Relativistic Quantum Mechanics: from Dirac Equation to Quantum Field Theory

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Abstract

Following the path from the Schrödinger Equation, we aim to present the predictions and limitations that lead to Quantum Field Theory.
We first develop the Klein-Gordon Equation, which describes relativistic spin-zero particles and look at its properties. The model of an atom where the orbiting electron has no spin will permit us to see the effects of relativity on the angular momentum quantum number. We derive the radial form of the Klein-Gordon Equation and solve it for the Coulomb potential. This is the direct generalisation of the non-relativistic hydrogen atom theory.
The Klein-Gordon Equation is only appropriate for particles with spin zero, but in reality fermions (such as proton, electron and neutron) have spin $\frac{1}{2}$. We develop the Dirac equation that describes particles with spin $\frac{1}{2}$ and explore its properties and solutions. The fundamental equation must look the same in any Lorentz frame of reference, therefore we show that the Dirac Equation is Lorentz invariant. We also derive the radial form of the Dirac equation and solve it for the Coulomb potential, which will accurately predict the hydrogen atom energy levels.
In Quantum Mechanics, wavefunctions describe a single particle state, which maintains its integrity during an interaction, therefore we do not have a way to treat transmutations of particles. In Quantum Field Theory, we will interpret the solutions as operators that create or destroy states, therefore it will provide us with a framework where particles can be annihilated, created or transmigrated from one type to another. Additionally, Quantum Field Theory will solve the problem of negative energy state solutions from Relativistic Quantum Mechanics, because the creation and destruction operator solutions can create and destroy both particles and antiparticles.

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Contents

List of Figures

List of Tables

1 Introduction

Beginning with non-relativistic quantum mechanics and its one-particle interpretation, it was already clear that the validity of this theory is restricted by the principles of special relativity. Attempts to extend it in such a way that it becomes Lorentz-covariant led to the formulation of the Klein-Gordon equation as a relativistic description of spin-0 particles. However, this equation leads to solutions with negative energy. Apart from the fact that they seem to have no physical interpretation, their existence implies that atoms are unstable, because an electron would fall deeper and deeper within the unbounded negative energy spectrum via continuous radiative transitions. Another problem of this equation is the absence of a positive definite probability density which is of fundamental importance for the usual quantum mechanical statistical interpretation. In his efforts to find an equation that leads to a positive definite probability density, Dirac developed an equation for the description of electrons (generally spin-1/2 particles) which also yields solutions with negative energy. However, the Dirac equation was experimentally proven to accurately predict the energy levels of the hydrogen atom, hence it could not be ignored.
In order to prevent electrons from falling into negative energy states, Dirac claimed that the vacuum consists of a completely occupied "sea" of electrons with negative energy which, due to Pauli's exclusion principle, cannot be filled further by a particle. This idea also introduced the pair creation and annihilation processes, successfully proven by Anderson's cloud chamber experiment. [4],[11]

2 Review of Special Relativity

2.1 Fundamental Principles of Special Relativity Theory

Beginning with the Michelson-Morley experiment in 1880, it has been accepted as a fact that the velocity of light $c = 2.9979 \times 10^8$ is an absolute of nature. This led Einstein to formulate the theory of special relativity, which introduces the following postulates: the laws of physics are the same in all inertial frames and the speed of light is invariant across all inertial frames.
The general setting for special relativity consists of a four-dimensional space whose points are called events and are coordinatized by $(x^\mu) = (x^0, x^1, x^2, x^3)$, where $x^0 = ct$ is the time coordinate and $(x^1, x^2, x^3) = (x, y, z)$ are the spatial coordinates. We usually consider two or more observers moving at constant velocities relative to each other that set up space-time coordinate systems in order to make calculations. Such coordinate systems in uniform relative motion are called inertial frames and are assumed to have a common origin at some $t = 0$. [3]

Consider two events $\mathcal{E}$ and $\mathcal{P}$ on the world line (i.e. four-dimensional path) of the same light beam. We have that, in a frame $\mathcal{O}$, the differences between the spacetime coordinates of $\mathcal{E}$ and $\mathcal{P}$ satisfy

$$(ct)^2 - (x)^2 - (y)^2 - (z)^2 = 0. \tag{2.1}$$

By universality of speed of light, the coordinate differences between the same two events in frame $\mathcal{O}'$ also satisfy

$$(ct')^2 - (x')^2 - (y')^2 - (z')^2 = 0. \tag{2.2}$$

We define the interval between any two events separated by coordinate increments (dx, dy, dz, dt) to be

$$ds^2 = (cdt)^2 - (dx)^2 - (dy)^2 - (dz)^2. \tag{2.3}$$

It follows that if $ds^2 = 0$ for the coordinates in $\mathcal{O}$, then the same must hold true for the coordinates in $\mathcal{O}'$, hence

$$ds'^2 = (cdt')^2 - (dx')^2 - (dy')^2 - (dz')^2. \tag{2.4}$$

A typical vector is the four-vector, which points from one event to another and has components equal to the coordinate differences. We denote its components

$$x^\mu \equiv (x^0, x^1, x^2, x^3) \equiv (ct, x, y, z). \tag{2.5}$$

For the coordinates in a frame $\mathcal{O}'$, this is

$$x'^\mu \equiv (x'^0, x'^1, x'^2, x'^3) \equiv (ct', x', y', z'). \tag{2.6}$$

The new components x'^μ are obtained from the Lorentz transformations. In general, we write these as

$$x'^\mu = \sum_{\nu=0}^{3} \Lambda^\mu{}_\nu x^\nu \tag{2.7}$$

where $\{\Lambda^\mu{}_\nu\}$ is a collection of 16 numbers which constitutes the Lorentz transformation matrix. This is always constructed using the velocity of the upper index frame relative to the lower index frame. For a boost in the x direction, this is a linear transformation which given coordinates of an event in one reference frame allows one to determine the coordinates in a frame of reference moving with respect to the first reference frame at velocity v in the x direction. This can explicitly be written as

$$\Lambda^\mu{}_\nu = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ \beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{2.8}$$

where

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}, \tag{2.9}$$

$$\beta = \frac{v}{c}. \tag{2.10}$$

A very useful notational convention for simplifying expressions including summations of vectors, matrices, and general tensors is the Einstein summation convention, which consists of the following rules: repeated indices are implicitly summed over, each index can appear at most twice in any term and each term must contain identical non-repeated indices. [13] Using the Einstein summation convention, the Lorentz transformation can be abbreviated to [3]

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu \tag{2.11}$$

By convention,

$$\Lambda^\mu{}_\nu x^\nu = \Lambda^\mu{}_0 x^0 + \Lambda^\mu{}_i x^i \tag{2.12}$$

i.e. we will use Greek indices to refer to the coordinates (ct, x, y, z) as a whole and Latin indices to refer only to the spatial coordinates.
A general four-vector is defined by

$$A^\mu = (A^0, A^1, A^2, A^3) \tag{2.13}$$

and by the rule that its components in a frame $\mathcal{O}'$ are

$$A'^{\mu} = \Lambda^{\mu}{}_{\nu} A^{\nu}. \tag{2.14}$$

That is, its components transform in the same way that coordinates do. For a Lorentz boost, the Lorentz transformation depends only on the relative velocity v of the two frames, i.e.

$$\Lambda^{\nu}{}_{\mu} = \Lambda^{\nu}{}_{\mu}(v), \tag{2.15}$$

$$\vec{e}_{\mu} = \Lambda^{\nu}{}_{\mu}(v) \vec{e'}_{\nu}. \tag{2.16}$$

If the coordinate basis of $\mathcal{O}$ is obtained from that of $\mathcal{O}'$ by the transformation with velocity v, then the reverse must be true if we use $-v$. Hence

$$\Lambda^{\alpha}{}_{\nu}(-v)\Lambda^{\nu}{}_{\mu}(v) = \delta^{\alpha}{}_{\mu} \tag{2.17}$$

This expresses the fact that the matrix $\Lambda^{\alpha}{}_{\nu}$ is the inverse of $\Lambda^{\nu}{}_{\mu}$, because the sum on ν is exactly the operation we perform when multiplying two matrices. The matrix $\delta^{\alpha}{}_{\mu}$ is the identity matrix. The expression for the change of a vector's components also has an inverse. Taking

$$A'^{\nu} = \Lambda^{\nu}{}_{\mu}(v) A^{\mu}, \tag{2.18}$$

we multiply by $\Lambda^{\alpha}{}_{\nu}(-v)$ and sum on ν to get

$$\Lambda^{\alpha}{}_{\nu}(-v) A'^{\nu} = \Lambda^{\alpha}{}_{\nu}(-v)\Lambda^{\nu}{}_{\mu}(v) A^{\mu} = \delta^{\alpha}{}_{\mu} A^{\mu} = A^{\alpha}. \tag{2.19}$$

This says that the components of A in frame $\mathcal{O}$ are obtained from those in $\mathcal{O}'$ by the transformation with $-v$.

2.2 Vector Analysis in Special Relativity

By analogy with equation (2.1), we define

$$\vec{A}^2 = (A^0)^2 - (A^1)^2 - (A^2)^2 - (A^3)^2 \tag{2.20}$$

to be the "squared" magnitude of the vector $\vec{A}$. Because we defined the components to transform under a Lorentz transformation in the same way as (ct, x, y, z), this guarantees the magnitude is also frame-independent, i.e.

$$(A^0)^2 - (A^1)^2 - (A^2)^2 - (A^3)^2 = (A^{\bar{0}})^2 - (A^{\bar{1}})^2 - (A^{\bar{2}})^2 - (A^{\bar{3}})^2. \tag{2.21}$$

We define the scalar product of $\vec{A}$ and $\vec{B}$ to be

$$\vec{A} \cdot \vec{B} = A^0 B^0 - A^1 B^1 - A^2 B^2 - A^3 B^3 \tag{2.22}$$

and note that $\vec{A}^2$ is just $\vec{A} \cdot \vec{A}$, which is invariant. Since $(\vec{A} + \vec{B}) \cdot (\vec{A} + \vec{B})$ is the magnitude of $(\vec{A} + \vec{B})$, it follows that it is invariant. But from equations (2.21) and (2.22), we have

$$(\vec{A} + \vec{B}) \cdot (\vec{A} + \vec{B}) = \vec{A}^2 + \vec{B}^2 + 2\vec{A} \cdot \vec{B}. \tag{2.23}$$

As the LHS of (2.23) is the same in all frames, as well as the first two terms of the RHS, then it is required that the last term on RHS must be as well. This proves the frame invariance of the scalar product. It follows that the basis vectors of frame $\mathcal{O}$ satisfy

$$\vec{e}_0 \cdot \vec{e}_0 = 1, \tag{2.24}$$

$$\vec{e}_1 \cdot \vec{e}_1 = \vec{e}_2 \cdot \vec{e}_2 = \vec{e}_3 \cdot \vec{e}_3 = -1. \tag{2.25}$$

This can be summarized to

$$\vec{e_\mu} \cdot \vec{e_\nu} = \eta_{\mu\nu}, \tag{2.26}$$

where $\eta_{00} = 1, \eta_{11} = \eta_{22} = \eta_{33} = -1$ and 0 otherwise. As we will see, $\eta_{\mu\nu}$ is the Minkowski metric tensor, which associates with two vectors $\vec{A}$ and $\vec{B}$ a number, which we will call their scalar product. Note also that $\vec{e_i}$ have "unit" magnitude -1.

