ALBERT MESSIAH

QUANTUM MECHANICS

VOLUME II

JOHN WILEY & SONS, INC. • NEW YORK • LONDON • SYDNEY
A NORTH-HOLLAND BOOK

ORIGINAL TITLE: MÉCANIQUE QUANTIQUE, VOL. II

TRANSLATED FROM THE FRENCH

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MÉCANIQUE QUANTIQUE I AND II WERE PUBLISHED BY

DUNOD, PARIS

SIXTH PRINTING, SEPTEMBER, 1966

PUBLISHERS:

NORTH-HOLLAND PUBLISHING COMPANY, AMSTERDAM

JOHN WILEY & SONS, INC. – New York · London · Sydney

Printed in the United States of America

CHAPTER XX

THE DIRAC EQUATION

I. GENERAL INTRODUCTION

1. Relativistic Quantum Mechanics [1])

All of the applications made up to the present have been based on the Schrödinger equation. This equation, deduced by the correspondence principle from the Hamiltonian formalism of non-relativistic Classical Mechanics, has all the invariance properties of the Hamiltonian from which it derives. In particular, if the system is isolated, it is invariant under spatial rotations and translations. It can also be shown that it is invariant under Galilean transformations (cf. Problem XV.7). Therefore, the physical properties predicted by the Schrödinger theory are invariant in a Galilean change of referential, but they do not have the invariance under a Lorentz change of referential required by the principle of relativity. Since the Galilean transformation approximates to the Lorentz transformation only in the limit of small velocities, one expects – and experiment verifies – that this theory will correctly describe phenomena only when the velocities of the particles involved are negligible beside the velocity of light: $v \ll c$. In particular, all phenomena concerning the interaction between light and matter, such as emission, absorption or scattering of photons, is outside the framework of non-relativistic Quantum Mechanics.

One of the main difficulties in elaborating relativistic Quantum Mechanics comes from the fact that the *law of conservation of the number of particles ceases in general to be true*. Due to the equivalence of mass and energy, one of the most important consequences of relativity, there can be creation or absorption of particles whenever the interactions give rise to energy transfers equal or superior to the rest masses of these particles. To be a complete theory, Relativistic Quantum Mechanics must encompass in a single scheme dynamical

[1]) Knowledge of Sections I and II of Appendix D is recommended for reading this chapter.

states differing not only by the quantum state, but also by the *number* and the *nature* of the elementary particles of which they are composed. For this, we must turn to the concept of the quantized field, whence the name of Quantum Field Theory currently given to Relativistic Quantum Mechanics. This theory, in its present form, is exempt neither of difficulties nor even of contradictions, but it accounts for a very large body of experimental facts.

The fifth and last part of this book is designed to serve as an introduction to Quantum Field Theory and at the same time to furnish elementary methods for calculating certain relativistic effects concerning the dynamics of the electron and the interaction between the electromagnetic field and charged particles.

It is made up of two chapters.

The present chapter, the first of the two, is devoted to one of the simplest problems in Relativistic Quantum Mechanics, the problem of a particle of spin $\frac{1}{2}$ in a given force field. One of the most important examples is the electron in an electromagnetic field. The field is not quantized and one tries to describe the evolution of the system with a wave equation having the invariance properties required by the principle of relativity. This equation must also satisfy the correspondence principle and give the Pauli theory in the non-relativistic approximation. Such an equation exists: it is called the Dirac equation. After reviewing the Lorentz Group and Classical Relativistic Dynamics (Section I) we establish the Dirac equation (Section II), and make a detailed study of its invariance properties (Section III). In the remainder of this chapter we discuss the physical significance of the theory, and, in the course of reviewing its principal applications, examine how it is situated with respect to Classical Dynamics (Section IV), non-relativistic Quantum Mechanics (Section V) and Quantum Field Theory (Section VI).

The second chapter is devoted to the concept of the quantized field, and to the elementary Quantum theory of electromagnetic radiation and its interaction with atomic and nuclear systems.

