \cdot b) = \sigma_i a_i \sigma_j b_j = (\delta_{ij} + i\epsilon_{ijk}a_k)b_j = a \cdot b + i\sigma \cdot (a \times b),
\]

(129)

we have

\[
u^*_1 u_1 = (E + m) \chi_{E+m}^+ \left( 1 + \frac{|p|^2}{(E + m)^2} \right) \chi_+
\]

\[
= (E + m) \chi_{E+m}^+ \frac{E^2 + 2Em + m^2 + |p|^2}{(E + m)^2} \chi_+
\]

\[
= \chi_+ \frac{2E^2 + 2Em}{E + m} \chi_+
\]

\[
= 2E \chi_{E+m}^+ \chi_+ = 2E.
\]

(130)
Similarly for other $u_r$ we have $u_r^\dagger u_s = \delta_{rs}2E$, which reflects that $\rho = \psi^\dagger\psi$ is the zeroth component of a 4-vector.

One can also check that
\[
\overline{u}_r u_s = \pm 2m\delta_{rs}
\]  
where $+$ for $r = 1, 2$ and $-$ for $r = 3, 4$.

\begin{align}
\overline{u}_1 u_1 &= u_1^\dagger \gamma^0 u_1 \\
\gamma^0 &= \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \\
&= (E + m)\chi_+^\dagger \left( 1 - \frac{|p|^2}{(E + m)^2} \right) \chi_+ \\
&= (E + m)\chi_+^\dagger \frac{E^2 + 2Em + m^2 - |p|^2}{(E + m)^2} \chi_+ \\
&= \chi_+ \frac{2m^2 + 2Em}{E + m} \chi_+ \\
&= 2m\chi_+^\dagger \chi_+ = 2m
\end{align}

is invariant under Lorentz transformation.

**Orbital angular momentum and spin**

Orbital angular momentum
\[
L = r \times p \quad \text{or} \quad L_i = \epsilon_{ijk}r_jp_k.
\]  
(We don’t distinguish upper and lower indices when dealing with space dimensions only.)

\[
\frac{dL_i}{dt} = i[H, L_i] \\
= i[c\alpha \cdot p + \beta mc^2, L_i] \\
= ic\alpha_n[p_n, \epsilon_{ijk}r_jp_k] \\
= ic\alpha_n\epsilon_{ijk}[p_n, r_j]p_k \\
= ic\alpha_n\epsilon_{ijk}(-i\delta_{nj}\hbar)p_k \\
= c\hbar\epsilon_{ijk}\alpha_jp_k \\
= c\hbar(\alpha \times p)_i \neq 0.
\]  
(134)

We find that the orbital angular momentum of a free particle is not a constant of the motion.
Consider the spin $\frac{1}{2} \Sigma = \frac{1}{2} \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}$,

$$\frac{d \Sigma_i}{dt} = i[H, \Sigma_i]$$

$$= i[\alpha_j, \Sigma_i]p_j$$

$$= ic[\alpha_j, \Sigma_i]p_j$$

$$= ic\gamma_5(\Sigma_j, \Sigma_i)p_j$$

$$= ic\gamma_5(-2i\epsilon_{ijk}\Sigma_k)p_j$$

$$= 2c\gamma_5\epsilon_{ijk}\Sigma_kp_j$$

$$= 2\epsilon_{ijk}\alpha_kp_j$$

$$= -2c(\alpha \times p)_i.$$  \hspace{1cm} (135)

Comparing it with Eq. (134), we find

$$\frac{d(L_i + \frac{1}{2}h\Sigma_i)}{dt} = 0,$$ \hspace{1cm} (136)

so the total angular momentum $J = L + \frac{1}{2}h\Sigma$ is conserved.

### 7 Interactions of a Relativistic Electron with an External Electromagnetic Field

We make the usual replacement in the presence of external potential:

$$E \rightarrow E - e\phi = ih\frac{\partial}{\partial t} - e\phi, \quad e < 0 \text{ for electron}$$

$$p \rightarrow p - \frac{e}{c}A = -ih\nabla - \frac{e}{c}A.$$ \hspace{1cm} (137)

In covariant form,

$$\partial_{\mu} \rightarrow \partial_{\mu} + \frac{ie}{\hbar c}A_{\mu} \rightarrow \partial_{\mu} + ieA_{\mu} \quad \hbar = c = 1.$$ \hspace{1cm} (138)

Dirac equation in external potential:

$$i\gamma^\mu(\partial_{\mu} + ieA_{\mu})\psi - m\psi = 0.$$ \hspace{1cm} (139)