2.3 Tensor Analysis in Special Relativity

Consider the representation of two vectors $\vec{A}$ and $\vec{B}$ on the basis $\vec{e}_\mu$ of a frame $\mathcal{O}$

$$\vec{A} = A^\mu \vec{e}_\mu, \tag{2.27}$$

$$\vec{B} = B^\nu \vec{e}_\nu. \tag{2.28}$$

Their scalar product is therefore

$$\vec{A} \cdot \vec{B} = A^\mu B^\nu \eta_{\mu\nu}. \tag{2.29}$$

This is a frame-invariant way of writing equation (2.22).

We define a tensor of type $\begin{pmatrix} 0 \\ N \end{pmatrix}$ as a function of N vectors into the real numbers, which is linear in each of its N arguments. E.g. equation (2.29) is a type $\begin{pmatrix} 0 \\ 2 \end{pmatrix}$ tensor, since it takes two vectors and produces a single real number.
We define the metric tensor as

$$\mathbf{g}(\vec{A}, \vec{B}) \coloneqq \vec{A} \cdot \vec{B}. \tag{2.30}$$

Therefore we regard $\mathbf{g}$ as a linear function of two arguments, i.e.

$$\mathbf{g}(\alpha\vec{A} + \beta\vec{B}, \vec{C}) = \alpha\mathbf{g}(\vec{A}, \vec{C}) + \beta\mathbf{g}(\vec{B}, \vec{C}). \tag{2.31}$$

and similarly for the second argument. Note that the definition of a tensor does not mention its components, i.e. a tensor must be a rule which gives the same number independently of the reference frame in which the vectors' components are calculated. This means we can regard a tensor as a function of the vectors themselves, rather than of their components.
We define the components in a frame $\mathcal{O}$ of a type $\begin{pmatrix} 0 \\ N \end{pmatrix}$ tensor as the values of the function when its arguments are the basis vectors $\vec{e}_\mu$ of the frame $\mathcal{O}$. Therefore, for the Minkowski metric tensor,

$$\mathbf{g}(\vec{e}_\mu, \vec{e}_\nu) = \vec{e}_\mu \cdot \vec{e}_\nu = \eta_{\mu\nu}. \tag{2.32}$$

We have that the type $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ tensor is called a covariant vector, or a one-form. We denote it by $\tilde{p}$, then if we supply it with a vector $\vec{A}$, i.e. $\tilde{p}(\vec{A})$, the result is a real number.
If $\tilde{p}$ and $\tilde{q}$ are two one-forms, then if we define for $\alpha \in \mathbb{R}$

$$\tilde{s} = \tilde{p} + \tilde{q}, \tag{2.33}$$
$$\tilde{r} = \alpha\tilde{p}, \tag{2.34}$$

we have the rules

$$\tilde{s}(\vec{A}) = \tilde{p}(\vec{A}) + \tilde{q}(\vec{A}), \tag{2.35}$$
$$\tilde{r}(\vec{A}) = \alpha\tilde{p}(\vec{A}), \tag{2.36}$$

which imply that the set of all one-forms satisfies the axioms for a vector space, therefore we will call it the dual vector space. The components of $\tilde{p}$ are given by

$$p_\mu = \tilde{p}(\vec{e}_\mu), \tag{2.37}$$

and by convention, any component with a single lower index is the component of a one-form, whereas an upper index denotes the component of a vector. In terms of components,

$$\tilde{p}(\vec{A}) = \tilde{p}(\vec{A}^\mu \vec{e}_\mu) = A^\mu \tilde{p}(\vec{e}_\mu) = A^\mu p_\mu \tag{2.38}$$

which follows from linearity of tensors. The real number $\tilde{p}(\vec{A})$ is found to be the sum $A^0p_0 + A^1p_1 + A^2p_2 + A^3p_3$ and is called the contraction of $\vec{A}$ and $\tilde{p}$ and it is more fundamental in tensor analysis, because it can be performed between a one-form and a vector without reference to other tensors. By contrast, we have seen previously that the dot product of two vectors cannot yield a scalar without the help of the metric tensor.
The components of $\tilde{p}$ on a basis $\{\vec{e'}_\beta\}$ are

$$\tilde{p'} := \tilde{p}(\vec{e}_\nu) = \tilde{p}(\Lambda^\mu{}_\nu \vec{e}_\mu) = \Lambda^\mu{}_\nu \tilde{p}(\vec{e}_\mu) = \Lambda^\mu{}_\nu p_\mu. \tag{2.39}$$

By comparing this with

$$\vec{e'}_\nu = \Lambda^\mu{}_\nu \vec{e}_\mu, \tag{2.40}$$

we deduce that components of one-forms transform in exactly the same manner as basis vectors and in the opposite manner to components of vectors (i.e. using the inverse transformation matrix). We have that

$$A^\mu p_\mu = (\Lambda^\mu{}_\nu A^\nu)(\Lambda^\alpha{}_\mu p_\alpha) = \Lambda^\alpha{}_\mu \Lambda^\mu{}_\nu A^\nu p_\alpha = \delta^\alpha{}_\nu A^\nu p_\alpha = A^\nu p_\nu, \tag{2.41}$$

hence, the use of the inverse guarantees that $A^\mu p_\mu$ is frame-independent for any vector $\vec{A}$ and one-form $\tilde{p}$. This is the same way in which the vector $A^\mu \vec{e}_\mu$ is kept frame-independent. The use of this inverse is the reason why the set of all one-forms is called a dual vector space. The property of transforming with basis vectors is the reason why one-forms are also called covariant vectors. By contrast, components of vectors transform oppositely to basis vectors and are called contravariant vectors.

Since the set of all one-forms is a vector space, we can use a linearly independent set $\{\tilde{\omega}^\mu,\ \mu = 0, ..., 3\}$ as a basis, which we call the basis dual to $\{\vec{e}_\mu\}$. We denote the dual basis with upper indices in order to be able to use the summation convention. Therefore,

$$\tilde{p} = p_\mu \tilde{\omega}^\mu \tag{2.42}$$

Combining equations (2.42) and (2.38), we have

$$\tilde{p}(\vec{A}) = p_\mu \tilde{\omega^\mu}(\vec{A}) = p_\mu \tilde{\omega^\mu}(\vec{A^\nu} \vec{e_\nu}) = p_\mu A^\nu \tilde{\omega^\mu}(\vec{e}_\nu), \tag{2.43}$$

which can only equal $p_\mu A^\mu$ fo all A^ν and p_μ if

$$\tilde{\omega}^\mu(\vec{e}_\nu) = \delta^\mu{}_\nu. \tag{2.44}$$

This equation gives the ν^{th} component of the μ^{th} basis one-form, therefore defines the μ^{th} basis one-form.
Each of the frames $\mathcal{O}$ and $\mathcal{O}'$ has its own set of basis vectors. The formula which relates the two frames is

$$\tilde{\omega'}^\mu = \Lambda^\mu{}_\nu \tilde{\omega}^\nu. \tag{2.45}$$

This is the same as for components of a vector, and opposite to components of a one-form.
A typical example of a one-form is the gradient of a scalar field ϕ (see [1]). It is defined as

$$d\phi = \left(\frac{d\phi}{dt}, \frac{d\phi}{dx}, \frac{d\phi}{dy}, \frac{d\phi}{dz}\right). \tag{2.46}$$

Then, its components transform according to

$$(d\phi')_\mu = \Lambda^\nu{}_\mu (d\phi)_\nu \tag{2.47}$$

But since

$$\frac{\partial \phi}{\partial x'^\mu} = \frac{\partial \phi}{\partial x^\nu}\frac{\partial x^\nu}{\partial x'^\mu}, \tag{2.48}$$

we have

$$\frac{\partial x^\nu}{\partial x'^\mu} = (\Lambda^{-1})^\nu{}_\mu. \tag{2.49}$$

Equation (2.49) is fundamental. It shows that components of the gradient transform according to the inverse of the components of vectors, as expected for a one-form.

If we now consider the metric tensor as a mapping of one-forms into vectors, we define a one-form vector $\tilde{V}$,

$$\tilde{V}(\vec{A}) := \mathbf{g}(\vec{V}, \vec{A}) = \vec{V} \cdot \vec{A}. \tag{2.50}$$

Then, its components are given by

$$V_\mu := \tilde{V}(\vec{e}_\mu) = \vec{V} \cdot \vec{e_\mu} = \vec{e}_\mu \cdot \vec{V} = \vec{e}_\mu \cdot (\vec{V}^\nu \vec{e}_\nu) = (\vec{e}_\mu \cdot \vec{e}_\nu) V^\nu, \tag{2.51}$$

therefore

$$V_\mu = \eta_{\mu\nu} V^\nu. \tag{2.52}$$

Since this metric tensor has an inverse (i.e. its determinant $\neq 0$), we can write

$$\eta_{\mu\nu}\eta^{\nu\alpha} = \delta^\nu{}_\alpha. \tag{2.53}$$

Hence,

$$A^\mu := \eta^{\mu\nu} A_\nu. \tag{2.54}$$

In particular, the defined Minkowski metric tensor $\eta_{\mu\nu}$ and its inverse $\eta^{\mu\nu}$ are identical. This means the components of a one-form are obtained from the ones of a vector by simply changing the sign of the spatial components. [1], [9]

3 Klein-Gordon Equation

Early efforts to include special relativity into quantum mechanics started with the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\phi = H\phi, \tag{3.1}$$

where the Hamiltonian H is given by

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V. \tag{3.2}$$

Since this equation has different orders for the spatial and temporal derivatives, it is not Lorentz-covariant. Therefore, in order to arrive at a relativistic quantum mechanical wave equation, we start from the energy-momentum relation for free particles,

$$E^2 = \mathbf{p}^2c^2 + m_0^2c^4, \tag{3.3}$$

where m_0 is the rest mass of the particle.