2. Notation, Various Conventions and Definitions

UNITS. Except for a few obvious exceptions, all expressions appearing in what follows are written with

$$\hbar = c = 1.$$

With this particular choice of units, time appears to have the dimension of a length; energies, momenta and masses the dimension of an inverse length; electric charges appear as dimensionless quantities ($e^2 \equiv e^2/\hbar c \simeq 1/137$). The general expressions may be re-established by simple considerations of homogeneity.

Coordinates. Specification of an instant t and a point $\boldsymbol{r} \equiv (x, y, z)$ of ordinary space defines a point of space-time. We denote the coordinates of this point by x^0, x^1, x^2, x^3; $x^0 \equiv ct$ is the time coordinate; x^1, x^2, x^3 the three spatial coordinates: $x^1 \equiv x, x^2 \equiv y, x^3 \equiv z$. More generally, we use the indices 0, 1, 2, 3 to denote the components of four-vectors or tensors along the axes t, x, y, z respectively. Greek indices denote the space-time components of four-vectors or tensors and therefore take the four values 0, 1, 2, 3; roman indices are reserved for the components of ordinary space and therefore take the three values 1, 2, 3. Thus:

$$x^\mu \equiv (x^0, x^k) \equiv (x^0, x^1, x^2, x^3)$$
$$(\mu = 0, 1, 2, 3) \qquad (k = 1, 2, 3).$$

Metric tensor, covariant and contravariant indices

The space-time metric is a pseudo-euclidian metric defined by the *metric tensor*

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

or again

$$g_{00} = 1, \quad g_{kk} = -1, \quad g_{\mu\nu} = 0 \text{ if } \mu \neq \nu. \qquad \text{(XX.1)}$$

We distinguish between *covariant* vectors (that transform like $\partial/\partial x^\mu$) and *contravariant* vectors (that transform like x^μ), and more generally between covariant tensor components and contravariant tensor components. Following the usual convention, covariant indices are placed as subscripts, contravariant indices as superscripts. Thus a^μ denotes a contravariant vector. The corresponding covariant vector a_μ is obtained by application of the metric tensor:

$$a_\mu = \sum g_{\mu\nu} a^\nu,$$

which gives

$$a_0 = a^0, \qquad a_k = -a^k.$$

We shall always follow *the convention of summing over repeated indices*. With this convention the preceding relation becomes simply

$$a_\mu = g_{\mu\nu} a^\nu.$$

Similarly, indices are raised by applying the tensor $g^{\mu\nu}$:

$$a^\mu = g^{\mu\nu} a_\nu.$$

In the present case, we also have

$$g^{\mu\nu} = g_{\mu\nu}.$$

In addition:

$$g_\mu^{\ \nu} = g_{\mu\varrho} g^{\varrho\nu} = g^\mu_{\ \nu} = \delta_\mu^{\ \nu},$$

where $\delta_\mu^{\ \nu}$ is the Kronecker symbol:

$$\delta_\mu^{\ \nu} = \begin{cases} 1 & \text{if} \quad \mu = \nu \\ 0 & \text{if} \quad \mu \neq \nu. \end{cases}$$

THREE-VECTORS, FOUR-VECTORS, SCALAR PRODUCT

For three-vectors, or vectors of ordinary space, we retain the usual notation; each of them is denoted by a bold-face letter and its length by the corresponding character in ordinary print.

The three space components of a contravariant four-vector a^μ form a three-vector. With the above notations, we therefore have

$$a^\mu \equiv (a^0, a^1, a^2, a^3) \equiv (a^0, \mathbf{a}) \quad \mathbf{a} \equiv (a_x, a_y, a_z)$$

$$a^1 = a_x \quad a^2 = a_y \quad a^3 = a_z \quad a \equiv (\mathbf{a}\cdot\mathbf{a})^{\frac{1}{2}} \equiv [a_x{}^2 + a_y{}^2 + a_z{}^2]^{\frac{1}{2}}.$$

When no confusion is possible with the length of the three-vector $\mathbf{a}$, we shall sometimes omit the index and denote the four-vector a^μ simply by a.