Two component reduction of Dirac equation in Pauli-Dirac basis:

$$\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} (E - e\phi) \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} - \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} (p - eA) \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} - m \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = 0,$$

$$\Rightarrow (E - e\phi)\psi_A - \sigma \cdot (p - eA)\psi_B - m\psi_A = 0$$ \hspace{1cm} (140)

$$-(E - e\phi)\psi_B + \sigma \cdot (p - eA)\psi_A - m\psi_B = 0$$ \hspace{1cm} (141)
where $E$ and $p$ represent the operators $i\partial_t$ and $-i\nabla$ respectively. Define $W = E - m$, $\pi = p - eA$, then we have

\[ \begin{align*}
\sigma \cdot \pi \psi_B &= (W - e\phi)\psi_A \quad (142) \\
\sigma \cdot \pi \psi_A &= (2m + W - e\phi)\psi_B \quad (143)
\end{align*} \]

From Eq. (143),

\[ \psi_B = (2m + W - e\phi)^{-1}\sigma \cdot \pi \psi_A. \quad (144) \]

Substitute it into Eq. (142),

\[ \frac{(\sigma \cdot \pi)(\sigma \cdot \pi)}{2m + W - e\phi} \psi_A = (W - e\phi)\psi_A. \quad (145) \]

In non-relativistic limit, $W - e\phi \ll m$,

\[ \frac{1}{2m + W - e\phi} = \frac{1}{2m} \left( 1 - \frac{W - e\phi}{2m} + \cdots \right). \quad (146) \]

In the lowest order approximation we can keep only the leading term $\frac{1}{2m}$,

\[ \frac{1}{2m}(\sigma \cdot \pi)(\sigma \cdot \pi)\psi_A \simeq (W - e\phi)\psi_A. \quad (147) \]

Using Eq. (129),

\[ (\sigma \cdot \pi)(\sigma \cdot \pi)\psi_A = [\pi \cdot \pi + i\sigma \cdot (\pi \times \pi)]\psi_A. \quad (148) \]

\[ (\pi \times \pi)\psi_A = [(p - eA) \times (p - eA)]\psi_A \\
= [-eA \times p - ep \times A]\psi_A \\
= [ieA \times \nabla + ie\nabla \times A]\psi_A \\
= ie\psi_A(\nabla \times A) \\
= ieB\psi_A, \quad (149) \]

so

\[ \frac{1}{2m}(p - eA)^2\psi_A - e\frac{1}{2m}\sigma \cdot B\psi_A + e\phi\psi_A = W\psi_A. \quad (150) \]

Restoring $\hbar$, $c$,

\[ \frac{1}{2m}(p - \frac{e}{c}A)^2\psi_A - \frac{e\hbar}{2mc}\sigma \cdot B\psi_A + e\phi\psi_A = W\psi_A. \quad (151) \]

This is the “Pauli-Schrödinger equation” for a particle with the spin-magnetic moment,

\[ \mu = \frac{e\hbar}{2mc}\sigma = 2\frac{e}{2mc}S. \quad (152) \]
In comparison, the relation between the angular momentum and the magnetic moment of a classical charged object is given by

\[ \mu = \frac{I \pi r^2}{c} = e \frac{\omega}{2\pi} \frac{\pi r^2}{c} = \frac{e\omega r^2}{2c} = \frac{e}{2mc} m \omega r^2 = \frac{e}{2mc} L. \]  

(153)

We can write

\[ \mu = g_s \frac{e}{2mc} S \]  

(154)

in general. In Dirac theory, \( g_s = 2 \). Experimentally,

\[ g_s(e^-) = 2 \times (1.0011596521859 \pm 38 \times 10^{-13}). \]  

(155)

The deviation from 2 is due to radiative corrections in QED, \( (g - 2)/2 = \frac{\alpha}{2\pi} + \cdots \).

The predicted value for \( g_s - 2 \) using \( \alpha \) from the quantum Hall effect is

\[ (g_s - 2)_{qH}/2 = 0.0011596521564 \pm 229 \times 10^{-13}. \]  

(156)

They agree down to the \( 10^{-11} \) level.