We know from special relativity that the four-momentum vector is Lorentz covariant (i.e. its length in four dimensional space is invariant). For a free particle ($V = 0$), we have

$$p^\mu p_\mu = m_0^2c^2 = \eta_{\mu\nu}p^\mu p^\nu = \begin{pmatrix} E/c, & p^1, & p^2, & p^3 \end{pmatrix}\begin{pmatrix} E/c \\ -p^1 \\ -p^2 \\ -p^3 \end{pmatrix} \tag{3.4}$$

We also note the relation

$$px = p_\mu x^\mu = p^\mu x_\mu = Et - p^i x^i = Et - \mathbf{p}\cdot\mathbf{x}, \tag{3.5}$$

$$\tag{3.6}$$

Hence, using the correspondence rule, we change the dynamical variables to operators, i.e.

$$E \to i\hbar\frac{\partial}{\partial t}, \quad p \to -i\hbar\nabla \iff p^\mu \to i\hbar\partial^\mu. \tag{3.7}$$

Hence, we find, from Equation (3.3) that

$$H = \sqrt{-\hbar^2c^2\partial_i\partial_i + m_0^2c^4}. \tag{3.8}$$

However, taking the square root of terms containing a derivative is problematic and difficult to correlate with the physical world.

3.1 Derivation of the Klein-Gordon Equation

In order to avoid the square root, we square the operators in the original Schrödinger equation, thus obtaining

$$\left(i\hbar\frac{\partial}{\partial t}\right)\left(i\hbar\frac{\partial}{\partial t}\right)\phi(x) = H^2\phi(x) = (\mathbf{p}^2c^2 + m_0^2c^4)\phi(x). \tag{3.9}$$

This gives the Klein-Gordon equation in canonical form, i.e.

$$-\hbar^2\frac{\partial^2}{\partial t^2}\phi(x) = (-c^2\hbar^2\nabla^2 + m_0^2c^4)\phi(x). \tag{3.10}$$

Since the Hamiltonian is given by Equation (3.8), we have

$$-\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2}\phi(x) = \Big(-\hbar^2\frac{\partial}{\partial X_i}\frac{\partial}{\partial X_i} + m^2c^2\Big)\phi(x)$$

Or, equivalently,

$$-\frac{\partial}{\partial x^0}\frac{\partial}{\partial x_0}\phi(x) = \Big(\frac{\partial}{\partial x^i}\frac{\partial}{\partial x_i} + \frac{m^2c^2}{\hbar^2}\Big)\phi(x),$$

where we changed from the three dimensional Cartesian coordinates X_i to the four-vector notation. Rearranging, we have the Klein-Gordon Equation in Lorentz-covariant form,

$$\Big(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x_\mu} + \mu^2\Big)\phi(x) = 0, \tag{3.11}$$

where $\mu = m_0^2c^2/\hbar^2$, which is equivalent to

$$(\partial_\mu\partial^\mu + \mu^2)\phi(x) = 0. \tag{3.12}$$

The operator $\partial_\mu\partial^\mu = \partial^\mu\partial_\mu$ is called the d'Alembert operator and it is the four-dimensional Minkowski coordinates analogue of the three-dimensional Laplace operator $\partial_i\partial_i = \partial^i\partial^i$ for Cartesian coordinates.
Contrary to the Schrödinger equation, the Klein-Gordon equation is of second order in time. This means we need two initial values, i.e. for ϕ and for $\partial\phi/\partial t$ in order to uniquely specify a state of the system. Furthermore, we can assert that the Klein-Gordon equation describes spin-0 particles, since the d'Alembertian only acts on the external degrees of freedom (i.e. space-time coordinates) of ϕ.

3.2 Solutions to the Klein-Gordon Equation

An equivalent formulation of (3.12) is

$$(p^\mu p_\mu - m_0^2c^2)\phi(x) = 0. \tag{3.13}$$

Then, the solutions are

$$\phi^{(1)}_{\mathbf{p}}(x) = e^{-i(cp_0t-\mathbf{p}\cdot\mathbf{x})/\hbar} \tag{3.14}$$

$$\phi^{(2)}_{\mathbf{p}}(x) = e^{i(cp_0t-\mathbf{p}\cdot\mathbf{x})/\hbar}. \tag{3.15}$$

The Klein-Gordon equation leads to solutions with positive energy eigenvalues $E = +cp_0$ and negative energy eigenvalues $E = -cp_0$. While the positive solutions can be interpreted as particle wave-functions, the physical meaning of the negative solutions is not yet clear. However, we will see that negative solutions can be related to antiparticles, which are experimentally observable, therefore we consider $\phi^{(2)}\mathbf{p}$ to be a negative solution with momentum index $\mathbf{p}$ and momentum eigenvalue $-\mathbf{p}$. So, the Klein-Gordon theory indeed provides a valuable generalisation of Schrödinger's theory.

3.3 Probability Density

We start by post multiplying Equation (3.12) by $\phi^\dagger$, then we subtract the complex conjugate equation post-multiplied by ϕ,

$$\phi^\dagger\frac{\partial^2}{\partial t^2}\phi = \phi^\dagger(\nabla^2 - \mu^2)\phi$$

$$\frac{\partial^2}{\partial t^2}\phi^\dagger = (\nabla^2 - \mu^2)\phi^\dagger\phi. \tag{3.16}$$

Since $\mu^2\phi^\dagger\phi - \mu^2\phi\phi^\dagger = 0$, the LHS of (3.16) is

$$\frac{\partial^2\phi}{\partial t^2}\phi^\dagger - \frac{\partial^2\phi^\dagger}{\partial t^2}\phi + \frac{\partial\phi}{\partial t}\frac{\partial\phi^\dagger}{\partial t} - \frac{\partial\phi^\dagger}{\partial t}\frac{\partial\phi}{\partial t} = \frac{\partial}{\partial t}\bigg(\frac{\partial\phi}{\partial t}\phi^\dagger - \frac{\partial\phi^\dagger}{\partial t}\phi\bigg), \tag{3.17}$$

and the RHS is

$$(\nabla^2\phi)\phi^\dagger - (\nabla^2\phi^\dagger)\phi + \nabla\phi\cdot\nabla\phi^\dagger - \nabla\phi^\dagger\cdot\nabla\phi = \nabla\cdot\bigg((\nabla\phi)\phi^\dagger - (\nabla\phi^\dagger)\phi\bigg). \tag{3.18}$$

By equating (3.17) and (3.18) above and multiplying both sides by i (in order to have a real current), we have

$$i\frac{\partial}{\partial t}\bigg(\frac{\partial\phi}{\partial t}\phi^\dagger - \frac{\partial\phi^\dagger}{\partial t}\phi\bigg) = i\nabla\cdot\bigg((\nabla\phi)\phi^\dagger - (\nabla\phi^\dagger)\phi\bigg). \tag{3.19}$$

This yields the form of the continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0, \tag{3.20}$$

where the probability density and the probability current for a Klein-Gordon particle are

$$\rho = j^0 = \frac{i}{c}\bigg(\frac{\partial\phi}{\partial t}\phi^\dagger - \frac{\partial\phi^\dagger}{\partial t}\phi\bigg), \tag{3.21}$$

$$j^i = i\bigg(\phi^\dagger\partial^i\phi - \partial^i\phi^\dagger\phi\bigg). \tag{3.22}$$

We now define the scalar four-current as

$$j^\mu = \begin{pmatrix} \rho \\ \mathbf{j} \end{pmatrix} = \begin{pmatrix} \rho \\ j^i \end{pmatrix} = \begin{pmatrix} j^0 \\ j^i \end{pmatrix} = i(\phi^\dagger\partial^\mu\phi - \partial^\mu\phi^\dagger\phi). \tag{3.23}$$

The four-dimensional continuity equation is then

$$\frac{\partial j^\mu}{\partial x^\mu} = \partial_\mu j^\mu = 0. \tag{3.24}$$

This tells us that the four-divergence of the four-current of any conserved quantity (total probability in this case) is zero. Note, however, that j^0 is not positive-definite, hence cannot be identified with a probability density. [6], [4]

3.4 Interaction with electromagnetic fields and gauge invariance

In the Klein-Gordon equation, the interaction of a relativistic spin-0 particle with an electromagnetic field can be taken into account by the following operator replacement, called minimal coupling [7]

$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - eA^0, \quad \frac{\hbar}{i}\nabla \to \frac{\hbar}{i}\nabla - \frac{e}{c}A \iff p^\mu \to p^\mu - \frac{e}{c}A^\mu, \tag{3.25}$$

where A^μ is the electromagnetic four-potential and e is the electric charge of the particle. With this, equations (3.10) and (3.13) become

$$\bigg[\bigg(i\hbar\frac{\partial}{\partial t} - eA^0\bigg)^2 - c^2\bigg(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\bigg)^2 - m_0^2c^4\bigg]\phi = 0, \tag{3.26}$$

and

$$\left[\left(p_\mu - \frac{e}{c}A_\mu\right)\left(p^\mu - \frac{e}{c}A^\mu\right) - m_0^2c^2\right]\phi = 0. \tag{3.27}$$

We know that Maxwell's equations are invariant under local gauge transformations of the kind

$$A^0 \to A'^0 = A^0 - \frac{1}{c}\frac{\partial \chi}{\partial t}, \quad \mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\chi, \tag{3.28}$$

or

$$A^\mu \to A'^\mu - \partial^\mu \chi, \tag{3.29}$$

where χ is an arbitrarily chosen real scalar function of the space-time coordinates.

As in the non relativistic case, the local gauge invariance can be carried over to the Klein-Gordon equation by multiplying the wavefunction ϕ by a phase $e^{i\Lambda(x)}$. In order to find the function Λ, we express equation (3.27) in terms of the primed quantities and calculate

$$\begin{aligned} 0 &= \left[\left(p_\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial_\mu\chi\right)\left(p^\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial^\mu\chi\right) - m_0^2c^2\right]\phi e^{i\Lambda} \\ &= \left[\left(p_\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial_\mu\chi\right)e^{i\Lambda}\left(p^\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial^\mu\chi + \hbar\partial^\mu\Lambda\right) - m_0^2c^2e^{i\Lambda}\right]\phi \\ &= e^{i\Lambda}\left[\left(p_\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial_\mu\chi + \hbar\partial_\mu\Lambda\right)\left(p^\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial^\mu\chi + \hbar\partial^\mu\Lambda\right) - m_0^2c^2\right]\phi, \end{aligned}$$

where we have used the chain rule for the momentum operator,

$$p^\mu(e^{i\Lambda}\phi) = e^{i\Lambda}(p^\mu + \hbar\partial^\mu\Lambda)\phi. \tag{3.30}$$

Choosing

$$\Lambda(x) = \frac{e}{\hbar c}\chi(x), \tag{3.31}$$

the equation above becomes

$$e^{i\Lambda}\left[\left(p_\mu - \frac{e}{c}A'_\mu\right)\left(p^\mu - \frac{e}{c}A'^\mu\right) - m_0^2c^2\right]\phi = 0. \tag{3.32}$$

In general, in order to calculate expectation values of observables, we need the phase factor to vanish; this corresponds to measurable quantities. This is true for a global phase factor of the form $e^{i\varphi}$ independent of position, because the phase angle φ only changes the direction of vectors, leaving their norm unchanged. In our case, if a wavefunction ϕ interacts with the electromagnetic field, the phase factor $\Lambda(x)$ varies with position, hence it is not invariant under a local transformation. This equation can be made invariant only if ϕ also transforms according to

$$\phi(x) \to \phi'(x) = e^{i\Lambda(x)}\phi(x). \tag{3.33}$$

In this case, the equation

$$\left[\left(p_\mu - \frac{e}{c}A'_\mu\right)\left(p^\mu - \frac{e}{c}A'^\mu\right) - m_0^2c^2\right]\phi' = 0 \tag{3.34}$$

is formally identical to the Klein-Gordon equation, i.e. the Klein-Gordon equation with minimal coupling is invariant under local gauge transformations of the electromagnetic field.

3.5 Radial Klein-Gordon Equation

If we consider a centrally symmetric potential of the form $eA^0(x) = V(x) = V(|x|), \mathbf{A} = 0$, then the Klein-Gordon equation possesses a central symmetry. Similar to the non-relativistic case, we can rewrite it in terms of spherical coordinates,

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta, \quad r = |x|, \tag{3.35}$$

in order to separate the radial and angular parts. Starting with the Klein-Gordon equation

$$\left(i\hbar\frac{\partial}{\partial t} - V\right)^2 \phi(x) + (c^2\hbar^2\nabla^2 - m_0^2c^4)\phi(x) = 0, \tag{3.36}$$

we derive the time independent form, i.e.

$$[(E-V)^2 + c^2\hbar^2\nabla^2 - m_0c^4]\Phi(x) = 0, \tag{3.37}$$

where

$$\phi(x) = \Phi(x)e^{-iEt/\hbar}. \tag{3.38}$$

We now write the momentum term as

$$\hbar^2\nabla^2 = -p_r^2 - \frac{\mathbf{L}^2}{r^2}, \tag{3.39}$$

where

$$p_r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right), \quad p_r^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \tag{3.40}$$

denotes the radial momentum and $\mathbf{L} = \mathbf{x}\times\mathbf{p}$ is the angular momentum whose eigenfunctions are given by the spherical harmonics $Y_{l,m}(\theta,\varphi)$

$$\mathbf{L}^2 Y_{l,m} = \hbar^2 l(l+1)Y_{l,m}, \quad l = 0,1,2,... \tag{3.41}$$

$$L_z Y_{l,m} = \hbar m Y_{l,m}, \qquad m = -l,...,l. \tag{3.42}$$

Consequently, equation (3.37) becomes

$$\left[(E-V)^2 + c^2\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) - \frac{c^2\mathbf{L}^2}{r^2} - m_0^2c^4\right]\Phi(x) = 0. \tag{3.43}$$

We can separate the radial and angular parts by writing

$$\Phi(x) = g_l(r)Y_{l,m}(\theta,\varphi), \tag{3.44}$$

then the functions g_l obey the radial Klein-Gordon equation

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right]g_l(r) = 0, \quad k^2 = \frac{(E-V)^2 - m_0^2c^4}{c^2\hbar^2}, \tag{3.45}$$

or, using $g_l = u_l(r)/r$,

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right]u_l(r) = 0. \tag{3.46}$$

These solutions also satisfy the relations

$$\mathbf{L}^2\Phi_{l,m}(r,\theta,\varphi) = \hbar^2 l(l+1)\Phi_{l,m}(r,\theta,\varphi), \quad l = 0,1,2,.... \tag{3.47}$$

$$L_z\Phi_{l,m}(r,\theta,\varphi) = \hbar m\Phi_{l,m}(r,\theta,\varphi), \quad m = -l,...,l \tag{3.48}$$

$$[\Phi_{l,m}]_P(r,\theta,\phi) = (-1)^l\Phi_{l,m}(r,\theta,\varphi). \tag{3.49}$$

Note that equations (3.45) and (3.46) are formally identical to the corresponding radial equations of non-relativistic theory, with $k^2 = 2m_0(E-V)/\hbar^2$.

3.6 Coulomb Potential

Considering the problem of a spin-0 particle within a Coulomb potential of the form

$$eA^0(r) = V(r) = -\frac{Ze^2}{r} = -\frac{Z\hbar c\alpha_e}{r}, \tag{3.50}$$

where $\alpha_e \approx 1/137$ denotes the fine-structure constant, the radial Klein-Gordon equation given in (3.46) becomes

$$\left[\frac{d}{dr^2} - \frac{l(l+1)-(Z\alpha_e)^2}{r^2} + \frac{2EZ\alpha_e}{\hbar cr} - \frac{m_0^2c^4 - E^2}{\hbar^2c^2}\right]u_l(r) = 0. \tag{3.51}$$

We want to restrict the discussion to bound states, i.e. to the interval $-m_0c^2 < E < m_0c^2$, hence we introduce the following quantities:

$$\rho = \beta r, \quad u_l(r) = \hat{u}_l(\rho), \quad \beta = 2\sqrt{\frac{m_0^2c^4 - E^2}{\hbar^2c^2}}, \quad \lambda = \frac{2EZ\alpha_e}{\beta\hbar c}. \tag{3.52}$$

Therefore, (3.51) is

$$\left[\frac{d^2}{d\rho^2} - \frac{l'(l'+1)}{\rho^2} + \frac{\lambda}{\rho} - \frac{1}{4}\right]\hat{u}_l(\rho) = 0, \tag{3.53}$$

with

$$l'(l'+1) = l(l+1) - (Z\alpha_e)^2, \tag{3.54}$$

which implies

$$l' = -\frac{1}{2} \pm \sqrt{\left(l+\frac{1}{2}\right)^2 - (Z\alpha_e)^2}. \tag{3.55}$$

Equation (3.53) is formally identical to the radial Schrödinger equation with Coulomb potential. Therefore, we follow the same approach and consider (3.53) for asymptotic regions $\rho \to 0$ and $\rho \to \infty$.

For $\rho \to 0$, equation (3.53) reduces to

$$\left[\frac{d^2}{d\rho^2} - \frac{l'(l'+1)}{\rho^2}\right]\hat{u}_l(\rho) = 0, \tag{3.56}$$

having solutions $\hat{u}_l(\rho) = \rho^{l'+1}$ and $\hat{u}_l(\rho) = \rho^{-l'}$.

Physical solutions exist only for real values of (3.55), otherwise the quantity $l' = -1/2 \pm \tau$, where $\tau = \sqrt{(Z\alpha_e)^2 - (l+1/2)^2}$ yields wavefunctions of the form $\hat{u}_l(\rho) = \rho^{1/2}\exp(\pm i\tau \ln\rho)$. These would oscillate infinitely often as $\rho \to 0$ and give divergent energy values. Therefore, we need the constraint

$$l + \frac{1}{2} > Z\alpha_e. \tag{3.57}$$

Also, because of the $1/r$ behaviour of the Coulomb potential, another constraint is

$$l' + 1 > 0. \tag{3.58}$$

Hence, the solution that satisfies (3.6) is

$$\hat{u}_l(\rho) = \rho^{l'+1}, \quad l' = -\frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right) - (Z\alpha_e)^2}. \tag{3.59}$$

For $\rho \to \infty$, equation (3.53) becomes

$$\left(\frac{d^2}{d\rho^2} - \frac{1}{4}\right)\hat{u}_l(\rho) = 0. \tag{3.60}$$

Its bounded solution at infinity is

$$\hat{u}(\rho) = e^{-\rho/2}. \tag{3.61}$$

Putting together the asymptotic regions yields that the solution of (3.53) must be

$$\hat{u}_l(\rho) = \rho^{l'+1} e^{-\rho/2} f(\rho). \tag{3.62}$$

Calculating the necessary derivatives and substituting them into (3.53) leads to the following differential equation:

$$\rho\frac{d^2 f}{d\rho^2} + (2l' + 2 - \rho)\frac{df}{d\rho} + (\lambda - l' - 1)f(\rho) = 0. \tag{3.63}$$

Expanding $f(\rho)$ as a power series, i.e.

$$f(\rho) = \sum_{k=0}^{\infty} a_k \rho_k, \tag{3.64}$$

yields

$$\sum_{k=0}^{\infty}[(k+1)(k+2l'+2)a_{k+1} + (\lambda - l' - 1 - k)a_k]\rho^k = 0. \tag{3.65}$$