There are also spin-1/2 particles with anomalous magnetic moments, e.g.,

\[ \mu_{\text{proton}} = 2.79 \frac{|e|}{2m_p c}, \quad \mu_{\text{neutron}} = -1.91 \frac{|e|}{2m_n c}. \]  

(157)

This can be described by adding the Pauli moment term to the Dirac equation,

\[ i\gamma^\mu (\partial_\mu + iqA_\mu) \psi - m\psi + k\sigma_{\mu\nu} F^{\mu\nu} \psi = 0. \]  

(158)

Recall

\[ \sigma_{\mu\nu} = \frac{i}{2} (\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu), \]

\[ \sigma_{0i} = i\gamma_0 \gamma_i = i \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} 0 & -\sigma^i \\ -\sigma^i & 0 \end{pmatrix} = i \begin{pmatrix} 0 & -\sigma^i \\ -\sigma^i & 0 \end{pmatrix} = -i\alpha^i, \]

\[ \sigma_{ij} = i\gamma_i \gamma_j = \epsilon_{ijk} \Sigma^k = \epsilon_{ijk} \begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}, \]

\[ F^{0i} = -E^i, \]

\[ F^{ij} = -\epsilon^{ijk} B^k. \]  

(159)

Then the Pauli moment term can be written as

\[ i\gamma^\mu (\partial_\mu + iqA_\mu) \psi - m\psi + 2ik \alpha \cdot E \psi - 2k \Sigma \cdot B \psi = 0. \]  

(160)

The two component reduction gives

\[ (E - q\phi) \psi_A - \sigma \cdot \pi \psi_B - m\psi_A + 2ik\sigma \cdot E \psi_B - 2k\sigma \cdot B \psi_A = 0, \]  

(161)

\[ -(E - q\phi) \psi_B + \sigma \cdot \pi \psi_A - m\psi_B + 2ik\sigma \cdot E \psi_A - 2k\sigma \cdot B \psi_B = 0. \]  

(162)
\[
\begin{align*}
(\sigma \cdot \pi - 2ik\sigma \cdot E)\psi_B &= (W - q\phi - 2k\sigma \cdot B)\psi_A, \quad (163) \\
(\sigma \cdot \pi + 2ik\sigma \cdot E)\psi_A &= (2m + W - q\phi + 2k\sigma \cdot B)\psi_B. \quad (164)
\end{align*}
\]

Again taking the non-relativistic limit,

\[
\psi_B \simeq \frac{1}{2m}(\sigma \cdot \pi + 2ik\sigma \cdot E)\psi_A, \quad (165)
\]

we obtain

\[
(W - q\phi - 2k\sigma \cdot B)\psi_A = \frac{1}{2m}(\sigma \cdot \pi - 2ik\sigma \cdot E)(\sigma \cdot \pi + 2ik\sigma \cdot E)\psi_A. \quad (166)
\]

Let’s consider two special cases.

(a) \( \phi = 0, \ E = 0 \)

\[
(W - 2k\sigma \cdot B)\psi_A = \frac{1}{2m}(\sigma \cdot \pi)^2 \psi_A
\]

\[
\Rightarrow \ W\psi_A = \frac{1}{2m}\pi^2 \psi_A - \frac{q}{2m}\sigma \cdot B\psi_A + 2k\sigma \cdot B\psi_A
\]

\[
\Rightarrow \ \mu = \frac{q}{2m} - 2k. \quad (167)
\]

(b) \( B = 0, \ E \neq 0 \) for the neutron \( q = 0 \)

\[
W\psi_A = \frac{1}{2m}\sigma \cdot (p + i\mu_n E) \sigma \cdot (p - i\mu_n E)\psi_A
\]

\[
= \frac{1}{2m}[(p + i\mu_n E) \cdot (p + i\mu_n E) + i\sigma \cdot (p + i\mu_n E) \times (p - i\mu_n E)] \psi_A
\]

\[
= \frac{1}{2m}\left[p^2 + \mu_n^2 E^2 + i\mu_n E \cdot p - i\mu_n p \cdot E + i\sigma \cdot (i\mu_n p \times E - i\mu_n E \times p)\right] \psi_A
\]

\[
= \frac{1}{2m}\left[p^2 + \mu_n^2 E^2 - \mu_n (\nabla \cdot E) + 2\mu_n \sigma \cdot (E \times p) + i\mu_n \sigma \cdot (\nabla \times E)\right] \psi_A
\]

\[
= \frac{1}{2m}\left[p^2 + \mu_n^2 E^2 - \mu_n p + 2\mu_n \sigma \cdot (E \times p)\right] \psi_A. \quad (168)
\]

The last term is the spin-orbit interaction,

\[
\sigma \cdot (E \times p) = -\frac{1}{r} \frac{d\phi}{dr} \sigma \cdot (r \times p) = -\frac{1}{r} \frac{d\phi}{dr} \sigma \cdot L. \quad (169)
\]

The second to last term gives an effective potential for a slow neutron moving in the electric field of an electron,

\[
V = -\frac{\mu_n p}{2m} = \frac{\mu_n}{2m}(-e)\delta^3(r). \quad (170)
\]

It’s called “Foldy” potential and does exist experimentally.
8 Foldy-Wouthuysen Transformation

We now have the Dirac equation with interactions. For a given problem we can solve for the spectrum and wavefunctions (ignoring the negative energy solutions for a moment), for instance, the hydrogen atom. We can compare the solutions to those of the Schrödinger equation and find out the relativistic corrections to the spectrum and the wavefunctions. In fact, the problem of hydrogen atom can be solved exactly. However, the exact solutions are problem-specific and involve unfamiliar special functions, hence they not very illuminating. You can find the exact solutions in many textbooks and also in Shulten’s notes. Instead, in this section we will develop a systematic approximation method to solve a system in the non-relativistic regime ($E - m \ll m$). It corresponds to take the approximation we discussed in the previous section to higher orders in a systematic way. This allows a physical interpretation for each term in the approximation and tells us the relative importance of various effects. Such a method has more general applications for different problems.

In Foldy-Wouthuysen transformation, we look for a unitary transformation $U_F$ removes operators which couple the large to the small components.

Odd operators (off-diagonal in Pauli-Dirac basis): $\alpha^i, \gamma^i, \gamma^5, \cdots$

Even operators (diagonal in Pauli-Dirac basis): $\mathbf{1}, \beta, \Sigma, \cdots$

$\psi' = U_F \psi = e^{iS} \psi, \quad S = \text{hermitian}$ (171)

First consider the case of a free particle, $H = \alpha \cdot \mathbf{p} + \beta m$ not time-dependent.

\[
\frac{i}{\hbar} \frac{\partial \psi'}{\partial t} = e^{iS} H \psi = e^{iS} H e^{-iS} \psi' = H' \psi'
\] (172)

We want to find $S$ such that $H'$ contains no odd operators. We can try

\[e^{iS} = e^{\beta \mathbf{p} \cdot \hat{\mathbf{p}} \sin \theta} = \cos \theta + \beta \mathbf{p} \cdot \hat{\mathbf{p}} \sin \theta, \quad \text{where } \hat{\mathbf{p}} = \mathbf{p}/|\mathbf{p}|.\] (173)

\[
H' = (\cos \theta + \beta \mathbf{p} \cdot \hat{\mathbf{p}} \sin \theta) (\mathbf{p} \cdot \mathbf{p} + \beta m) (\cos \theta - \beta \mathbf{p} \cdot \hat{\mathbf{p}} \sin \theta)^2
\]

\[
= (\mathbf{p} \cdot \mathbf{p} + \beta m) (\cos \theta - \beta \mathbf{p} \cdot \hat{\mathbf{p}} \sin \theta)^2
\]

\[
= (\mathbf{p} \cdot \mathbf{p} + \beta m) \exp (-2\beta \mathbf{p} \cdot \hat{\mathbf{p}} \theta)
\]

\[
= (\mathbf{p} \cdot \mathbf{p}) \left( \cos 2\theta - \frac{m}{|\mathbf{p}|} \sin 2\theta \right) + \beta (m \cos 2\theta + |\mathbf{p}| \sin 2\theta).\] (174)

To eliminate $(\mathbf{p} \cdot \mathbf{p})$ term we choose $\tan 2\theta = |\mathbf{p}|/m$, then

\[H' = \beta \sqrt{m^2 + |\mathbf{p}|^2}.\] (175)

This is the same as the first Hamiltonian we tried except for the $\beta$ factor which also gives rise to negative energy solutions. In practice, we need to expand the Hamiltonian for $|\mathbf{p}| \ll m$. 


General case:
\[ H = \alpha \cdot (p - eA) + \beta m + e\Phi \]
\[ = \beta m + O + \mathcal{E}, \quad (176) \]
\[ O = \alpha \cdot (p - eA), \quad \mathcal{E} = e\Phi, \quad \beta O = -O\beta, \quad \beta\mathcal{E} = \mathcal{E}\beta \]
\[ \quad (177) \]

\( H \) time-dependent \( \Rightarrow \) \( S \) time-dependent

We can only construct \( S \) with a non-relativistic expansion of the transformed Hamiltonian \( H' \) in a power series in \( 1/m \).