Hence we obtain the recursion formula for the coefficients

$$a_{k+1} = \frac{k + l' + 1 - \lambda}{(k+1)(k+2l'+2)} a_k. \tag{3.66}$$

Since the wavefunction u_l must converge at infinity, the expansion must break at some $k = n'$, which means

$$\lambda = n' + l' + 1, \quad n' = 0, 1, 2, ... \tag{3.67}$$

This is the quantization condition for λ, hence for the energy levels of bound spin-0 particles. Using the previous definition of λ, it follows that

$$\frac{E^2(Z\alpha_e)^2}{m_0 c^4 - E^2} = \left[n' + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - (Z\alpha_e)^2}\right]^2, \tag{3.68}$$

hence

$$E_{n',l} = \frac{m_0 c^2}{\sqrt{1 + \frac{(Z\alpha_e)^2}{\left(n + \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - (Z\alpha_e)^2}\right)}}} \tag{3.69}$$

for $n' = 1, 2, 3, ...$ and $l = 0, 1, ..., n-1$. Note that the earlier constraint we had on l is also necessary here in order to have real (i.e. physical) energy eigenvalues.
Introducing the principal quantum number,

$$n = n' + l + 1, \tag{3.70}$$

we finally obtain

$$E_{n,l} = \frac{m_0c^2}{\sqrt{1 + \frac{(Z\alpha_e)^2}{\left(n-(l+\frac{1}{2})+\sqrt{(l+\frac{1}{2})^2-(Z\alpha_e)^2}\right)}}}, \tag{3.71}$$

for $n = 1, 2, 3...$ and $l = 0, 1, ..., n-1$. Expanding (3.71) in powers of $Z\alpha_e$ yields

$$E_{n,l} = m_0c^2\left[1 - \frac{(Z\alpha_e)^2}{2n^2} - \frac{(Z\alpha_e)^4}{2n^4}\left(\frac{n}{l+\frac{1}{2}} - \frac{3}{4}\right) + ...\right]. \tag{3.72}$$

[4]

4 Dirac Equation

4.1 Derivation of Dirac Equation

Dirac's primary goal was finding a relativistic generalisation for the Schrödinger equation, therefore he postulated that if it existed, it must satisfy the following constraints:

1. The equation must be Lorentz-covariant. Since its temporal derivative is of first order, the spatial derivatives must also be of first order.
2. The equation must yield the energy-momentum relation in operator form.
3. The quantity $\rho = \psi^\dagger\psi$ must be the temporal component of a conserved four-vector j^μ. That is, there must exist a Lorentz-covariant continuity equation so that its integral over the whole space is invariant.

Hence, the equation must have the general form

$$i\hbar\frac{\partial}{\partial t}\psi = H\psi = (c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m_0c^2)\psi, \tag{4.1}$$

where $\mathbf{p}$ is the particle momentum operator and the vector $\boldsymbol{\alpha}$ and the scalar β have to be determined. Also, the relativistic free particle Hamiltonian would be a linear function of both $\mathbf{p}$ and mass m_0. The key problem then is to find $\boldsymbol{\alpha}$ and β in order for this equation to be true.
To find the answer, Dirac reasoned that H^2 and ψ must also satisfy the usual relativistic energy-momentum relation (and therefore the Klein-Gordon Equation):

$$-\hbar^2\frac{\partial^2}{\partial t}\psi = H^2\psi = (c^2\mathbf{p}^2 + m_0^2c^4)\psi \tag{4.2}$$

Squaring the operators in Equation (4.1) and inserting the results into Equation (4.2), we get:

$$\begin{aligned}-\hbar^2\frac{\partial^2}{\partial t}\psi = H^2\psi &= (\alpha_ip_i + \beta m)(\alpha_jp_j + \beta m)\psi = \\ &= \left(\alpha_i^2p_i^2 + (\alpha_i\alpha_j + \alpha_j\alpha_i)p_ip_j + (\alpha_i\beta + \beta\alpha_i)p_im + \beta^2m^2\right)\psi\end{aligned} \tag{4.3}$$

Comparison with the RHS of Equation (4.2) shows that the quantities in brackets above must equal zero. Moreover, we must have $\alpha_i^2 = 1$ and $\beta_i^2 = 1$. To summarize, we have:

$$[\alpha_i, \alpha_j]_+ = [\alpha_i, \beta]_+ = 0, \quad i \neq j, \tag{4.4}$$

$$(\alpha_1)^2 = (\alpha_2)^2 = (\alpha_3)^2 = (\beta)^2 = 1, \tag{4.5}$$

where anti-commutators are defined as $[\alpha_i, \alpha_j]_+ = \alpha_i\alpha_j + \alpha_j\alpha_i$.
We have that $\alpha_1, \alpha_2, \alpha_3, \beta$ all anti-commute with each other. Using these requirements, we can show that α_i and β matrices are traceless. By the cyclic property of traces, we have

$$Tr(\alpha_i) = Tr(\alpha_i\beta\beta) = Tr(\beta\alpha_i\beta) = -Tr(\alpha_i\beta\beta) = -Tr(\alpha_i). \tag{4.6}$$

Furthermore, it can be shown that the eigenvalues of α_i and β are ± 1. This follows from multiplying the eigenvalue equation,

$$\alpha_i X = \lambda X \tag{4.7}$$

by α_i and using $\alpha_i^2 = I$, which implies

$$X = \lambda^2 X \tag{4.8}$$

and therefore $\lambda = \pm 1$. Because the sum of the eigenvalues of a matrix is equal to its trace, and these matrices have eigenvalues ± 1, the only way the trace can be zero is if α_i and β are of even dimension.
Because the Dirac Hamiltonian operator of (4.1), i.e.

$$H = (c\boldsymbol{\alpha} \cdot \boldsymbol{\beta} + \beta m_0 c^2) \tag{4.9}$$

must be Hermitian in order to have real eigenvalues, α_i and β also must be Hermitian, i.e. $\alpha_i = \alpha_i^\dagger$ and $\beta = \beta^\dagger$. Because there are only three mutually anticommuting 2×2 traceless matrices, e.g. the Pauli matrices, the lowest dimension object that can represent the above are 4×4 matrices. Therefore, the Dirac Hamiltonian is a 4×4 matrix of operators that must act on a four-component wavefunction, known as a Dirac spinor,

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}. \tag{4.10}$$

Thus, the consequence of requiring the wavefunctions for a relativistic particle to satisfy the Dirac equation and to be consistent with the Klein-Gordon equation is that the wavefunctions are forced to have four degrees of freedom.

Note: the four-dimensional space here does not have the meaning of a four-dimensional physical space, but of an abstract one called spinor space.

The matrices Dirac found for the spinor space are

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \ \alpha_1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}, \ \alpha_2 = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \ \alpha_3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \tag{4.11}$$

where $0 \equiv O_2$, the 2×2 null matrix, and σ_i are the Pauli matrices.
Note: the Klein-Gordon Equation can be viewed as the "square" of the Dirac Equation, hence any solution ψ of the latter will also satisfy the former.

4.2 Radial Dirac Equation

In the case of a spin-1/2 particle in a centrally symmetric potential of the form $eA^0(x) = V(x) = V(|x|), \mathbf{A} = 0$, we can again use spherical coordinates,

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta, \quad r = |x|, \tag{4.12}$$

in order to separate radial and angular parts. Starting with the Dirac equation

$$i\hbar\frac{\partial\psi}{\partial t} = [c\boldsymbol{\alpha} + \beta m_0 c^2 + V(r)]\psi(x), \quad r = |x|, \tag{4.13}$$

we derive the time-independent form

$$H\Psi(\mathbf{x}) = E\Psi(\mathbf{x}), \quad H = c\boldsymbol{\alpha}\mathbf{p} + \beta m_0 c^2 + V(r), \tag{4.14}$$

where

$$\Psi(\mathbf{x}) = \psi(x)e^{-iEt/\hbar}. \tag{4.15}$$

In order to separate the radial and angular parts of $\boldsymbol{\alpha}\mathbf{p}$, we introduce the radial momentum,

$$p_r = i - \hbar\frac{1}{r}\frac{\partial}{\partial r} = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \tag{4.16}$$

and the radial velocity

$$\alpha_r = \frac{\boldsymbol{\alpha}\mathbf{x}}{r}. \tag{4.17}$$

Using the identities

$$(\boldsymbol{\sigma}\mathbf{A})(\boldsymbol{\sigma}\mathbf{B}) = \mathbf{AB} + i\boldsymbol{\sigma}(\mathbf{A}\times\mathbf{B}), \tag{4.18}$$

$$x\nabla = r\frac{\partial}{\partial r}, \tag{4.19}$$

we have that

$$(\boldsymbol{\alpha}\mathbf{x})(\boldsymbol{\alpha}\mathbf{p}) = \mathbf{xp} + i\hat{\boldsymbol{\sigma}}\mathbf{L} = rp_r + i\left(\hbar + \frac{2SL}{\hbar}\right). \tag{4.20}$$

Multiplying the above from the left by α_r/r yields

$$\boldsymbol{\alpha}\mathbf{p} = \alpha_r\left[p_r + \frac{i}{r}\left(\hbar + \frac{\mathbf{J^2} - \mathbf{S}^2 - \mathbf{L}^2}{\hbar}\right)\right], \tag{4.21}$$

where $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is the total angular momentum of the particle. We can show that $\{H, \mathbf{J}, J_z\}$ and the parity transformation P all commute with each other, therefore solutions will be eigenfunctions of $\mathbf{J}^2$ and J_z (and hence of $\mathbf{L}^2$,$\mathbf{S}^2$) given by

$$\mathcal{Y}^{(l)}_{J,M}(\theta,\varphi) = \sum_{m+m_s=M}\left\langle l, m_l; \frac{1}{2}, m_s\middle| J, M\right\rangle Y_{l,m}(\theta,\varphi)\chi(m_s), \quad l = J \mp \frac{1}{2}, \tag{4.22}$$

with

$$\mathbf{J}^2\mathcal{Y}^{(l)}_{J,M} = \hbar^2 J(J+1)\mathcal{Y}^{(l)}_{J,M}, \quad J_z\mathcal{Y}^{(l)}_{J,M} = \hbar M\mathcal{Y}^{(l)}_{J,M}, \quad M = -J, ..., J. \tag{4.23}$$

These spinor spherical harmonics are composed of the spherical harmonics $Y_{l,m}(\theta,\varphi)$, with

$$\mathbf{S}^2\chi(m_s) = \frac{3\hbar^2}{4}\chi(m_s), \quad S_z\chi(m_s) = \hbar m_s\chi(m_s), \quad \mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}, \quad m_s = \pm\frac{1}{2}. \tag{4.24}$$

The coefficients in (4.22) are called Clebsch-Gordan coefficients and can be found in [10].