We’ll expand to \( \frac{p^4}{m^3} \) and \( \frac{p \times (E, B)}{m^2} \).

\[ H_\psi = i\frac{\partial}{\partial t} (e^{iS} \psi') = e^{-iS} i\frac{\partial \psi'}{\partial t} + \left( i\frac{\partial}{\partial t} e^{-iS} \right) \psi' \]
\[ \Rightarrow \frac{\partial \psi'}{\partial t} = e^{iS} \left( H - i\frac{\partial}{\partial t} \right) e^{-iS} \psi' = H'\psi' \quad (178) \]

\( S \) is expanded in powers of \( 1/m \) and is “small” in the non-relativistic limit.

\[ e^{iS}He^{-iS} = H + i[S, H] + \frac{i^2}{2!}[S, [S, H]] + \cdots + \frac{i^n}{n!}[S, [S, [S, H]]]. \quad (179) \]

\( S = O(\frac{1}{m}) \) to the desired order of accuracy

\[ H' = H + i[S, H] - \frac{1}{2}[S, [S, H]] - \frac{i}{6}[S, [S, [S, H]]] + \frac{1}{24}[S, [S, [S, [S, \beta m]]]] \]
\[ -\dot{S} - \frac{i}{2}[S, \dot{S}] + \frac{1}{6}[S, [S, \dot{S}]] \quad (180) \]

We will eliminate the odd operators order by order in \( 1/m \) and repeat until the desired order is reached.

First order \( [O(1)] \):
\[ H' = \beta m + \mathcal{E} + O + i[S, \beta m]. \quad (181) \]

To cancel \( O \), we choose \( S = -\frac{i\beta O}{2m} \).

\[ i[S, H] = -O + \frac{\beta}{2m} [O, \mathcal{E}] + \frac{1}{m} \beta O^2 \quad (182) \]
\[ \frac{i^2}{2}[S, [S, H]] = -\frac{\beta O^2}{2m} - \frac{1}{8m^2} [O, [O, \mathcal{E}]] - \frac{1}{2m^2} O^3 \quad (183) \]
\[ \frac{i^3}{3!}[S, [S, [S, H]]] = \frac{\beta O^3}{6m^2} - \frac{1}{6m^3} \beta O^4 \quad (184) \]
\[ \frac{i^4}{4!}[S, [S, [S, H]]]] = \frac{\beta O^4}{24m^3} \quad (185) \]
\[ -\dot{S} = \frac{i\beta \dot{O}}{2m} \quad (186) \]
\[ -\frac{i}{2}[S, \dot{S}] = -\frac{i}{8m^2} [O, \dot{O}] \quad (187) \]
Collecting everything,

\[ H' = \beta \left( m + \frac{\mathcal{O}^2}{2m} - \frac{\mathcal{O}^4}{8m^3} \right) + \mathcal{E} - \frac{1}{8m^2} [\mathcal{O}, [\mathcal{O}, \mathcal{E}]] - \frac{i}{8m^2} [\mathcal{O}, \hat{\mathcal{O}}] \]

\[ + \frac{\beta}{2m} [\mathcal{O}, \mathcal{E}] - \frac{\mathcal{O}^3}{3m^2} + \frac{i \beta \mathcal{O}}{2m} \]

\[ = \beta m + \mathcal{E}' + \mathcal{O}' \] \hfill (189)

Now \( \mathcal{O}' \) is \( O(\frac{1}{m}) \), we can transform \( H' \) by \( S' \) to cancel \( \mathcal{O}' \),

\[ S' = -\frac{i \beta}{2m} \mathcal{O}' = -\frac{i \beta}{2m} \left( \frac{\beta}{2m} [\mathcal{O}, \mathcal{E}] - \frac{\mathcal{O}^3}{3m^2} + \frac{i \beta \mathcal{O}}{2m} \right) \]

\[ \text{(190)} \]