We now combine two spinor spherical harmonics with the same J and M in order to get a bispinor with a defined parity. Since the spherical harmonics obey

$$Y_{l,m}(\pi-\theta,\varphi+\pi)=(-1)^{l}Y_{l,m}^{(l)}(\theta,\varphi), \tag{4.25}$$

we have for the spinor spherical harmonics that

$$\mathcal{Y}_{J,M}^{(l)}(\pi-\theta,\varphi+\pi)=(-1)^{l}Y_{J,M}^{(l)}(\theta,\varphi). \tag{4.26}$$

Also, if we apply the parity transformation to a bispinor, this yields

$$\begin{pmatrix}\Psi_u(x)\\ \Psi_d(x)\end{pmatrix}_P=\begin{pmatrix}\Psi_u(-x)\\ -\Psi_d(-x)\end{pmatrix}. \tag{4.27}$$

So in order to get a state with defined parity, we have to combine two states $\mathcal{Y}_{J,M}^{(l)}$ whose l-values differ by 1. Therefore, two possible combinations can be written as

$$\Psi_{J,M}^{(\omega)}(r,\theta,\varphi)=\frac{1}{r}\begin{pmatrix}F_{J+\omega/2}(r)\mathcal{Y}_{J,M}^{(J+\omega/2)}(\theta,\varphi)\\ iG_{J-\omega/2}(r)\mathcal{Y}_{J,M}^{(J-\omega/2)}(\theta,\varphi)\end{pmatrix},\quad \omega=\pm1, \tag{4.28}$$

where $[\Psi_{J,M}^{(\omega)}]_P(\theta,\varphi)=(-1)^{J+\omega/2}(r)\Psi_{J,M}^{(\omega)}(\theta,\varphi)$. We know that

$$\mathbf{L}^2\Psi_{J,M}^{(\omega)}=\hbar^2 l(l+1)\Psi_{J,M}^{(\omega)}=\hbar^2\left[J(J+1)+\frac{1}{4}+\frac{\omega}{2}\beta(2J+1)\right]\Psi_{J,M}^{(\omega)}, \tag{4.29}$$

hence the bracket term in (4.20) becomes

$$\left(\hbar+\frac{\mathbf{J}^2-\mathbf{S}^2-\mathbf{L}^2}{\hbar}\right)\Psi_{J,M}^{(\omega)}=-\frac{\hbar\omega}{2}(2J+1)\beta\Psi_{J,M}^{(\omega)}, \tag{4.30}$$

hence equation (4.14) becomes

$$\left[c\alpha_r\left(p_r-\frac{i\hbar\omega(J+\frac{1}{2})}{r}\beta\right)+\beta m_0c^2+V(r)\right]\Psi_{J,M}^{(\omega)}=E\Psi_{J,M}^{(\omega)} \tag{4.31}$$

Using the identities

$$\frac{\boldsymbol{\sigma}\mathbf{x}}{r}\mathcal{Y}_{J,M}^{(J\pm\omega/2)}=-\mathcal{Y}_{J,M}^{(J\mp\omega/2)},\quad p_r\left(\frac{f(r)}{r}\right)=-i\hbar\frac{1}{r}\frac{df}{dr}, \tag{4.32}$$

we conclude that the solutions of the time-independent Dirac equation with a centrally symmetric potential can be written in spherical coordinates (equation (4.28)), where the functions F_l and G_l satisfy the radial Dirac equations, i.e.

$$\left[-\frac{d}{dr}+\frac{\omega(J+\frac{1}{2})}{r}\right]G_{J-\omega/2}(r)=\frac{E-m_0c^2-V}{c\hbar}F_{J+\omega/2}(r), \tag{4.33}$$

$$\left[\frac{d}{dr}+\frac{\omega(J+\frac{1}{2})}{r}\right]F_{J+\omega/2}(r)=\frac{E+m_0c^2-V}{c\hbar}G_{J-\omega/2}(r). \tag{4.34}$$

Furthermore, these solutions satisfy

$$\mathbf{J}^2\Psi_{J,M}^{(\omega)}(r,\theta,\varphi)=\hbar^2J(J+1)\Psi_{J,M}^{(\omega)}(r,\theta,\varphi),\quad J=\frac{1}{2},\frac{3}{2},... \tag{4.35}$$

$$J_z\Psi_{J,M}^{(\omega)}(r,\theta,\varphi)=\hbar M\Psi_{J,M}^{(\omega)}(r,\theta,\varphi),\quad M=-J,...,J \tag{4.36}$$

$$[\Psi_{J,M}^{(\omega)}]_P(r,\theta,\varphi)=(-1)^{J+\omega/2}\Psi_{J,M}^{(\omega)}(r,\theta,\varphi),\quad \omega=\pm1. \tag{4.37}$$

[4]

4.3 Coulomb Potential

As in the Klein-Gordon case, we consider a bound spin-1/2 particle in a Coulomb Potential of the form

$$eA^0(r) = V(r) = -\frac{Ze^2}{r} = -\frac{Z\hbar c\alpha_e}{r}, \tag{4.38}$$

and look at the asymptotic regions of the radial Dirac equations in order to find a series expansion of the solution.

For $r \to \infty$, the radial Dirac equations (4.33), (4.34) become

$$-\frac{dG}{dr} = \frac{E - m_0c^2}{c\hbar}F, \tag{4.39}$$

$$\frac{dF}{dr} = \frac{E + m_0c^2}{c\hbar}G. \tag{4.40}$$

Combining the above, we have the relation

$$\frac{d^2F}{dr^2} = -\frac{E^2 - m_0^2c^4}{c^2\hbar^2}F. \tag{4.41}$$

Hence, the solution for $r \to \infty$ is

$$F = e^{-kr}, \quad k = \sqrt{\frac{m_0^2c^4 - E^2}{c^2\hbar^2}}. \tag{4.42}$$

Considering the radial Dirac equations for $r \to 0$, we obtain

$$\left[-\frac{d}{dr} + \frac{\omega(J+\frac{1}{2})}{r}\right]G = \frac{Z\alpha_e}{r}F, \tag{4.43}$$

$$\left[\frac{d}{dr} + \frac{\omega(J+\frac{1}{2})}{r}\right]F = \frac{Z\alpha_e}{r}G. \tag{4.44}$$

These can also be combined to yield

$$\left\{r\frac{d^2}{dr^2} + \frac{d}{dr} + \frac{1}{r}\left[(Z\alpha_e)^2 - \left(J + \frac{1}{2}\right)^2\right]\right\}F = 0. \tag{4.45}$$

Hence, the solution for $r \to 0$ is

$$F = r^s, \quad s = +\sqrt{\left(J + \frac{1}{2}\right)^2 - (Z\alpha_e)^2}. \tag{4.46}$$

We now introduce the substitutions

$$\begin{aligned} &\rho = kr, \quad (r) = \hat{F}(\rho), \quad G(r) = \hat{G}(\rho), \quad k = \sqrt{\frac{m_0^2c^4 - E^2}{c^2\hbar^2}}, \\ &\tau = \omega\left(J + \frac{1}{2}\right), \quad \nu = \sqrt{\frac{m_0c^2 - E}{m_0c^2 + E}}, \end{aligned} \tag{4.47}$$

so that the original radial equations become

$$\left(-\frac{d}{d\rho} + \frac{\tau}{\rho}\right)\hat{G} = \left(-\nu + \frac{Z\alpha_e}{\rho}\right)\hat{F}, \tag{4.48}$$

$$\left(\frac{d}{d\rho} + \frac{\tau}{\rho}\right)\hat{F} = \left(\frac{1}{\nu} + \frac{Z\alpha_e}{\rho}\right)\hat{G}. \tag{4.49}$$

Choosing

$$\hat{F}(\rho) = \rho^s e^{-\rho} \sum_i a_i \rho^i, \tag{4.50}$$

$$\hat{G}(\rho) = \rho^s e^{-\rho} \sum_i b_i \rho^i, \tag{4.51}$$

where $s = \sqrt{\tau^2 - (Z\alpha_e)^2}$, we obtain the following recursive formulae for the expansion coefficients

$$b_i = \frac{Z\alpha_e - \nu(\tau + s + i)}{\tau - s - i - \nu Z\alpha_e} a_i, \tag{4.52}$$

$$a_{i+1} \frac{(Z\alpha_e)^2 + (\tau + s + i + 1)(-\tau + s + i + 1)}{\tau - s - i - 1 - \nu Z\alpha_e} = a_i \frac{Z\alpha_e \nu^2 + 2\nu(s + i) - Z\alpha_e}{\nu(\tau - s - i - \nu Z\alpha_e)}. \tag{4.53}$$

Since $\hat{F}(\rho)$ and $\hat{G}(\rho)$ must converge at infinity, the power series expansion must break at some $i = n'$, which means

$$Z\alpha_e - 2\nu(n' + s) - \nu^2 Z\alpha_e = 0. \tag{4.54}$$

Hence, the quantization condition is

$$\nu = -\frac{n' + s}{Z\alpha_e} + \sqrt{\left(\frac{n' + s}{Z\alpha_e}\right)^2 + 1} \tag{4.55}$$

Using the previous substitutions from equation (4.47), the energy levels of bound spin-1/2 particles are

$$E_{n',J} = \frac{m_0 c^2}{\sqrt{1 + \frac{(Z\alpha_e)^2}{\left(n' + \sqrt{(J+\frac{1}{2}) - (Z\alpha_e)^2}\right)^2}}}. \tag{4.56}$$

Introducing the principal quantum number $n = n' + J + 1/2$, the final result is

$$E_{n,J} = \frac{m_0 c^2}{\sqrt{1 + \frac{(Z\alpha_e)^2}{\left(n - (J+\frac{1}{2}) + \sqrt{(J+\frac{1}{2})^2 - (Z\alpha_e)^2}\right)^2}}}, \tag{4.57}$$

where $n = 1, 2, 3, ...$ and $J = \frac{1}{2}, \frac{3}{2}, ..., n - \frac{1}{2}$. This can also be expanded in powers of $Z\alpha_e$ as

$$E_{n,J} = m_0 c^2 \left[1 - \frac{(Z\alpha_e)^2}{2n^2} - \frac{(Z\alpha_e)^4}{2n^4}\left(\frac{n}{J + \frac{1}{2}} - \frac{3}{4}\right) + ...\right]. \tag{4.58}$$

4.4 The Dirac Equation as Four Differential Equations

A more convenient way to express the Dirac Equation is by pre-multiplying Equation (4.1) by β. Then, we define the so-called Dirac matrices or gamma matrices as follows:

$$\gamma^0 = \beta, \quad \gamma^1 = \beta\alpha_1, \quad \gamma^2 = \beta\alpha_2, \quad \gamma^3 = \beta\alpha_3 \tag{4.59}$$

These equal

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \ \gamma^1 = \begin{pmatrix} 0 & \tau_1 \\ -\tau_1 & 0 \end{pmatrix}, \ \gamma^2 = \begin{pmatrix} 0 & \tau_2 \\ -\tau_2 & 0 \end{pmatrix}, \ \gamma^3 = \begin{pmatrix} 0 & \tau_3 \\ -\tau_3 & 0 \end{pmatrix}. \tag{4.60}$$

These matrices satisfy the hermiticity conditions

$$\gamma^{\mu\dagger} = \gamma^0\gamma^\mu\gamma^0. \tag{4.61}$$

as well as the relation

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}. \tag{4.62}$$

The Dirac Equation can then be written using the gamma matrices γ^μ as:

$$(i\hbar\gamma^\mu\partial_\mu - m_0c)\psi = 0. \tag{4.63}$$

We can write this as a matrix eigenvalue equation by moving the terms involving mc to the RHS and factoring out $i\hbar$ from the remaining terms in the LHS

$$i\hbar\begin{pmatrix} \partial_0 & 0 & \partial_3 & \partial_1 - i\partial_2 \\ 0 & \partial_0 & \partial_1 + i\partial_2 & -\partial_3 \\ -\partial_3 & -\partial_1 + i\partial_2 & -\partial_0 & 0 \\ -\partial_1 - i\partial_2 & \partial_3 & 0 & -\partial_0 \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = m_0c\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \tag{4.64}$$

When written out in its matrix components, this equation is, in fact, a system of four coupled differential equations:

$$(i\partial_0 - m_0c)\psi_1 + i\partial_3\psi_3 + (i\partial_1 + \partial_2)\psi_4 = 0, \tag{4.65}$$

$$(i\partial_0 - m_0c)\psi_2 + (i\partial_1 - \partial_2)\psi_3 - i\partial_3\psi_4 = 0, \tag{4.66}$$

$$-i\partial_3\psi_1 - (i\partial_1 + \partial_2)\psi_2 - (i\partial_0 + m_0c)\psi_3 = 0, \tag{4.67}$$

$$-i(\partial_1 + i\partial_2)\psi_1 + i\partial_3\psi_2 - (i\partial_0 + m_0c)\psi_4 = 0. \tag{4.68}$$

Since ψ is a four-component column vector in spinor space, the index j in ψ_j indicates which component in spinor space we are dealing with.
We now look at the four solutions satisfying the above equations, denoted by $\psi^{(n)}$ for $n = 1, 2, 3, 4$. Each of these is a full four-component vector in spinor space. Therefore, the superscript (n) indicates which complete vector we are dealing with. Thus, ${\psi^{(n)}}_j$ is the j^{th} component of the n^{th} vector.

4.4.1 Four Solution Vectors

We now look at the four solutions $\psi^{(n)}$ that satisfy Equation (4.64). First, we have

$$\psi^{(1)} = N_1\begin{pmatrix} 1 \\ 0 \\ \frac{p^3}{E+m_0} \\ \frac{p^1+ip^2}{E+m_0} \end{pmatrix} e^{-ipx} \equiv u_1 e^{-ipx}, \tag{4.69}$$

where u_1 is defined as the normalisation constant N_1 multiplied by the four-dimensional spinor factor.
Recall: px is in fact a four-component vector product, i.e.

$$px = p^\mu x_\mu = Et - \mathbf{p}\cdot\mathbf{x}. \tag{4.70}$$

All the derivatives in Equation (4.64) are with respect to space-time variables, hence they only act on e^{-ipx}; the spinor components are constants with respect to these derivatives.

The other three solutions are:

$$\psi^{(2)} = N_2 \begin{pmatrix} 0 \\ 1 \\ \frac{p^1 - ip^2}{E+m_0} \\ \frac{-p^3}{E+m_0} \end{pmatrix} e^{-ipx} \equiv u_2 e^{-ipx}, \tag{4.71}$$

$$\psi^{(3)} = N_3 \begin{pmatrix} \frac{p^3}{E+m_0} \\ \frac{p^1 + ip^2}{E+m_0} \\ 1 \\ 0 \end{pmatrix} e^{ipx} \equiv v_2 e^{ipx}, \tag{4.72}$$

$$\psi^{(4)} = N_4 \begin{pmatrix} \frac{p^1 - ip^2}{E+m_0} \\ \frac{-p^3}{E+m_0} \\ 0 \\ 1 \end{pmatrix} e^{ipx} \equiv v_1 e^{ipx}. \tag{4.73}$$

The symbol E is always a positive number equal to the energy and p^i is positive if it points in the positive direction of its respective axis. These are plane wave solutions where we have defined $u_r(\mathbf{p})$ and $v_r(\mathbf{p})$, $(r = 1, 2)$ as the column vectors multiplied by the constant shown. They are functions only of $\mathbf{p}$ for a given m_0 (since $E = \sqrt{\mathbf{p}^2 c^2 + m_0^2 c^4}$) and are called spinors, or four-spinors.
The four solutions are eigenstates of $\mathbf{p}$, since every measurement of the 3-momentum of the particles they represent results in the value $\mathbf{p}$. They are also eigenstates of energy, since for a given m_0, a free particle of 3-momentum $\mathbf{p}$ has a fixed E. As we will see, the solutions containing $u_r(\mathbf{p})$ are associated with particles and the solutions $v_r(\mathbf{p})$ with antiparticles. Note here the reverse order numbering on $v_{2,1}$ from $u_{1,2}$, which is customary.

4.5 Inner products of Spinors

We take all the spinors as functions of the same 3-momentum $\mathbf{p}$. Therefore, for the two pairs of spinors we have the general results:

$$u_r^\dagger(\mathbf{p}) u_s(\mathbf{p}) = v_r^\dagger(\mathbf{p}) v_s(\mathbf{p}) = \frac{E}{m_0} \delta_{rs}, \tag{4.74}$$

$$u_r^\dagger(\mathbf{p}) v_s(-\mathbf{p}) = 0. \tag{4.75}$$

4.5.1 Orthogonality of Eigensolutions

We can show that the eigensolutions (i.e. equations (4.69), (4.71)-(4.73)) to the Dirac Equation are orthogonal in the usual quantum mechanical way. For example, we can calculate the inner products

$$\langle \psi^{(1)} | \psi^{(2)} \rangle = \int \psi^{(1)\dagger} \psi^{(2)} \, d^3x = \int u_1^\dagger(\mathbf{p}) e^{ipx} u_2(\mathbf{p}) e^{-ipx} \, d^3x$$
$$= u_1^\dagger(\mathbf{p}) u_2(\mathbf{p}) \int e^{ipx} e^{-ipx} \, d^3x = 0 \tag{4.76}$$

$$\langle \psi^{(1)} | \psi^{(3)} \rangle = \int \psi^{(1)\dagger} \psi^{(3)} \, d^3x = \int u_1^\dagger(\mathbf{p}) e^{ipx} v_2(\mathbf{p}) e^{ipx} \, d^3x$$
$$= u_1^\dagger(\mathbf{p}) v_2(\mathbf{p}) \int e^{ipx} e^{ipx} \, d^3x = 0 \tag{4.77}$$

By continuing calculations with different solution pairs, we have that in general,

$$\langle\psi^{(m)}|\psi^{(n)}\rangle = 0, \quad m \neq n. \tag{4.78}$$

However, the Dirac Equation still gives both positive and negative energies for a free particle: applying the Hamiltonian operator $i\hbar\partial/\partial t$ to Equations (4.69) and (4.71), we have:

$$i\hbar\frac{\partial}{\partial t}(u_{1,2}e^{-ipx}) = p^0 u_{1,2}e^{-ipx} = +E_{\mathbf{p}}u_{1,2}e^{-ipx} \tag{4.79}$$

And applying to Equations (4.72) and (4.73), we have:

$$i\hbar\frac{\partial}{\partial t}(v_{2,1}e^{ipx}) = -p^0 v_{2,1}e^{ipx} = -E_{\mathbf{p}}v_{2,1}e^{ipx} \tag{4.80}$$

[2]

4.6 Interpretation of negative solutions

The Dirac equation provides a mathematical framework for the relativistic quantum mechanics of spin-1/2 fermions in which the properties of spin and magnetic moments are intrinsic, as seen in the description of the hydrogen atom. However, the presence of negative energy solutions is unavoidable. In quantum mechanics, a complete set of basis states is required to span the vector space, therefore the negative energy solutions cannot be discarded as being unphysical. It is therefore necessary to provide a physical interpretation for the negative energy solutions.

If negative energy solutions represented accessible negative energy particle states, we would expect all positive energy electrons to fall spontaneously into these lower energy states. To avoid this apparent contradiction, Dirac proposed that the vacuum corresponds to the state where all negative energy states are occupied. This is the "Dirac sea" picture, where the Pauli exclusion principle prevents positive energy electrons from falling into the fully occupied negative energy states. This assumption of a sea occupied by electrons has many consequences. For example, an electron with negative energy can shift into a state of positive energy by absorbing radiation. If this occurs, one observes an electron with charge $+e$ and energy $+E$. Additionally, a hole is created in the sea of negative energies indicating the absence of an electron with charge $+e$ and energy E. An observer relative to the vacuum perceives this hole as a particle of charge e and energy $+E$ (antiparticle). Thus, this theory also provides an explanation for the creation of particle-antiparticle pairs (pair creation).