After transformation with \( S' \),

\[ H'' = e^{iS'} \left( H' - i \frac{\partial}{\partial t} \right) e^{-iS'} = \beta m + \mathcal{E}' + \frac{\beta}{2m} [\mathcal{O}', \mathcal{E}'] + \frac{i \beta \mathcal{O}'}{2m} \]

\[ = \beta m + \mathcal{E}' + \mathcal{O}'', \] \hfill (191)

where \( \mathcal{O}'' \) is \( O(\frac{1}{m^2}) \), which can be cancelled by a third transformation, \( S'' = \frac{-i \beta \mathcal{O}''}{2m} \)

\[ \text{(192)} \]

\[ H''' = e^{iS''} \left( H'' - i \frac{\partial}{\partial t} \right) e^{-iS''} = \beta m + \mathcal{E}' \]

\[ = \beta \left( m + \frac{\mathcal{O}^2}{2m} - \frac{\mathcal{O}^4}{8m^3} \right) + \mathcal{E} - \frac{1}{8m^2} [\mathcal{O}, [\mathcal{O}, \mathcal{E}]] - \frac{i}{8m^2} [\mathcal{O}, \hat{\mathcal{O}}] \]

\[ \text{(193)} \]

Evaluating the operator products to the desired order of accuracy,

\[ \frac{\mathcal{O}^2}{2m} = \frac{(\alpha \cdot (p - eA))^2}{2m} = \left( \frac{p - eA}{2m} \right)^2 - \frac{e}{2m} \sum \mathbf{B} \] \hfill (195)

\[ \frac{1}{8m^2} \left( [\mathcal{O}, \mathcal{E}] + i \dot{\mathcal{O}} \right) = \frac{e}{8m^2} \left( -i \alpha \cdot \nabla \Phi - i \alpha \cdot \dot{A} \right) = \frac{ie}{8m^2} \alpha \cdot \mathbf{E} \] \hfill (196)

\[ \left[ \mathcal{O}, \frac{ie}{8m^2} \alpha \cdot \mathbf{E} \right] = \frac{ie}{8m^2} [\alpha \cdot \mathbf{p}, \alpha \cdot \mathbf{E}] \]

\[ = \frac{ie}{8m^2} \sum_{i,j} \alpha^i \alpha^j \left( -i \frac{\partial E^j}{\partial x^i} \right) + \frac{e}{4m^2} \sum \mathbf{E} \times \mathbf{p} \] \hfill (197)

\[ = \frac{e}{8m^2} (\nabla \cdot \mathbf{E}) + \frac{ie}{8m^2} \sum (\nabla \times \mathbf{E}) + \frac{e}{4m^2} \sum \mathbf{E} \times \mathbf{p} \]

So, the effective Hamiltonian to the desired order is

\[ H''' = \beta \left( m + \left( \frac{p - eA}{2m} \right)^2 - \frac{p^4}{8m^3} \right) + e \Phi - \frac{e}{2m} \beta \sum \mathbf{B} \]

\[- \frac{ie}{8m^2} \sum (\nabla \times \mathbf{E}) - \frac{e}{4m^2} \sum \mathbf{E} \times \mathbf{p} - \frac{e}{8m^2} (\nabla \cdot \mathbf{E}) \] \hfill (198)
The individual terms have a direct physical interpretation.

The first term in the parentheses is the expansion of

$$\sqrt{(p - eA)^2 + m^2}$$

(199)

and $-p^4/(8m^3)$ is the leading relativistic corrections to the kinetic energy.

The two terms

$$-\frac{ie}{8m^2} \Sigma \cdot (\nabla \times E) - \frac{e}{4m^2} \Sigma \cdot E \times p$$

(200)
together are the spin-orbit energy. In a spherically symmetric static potential, they take a very familiar form. In this case $\nabla \times E = 0$,

$$\Sigma \cdot E \times p = -\frac{1}{r} \frac{\partial \Phi}{\partial r} \Sigma \cdot r \times p = -\frac{1}{r} \frac{\partial \Phi}{\partial r} \Sigma \cdot L,$$

(201)

and this term reduces to

$$H_{\text{spin-orbit}} = \frac{e}{4m^2} \frac{1}{r} \frac{\partial \Phi}{\partial r} \Sigma \cdot L.$$ 

(202)

The last term is known as the Darwin term. In a coulomb potential of a nucleus with charge $Ze$, it takes the form

$$-\frac{e}{8m^2} (\nabla \cdot E) = -\frac{e}{8m^2} Z|e|\delta^3(r) = \frac{Ze^2}{8m^2} \delta^3(r) = \frac{Z\alpha \pi}{2m^2} \delta^3(r),$$

(203)

so it can only affect the $S$ ($l = 0$) states whose wavefunctions are nonzero at the origin.

For a Hydrogen-like (single electron) atom,

$$e\Phi = -\frac{Ze^2}{4\pi r}, \quad A = 0.$$ 

(204)

The shifts in energies of various states due to these correction terms can be computed by taking the expectation values of these terms with the corresponding wavefunctions.

Darwin term (only for $S$ ($l = 0$) states):

$$\langle \psi_{ns} | \frac{Z\alpha \pi}{2m^2} \delta^3(r) | \psi_{ns} \rangle = \frac{Z\alpha \pi}{2m^2} |\psi_{ns}(0)|^2 = \frac{Z^4\alpha^4 m}{2n^3}.$$ 

(205)

Spin-orbit term (nonzero only for $l \neq 0$):

$$\langle \frac{Z\alpha}{4m^2} \frac{1}{r^3} \sigma \cdot r \times p \rangle = \frac{Z^4\alpha^4 m}{4n^3} \frac{[j(j + 1) - l(l + 1) - s(s + 1)]}{l(l + 1)(l + \frac{1}{2})}.$$ 

(206)
Relativistic corrections:
\[ \left\langle -\frac{p^4}{8m^3} \right\rangle = \frac{Z^4\alpha^4 m}{2n^4} \left( \frac{3}{4} - \frac{n}{l + \frac{1}{2}} \right). \] (207)

We find
\[ \Delta E(l = 0) = \frac{Z^4\alpha^4 m}{2n^4} \left( \frac{3}{4} - n \right) \] (208)
\[ = \Delta E(l = 1, j = \frac{1}{2}), \] (209)

so \(2S_{1/2}\) and \(2P_{1/2}\) remain degenerate at this level. They are split by Lamb shift \((2S_{1/2} > 2P_{1/2})\) which can be calculated after you learn radiative corrections in QED. The \(2P_{1/2}\) and \(2P_{3/2}\) are split by the spin-orbit interaction (fine structure) which you should have seen before.

\[ \Delta E(l = 1, j = \frac{3}{2}) - \Delta E(l = 1, j = \frac{1}{2}) = \frac{Z^4\alpha^4 m}{4n^3} \] (210)

9 Klein Paradox and the Hole Theory

So far we have ignored the negative solutions. However, the negative energy solutions are required together with the positive energy solutions to form a complete set. If we try to localize an electron by forming a wave packet, the wavefunction will be composed of some negative energy components. There will be more negative energy components if the electron is more localized by the uncertainty relation \(\Delta x \Delta p \sim \hbar\). The negative energy components can not be ignored if the electron is localized to distances comparable to its Compton wavelength \(\hbar/mc\), and we will encounter many paradoxes and dilemmas. An example is the Klein paradox described below.

In order to localize electrons, we must introduce strong external forces confining them to the desired region. Let’s consider a simplified situation that we want to confine a free electron of energy \(E\) to the region \(z < 0\) by a one-dimensional step-function potential of height \(V\) as shown in Fig. 1. Now in the \(z < 0\) half space there is an incident positive energy plan wave of momentum \(k > 0\) along the \(z\) axis,

\[ \psi_{\text{inc}}(z) = e^{ikz} \left( \begin{array}{c} 1 \\ 0 \\ \frac{E+m}{k} \\ 0 \end{array} \right), \text{ (spin-up)}. \] (211)
Figure 1: Electrostatic potential idealized with a sharp boundary, with an incident free electron wave moving to the right in region I.

The reflected wave in $z < 0$ region has the form

$$\psi_{\text{ref}}(z) = a e^{-ikz} \begin{pmatrix} 1 \\ 0 \\ \frac{\sqrt{E+m}}{k} \\ 0 \end{pmatrix} + b e^{-ikz} \begin{pmatrix} 0 \\ 1 \\ \frac{\sqrt{E+m}}{k} \\ 0 \end{pmatrix}, \quad (212)$$

and the transmitted wave in the $z > 0$ region (in the presence of the constant potential $V$) has a similar form

$$\psi_{\text{trans}}(z) = c e^{iqz} \begin{pmatrix} 1 \\ 0 \\ \frac{\sqrt{E-V+m}}{q} \\ 0 \end{pmatrix} + d e^{iqz} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{\sqrt{E-V+m}}{-q} \end{pmatrix}, \quad (213)$$

with an effective momentum $q$ of

$$q = \sqrt{(E-V)^2 - m^2}. \quad (214)$$

The total wavefunction is

$$\psi(z) = \theta(-z)[\psi_{\text{inc}}(z) + \psi_{\text{ref}}(z)] + \theta(z)\psi_{\text{trans}}(z). \quad (215)$$