The effect opposite to pair creation, the particle-antiparticle annihilation (pair annihilation), can equally be described within the hole theory. Here, a light emitting electron falls into an electron hole in the sea of negative energies and hence destroys the positron associated with the hole. [11], [4]

4.7 Interaction with electromagnetic fields and gauge invariance

We know that the electric and magnetic fields, which are obtained from the scalar and vector potentials ϕ and $\mathbf{A}$ do not change under the gauge transformation

$$\phi \to \phi' = \phi - \frac{1}{c}\frac{\partial\chi}{\partial t}, \quad \mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\chi, \tag{4.81}$$

which can be written more succintly as

$$A_\mu \to A'_\mu = A_\mu - \partial_\mu\chi. \tag{4.82}$$

In relativistic quantum mechanics, we can relate the gauge invariance of electromagnetism to a local gauge principle defined by

$$\psi(x) \to \psi'(x) = e^{ie\chi(x)}\psi(x), \tag{4.83}$$

where e is the electric charge of the particle. For this local phase transformation, the free-particle Dirac equation

$$i\hbar\gamma^\mu \partial_\mu \psi = m_0 c\psi \tag{4.84}$$

becomes

$$i\hbar\gamma^\mu \partial_\mu (e^{ie\chi(x)}\psi) = m_0 c e^{ie\chi(x)}\psi, \tag{4.85}$$

or equivalently,

$$i\hbar\gamma^\mu (\partial_\mu + ie\partial_\mu \chi)\psi = m_0 c\psi. \tag{4.86}$$

This differs from the original equation by the term $-e\hbar\gamma^\mu(\partial_\mu \chi)\psi$. Therefore, the free-particle Dirac equation is not invariant under the local phase transformation given in (4.83). More generally, local phase invariance is not possible for a theory that does not include interactions. The required invariance can be established only by modifying the Dirac equation to include the interaction term $e\gamma^\mu A_\mu \psi$ such that the original equation becomes

$$i\hbar\gamma^\mu (\partial_\mu + ieA_\mu)\psi = m_0 c\psi. \tag{4.87}$$

This is invariant under the local phase transformation given in (4.83), provided that A_μ transforms according to equation (4.82). Therefore, the requirement that the Dirac equation is invariant under a local phase transformation implies the existence of a gauge field A_μ corresponding to photons which couples to spin-1/2 particles (fermions).

4.8 Conservation of probability

Taking the Hermitian conjugate of the Dirac equation, we have

$$-i\hbar\partial_\mu \psi^\dagger \gamma^{\mu\dagger} - m_0 c\psi^\dagger = 0. \tag{4.88}$$

Multiplying both sides from the right with γ^0 and defining the adjoint spinor of ψ as

$$\bar{\psi}(x) = \psi^\dagger(x)\gamma^0, \tag{4.89}$$

we find the adjoint Dirac equation

$$-i\hbar\partial_\mu \bar{\psi}\gamma^\mu - m_0 c\bar{\psi} = 0, \tag{4.90}$$

where we have used the hermiticity conditions for gamma matrices given in (4.61). If we now define the four-current

$$j^\mu = \bar{\psi}\gamma^\mu\psi \tag{4.91}$$

and assume that it is a Lorentz-covariant quantity (proof will be given in the next section), then using the Dirac equation, we have

$$\partial_\mu j^\mu = (\partial_\mu \bar{\psi})\gamma^\mu\psi + \bar{\psi}\gamma^\mu\partial_\mu\psi = i\frac{m_0 c}{\hbar}\bar{\psi}\psi - i\frac{m_0 c}{\hbar}\bar{\psi}\psi = 0. \tag{4.92}$$

This means that j^μ satisfies the continuity equation and hence it is a conserved four-current. Note here that $\rho = j^0 = \psi^\dagger\psi$ is positive definite, hence the Dirac equation removes the problem of negative probabilities given by the Klein-Gordon equation.

4.9 Lorentz covariance of Dirac equation

The Lorentz covariance of Dirac equation means that if in a given reference frame equation (4.63) holds, then in any other reference frame related to the former one by a Lorentz transformation, the same must hold, although in the transformed variables. We have that the Dirac equation is for a frame O' and a frame O respectively,

$$(i\hbar\gamma^\mu\partial'_\mu - m_0c)\psi'(x') = 0, \tag{4.93}$$

$$(i\hbar\gamma^\mu\partial_\mu - m_0c)\psi(x) = 0, \tag{4.94}$$

where $\partial'_\mu = \frac{\partial}{\partial x'_\mu}$ and $x'^\mu = \Lambda^\mu{}_\nu x^\nu$. The requirement that (4.93) holds in the new frame O' implies the existence of an invertible matrix $S \equiv S^\alpha{}_\beta$ acting as a Lorentz transformation on a spinor $\psi(x)$ as follows:

$$\psi'^\alpha(x') = S^\alpha{}_\beta\psi^\beta(x). \tag{4.95}$$

Since

$$\frac{\partial}{\partial x'^\mu} = \frac{\partial x^\nu}{\partial x'^\mu}\frac{\partial}{\partial x^\nu} = (\Lambda^{-1})^\nu{}_\mu\partial_\nu, \tag{4.96}$$

we have that

$$\Big(i\hbar\gamma^\mu\partial'_\mu - m_0c\Big)\psi'(x') = \Big(i\hbar\gamma^\mu(\Lambda^{-1})^\nu{}_\mu\partial_\nu - m_0c\Big)S\psi(x) = 0. \tag{4.97}$$

By multiplying both sides from the left with S^{-1}, we have

$$\Big[i\hbar(\Lambda^{-1})^\nu{}_\mu\Big(S^{-1}\gamma^\mu S\Big)\partial_\nu - m_0c\Big]\psi(x) = 0. \tag{4.98}$$

Provided that the matrix S satisfies the relation

$$(\Lambda^{-1})^\nu{}_\mu S^{-1}\gamma^\mu S = \gamma^\nu \iff S^{-1}\gamma^\nu S = \Lambda^\nu{}_\mu\gamma^\mu, \tag{4.99}$$

equation (4.98) becomes

$$(i\hbar\gamma^\nu\partial_\nu - m_0c)\psi(x) = 0, \tag{4.100}$$

i.e. we retrieve the Dirac equation.

Now we also check that the current j^μ is Lorentz covariant (transforms as a four-vector). From equation (4.95) and using the definition of an adjoint spinor, we have

$$\bar{\psi}'(x') = \overline{S\psi(x)} = \psi^\dagger(x)S^\dagger\gamma^0, \tag{4.101}$$

therefore using that $(\gamma^0)^2 = I$ we have

$$\bar{\psi}'(x')\gamma^\mu\psi'(x') = \psi^\dagger(x)\gamma^0(\gamma^0 S^\dagger\gamma^0)\gamma^\mu S\psi(x) = \bar{\psi}(\gamma^0 S^\dagger\gamma^0)\gamma^\mu S\psi \tag{4.102}$$

Assuming that

$$\gamma^0 S^\dagger\gamma^0 = S^{-1} \tag{4.103}$$

holds and using the relation satisfied by S from above, we arrive at

$$\bar{\psi}'(x')\gamma^\mu\psi'(x') = \bar{\psi}(x)S^{-1}\gamma^\mu S\psi = \Lambda^\mu{}_\nu\bar{\psi}(x)\gamma^\nu\psi(x), \tag{4.104}$$

which shows that the current j^μ transforms as a four-vector. A complete proof of the properties satisfied by the matrix S is found in [5].

5 Conclusions

The Klein-Gordon as well as the Dirac theory provides experimentally verifiable predictions as long as they are restricted to low energy phenomena where particle creation and annihilation processes do not play any role. However, as soon as one attempts to include high energy processes both theories exhibit deficiencies and contradictions. It is quantum field theories that are regarded as "not being demonstrably false" for the description of microscopic natural phenomena. They can be Lorentz-covariantly formulated, thus being in agreement with special relativity and they are many-particle theories with infinitely many degrees of freedom and can account for particle creation and annihilation processes.

Quantum Field Theory employs creation and destruction operators acting on wavefunctions and these creation/destruction operators are part of a mathematical relationship, called a transition amplitude, describing a transition from an initial set of particles to a final set (i.e. an interaction). The absolute value of the transition amplitude equals the probability of finding (upon measurement) that the interaction occurred. This is similar to the square of the absolute value of the wave function in NRQM equaling the probability density of finding the particle.
In Quantum Field Theory, we will use a function called the Lagrangian density. This will determine how the particles (their wavefunctions) evolve in time. By requiring a certain mathematical symmetry of the Lagrangian called gauge symmetry (invariance of the Lagrangian under a specific group of transformations), we will establish what gauge bosons must exist and this will determine how the particles interact. [11], [12]

References

[1] B. Schutz, *A First Course In General Relativity*, 2nd ed. (Cambridge University Press, Cambridge, 2009), pp. 9-12, 33-45, 56-66, 68-70.

[2] R. Klauber, *Student Friendly Quantum Field Theory*, 2nd ed. (Sandtrove Press, Fairfield, Iowa, 2013), pp. 40-47, 84-92.

[3] D. Schaum, W. Duffin and C. Merwe, *Schaum's Outline Of Theory And Problems Of College Physics* (McGraw-Hill Book Company, New York, 1977).

[4] A. Wachter, *Relativistische Quantenmechanik* (Springer, Berlin, 2011), pp. 5-11, 51-52, 66-68, 73-75, 86-92, 151-152, 163-166, 169-171.

[5] J. Bjorken and S. Drell, *Relativistic Quantum Mechanics* [By] James D. Bjorken [And] Sidney D. Drell (McGraw-Hill, New York, 1964).

[6] R. D'Auria and M. Trigiante, *From Special Relativity To Feynman Diagrams* (Springer International Publishing, Cham, 2016).

[7] D. Griffiths, *Introduction To Electrodynamics*.

[8] D. Kay, *Tensor Calculus* (McGraw-Hill, New York, 2011).

[9] D. Fleisch, *A Student's Guide To Vectors And Tensors* (Cambridge University Press, Cambridge, 2017).

[10] J. Sakurai, *Modern Quantum Mechanics* (Pearson, Harlow, 2013).

[11] M. Thomson, *Modern Particle Physics* (Cambridge University Press, Cambridge, 2018).

[12] Royal Holloway PH3520 *Lecture Notes on Particle Physics*

[13] http://mathworld.wolfram.com/EinsteinSummation.html