Requiring the continuity of $\psi(z)$ at $z = 0$, $\psi_{\text{inc}}(0) + \psi_{\text{ref}}(0) = \psi_{\text{trans}}(0)$, we obtain

$$1 + a = c \quad (216)$$

$$b = d \quad (217)$$

$$\frac{k}{E+m} = c \frac{q}{E-V+m} \quad (218)$$

$$b \frac{k}{E+m} = d \frac{-q}{E-V+m} \quad (219)$$
From these equations we can see

\[ b = d = 0 \quad \text{(no spin-flip)} \]  
\[ 1 + a = c \]  
\[ 1 - a = rc \quad \text{where} \quad r = \frac{q}{k} \frac{E + m}{E - V + m} \]  
\[ \Rightarrow c = \frac{2}{1 + r}, \quad a = \frac{1 - r}{1 + r}. \]  

As long as \(|E - V| < m\), \(q\) is imaginary and the transmitted wave decays exponentially. However, when \(V \geq E + m\) the transmitted wave becomes oscillatory again. The probability currents \(j = \psi^\dagger \alpha \psi = \psi^\dagger \alpha \psi \hat{z}\), for the incident, transmitted, and reflected waves are

\[ j_{\text{inc}} = 2 \frac{k}{E + M}, \]  
\[ j_{\text{trans}} = 2c^2 \frac{q}{E - V + m}, \]  
\[ j_{\text{ref}} = 2a^2 \frac{k}{E + m}. \]  

we find

\[ \frac{j_{\text{trans}}}{j_{\text{inc}}} = c^2 r = \frac{4r}{(1 + r)^2} \quad (< 0 \text{ for } V \geq E + m), \]  
\[ \frac{j_{\text{ref}}}{j_{\text{inc}}} = a^2 = \left( \frac{1 - r}{1 + r} \right)^2 \quad (> 1 \text{ for } V \geq E + m). \]  

Although the conservation of the probabilities looks satisfied: \(j_{\text{inc}} = j_{\text{trans}} + j_{\text{ref}}\), but we get the paradox that the reflected flux is larger than the incident one!

There is also a problem of causality violation of the single particle theory which you can read in Prof. Gunion’s notes, p.14–p.15.

**Hole Theory**

In spite of the success of the Dirac equation, we must face the difficulties from the negative energy solutions. By their very existence they require a massive reinterpretation of the Dirac theory in order to prevent atomic electrons from making radiative transitions into negative-energy states. The transition rate for an electron in the ground state of a hydrogen atom to fall into a negative-energy state may be calculated by applying semi-classical radiation theory. The rate for the electron to make a transition into the energy interval \(-mc^2\) to \(-2mc^2\) is

\[ \sim \frac{2\alpha^6 mc^2}{\pi} \frac{mc^2}{\hbar} \sim 10^8 \text{sec}^{-1} \]  

and it blows up if all the negative-energy states are included, which clearly makes no sense.
A solution was proposed by Dirac as early as 1930 in terms of a many-particle theory. (This shall not be the final standpoint as it does not apply to scalar particle, for instance.) He assumed that all negative energy levels are filled up in the vacuum state. According to the Pauli exclusion principle, this prevents any electron from falling into these negative energy states, and thereby insures the stability of positive energy physical states. In turn, an electron of the negative energy sea may be excited to a positive energy state. It then leaves a hole in the sea. This hole in the negative energy, negatively charged states appears as a positive energy positively charged particle—the positron. Besides the properties of the positron, its charge $|e| = -e > 0$ and its rest mass $m_e$, this theory also predicts new observable phenomena:

—The annihilation of an electron-positron pair. A positive energy electron falls into a hole in the negative energy sea with the emission of radiation. From energy momentum conservation at least two photons are emitted, unless a nucleus is present to absorb energy and momentum.

—Conversely, an electron-positron pair may be created from the vacuum by an incident photon beam in the presence of a target to balance energy and momentum. This is the process mentioned above: a hole is created while the excited electron acquires a positive energy.

Thus the theory predicts the existence of positrons which were in fact observed in 1932. Since positrons and electrons may annihilate, we must abandon the interpretation of the Dirac equation as a wave equation. Also, the reason for discarding the Klein-Gordon equation no longer hold and it actually describes spin-0 particles, such as pions. However, the hole interpretation is not satisfactory for bosons, since there is no Pauli exclusion principle for bosons.

Even for fermions, the concept of an infinitely charged unobservable sea looks rather queer. We have instead to construct a true many-body theory to accommodate particles and antiparticles in a consistent way. This is achieved in the quantum theory of fields which will be the subject of the rest of this course.