The scalar product of two four-vectors a^μ and b^μ is obtained by contracting the contravariant components of the one with the co-variant components of the other, i.e. it is given by either $a_\mu b^\mu$, or $a^\mu b_\mu$:

$$a_\mu b^\mu = a^\mu b_\mu = a^0 b^0 - \mathbf{a}\cdot\mathbf{b} \tag{XX.2}$$

The *norm* of a^μ is $a_\mu a^\mu = (a^0)^2 - a^2$.

Classifications of the four-vectors

The four-vectors may be put into three classes, according to the sign of their norm

$$\begin{aligned} a_\mu a^\mu &< 0 \qquad a^\mu = \text{space-like vector} \\ a_\mu a^\mu &= 0 \qquad a^\mu = \text{null vector} \\ a_\mu a^\mu &> 0 \qquad a^\mu = \text{time-like vector} \end{aligned}$$

This classification corresponds to the position of the vector with respect to the light cone $x_\mu x^\mu = 0$. The two latter cases can be further classified according to the sign of the time component:

$a^0 > 0$ the vector points towards the future;
$a^0 < 0$ the vector points towards the past.

Gradient, differential operators

We retain the notation $\nabla \equiv (\partial/\partial x, \partial/\partial y, \partial/\partial z)$ and $\triangle \equiv \nabla \cdot \nabla$.

The four partial-differentiation operators $\partial/\partial x^\mu$ form a *covariant* vector, called the gradient operator, which we denote by the symbol ∂_μ:

$$\begin{aligned} \partial_\mu \equiv \partial/\partial x^\mu &\equiv (\partial/\partial x^0, \partial/\partial x^1, \partial/\partial x^2, \partial/\partial x^3) \\ &\equiv (\partial/\partial ct, \nabla). \end{aligned} \tag{XX.3}$$

We shall also make use of the "contravariant gradient":

$$\partial^\mu \equiv g^{\mu\nu}\partial_\nu \equiv (\partial/\partial ct, -\nabla). \tag{XX.4}$$

The Dalembertian $\Box$ is defined [1]) by (cf. § II.12):

$$\Box \equiv \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \triangle \equiv \partial_\mu \partial^\mu. \tag{XX.5}$$

The $\varepsilon^{\lambda\mu\nu\varrho}$ tensor

$\varepsilon^{\lambda\mu\nu\varrho}$ denotes the completely antisymmetrical tensor with four indices, the components of which are equal to 0 if two of the indices are equal, to $+1$ if $(\lambda\mu\nu\varrho)$ is an even permutation of (0, 1, 2, 3), and to -1 if $(\lambda\mu\nu\varrho)$ is an odd permutation of (0, 1, 2, 3).

Electromagnetic field

The electromagnetic potential is made up of a vector term $\mathbf{A}(\mathbf{r}, t)$ and a scalar potential $\varphi(\mathbf{r}, t)$ which form a four-vector A^μ:

$$A^\mu \equiv (\varphi, \mathbf{A}). \tag{XX.6}$$

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[1]) Many authors use the symbol $\Box$ to denote the negative of the operator defined here.

The electric field $\mathscr{E}$ and the magnetic field $\mathscr{H}$ are given by

$$\mathscr{E} = -\nabla\varphi - \partial A/\partial x^0, \qquad \mathscr{H} = \text{curl}\,\mathbf{A}. \tag{XX.7}$$

The components of $\mathscr{E}$ and $\mathscr{H}$ form an antisymmetrical space-time tensor, $F_{\mu\nu}$, according to the definition

$$F_{\mu\nu} = \frac{\partial A_\nu}{\partial x^\mu} - \frac{\partial A_\mu}{\partial x^\nu} \tag{XX.8}$$

giving

$$F_{\mu\nu} \equiv \begin{pmatrix} 0 & \mathscr{E}_x & \mathscr{E}_y & \mathscr{E}_z \\ -\mathscr{E}_x & 0 & -\mathscr{H}_z & \mathscr{H}_y \\ -\mathscr{E}_y & \mathscr{H}_z & 0 & -\mathscr{H}_x \\ -\mathscr{E}_z & -\mathscr{H}_y & \mathscr{H}_x & 0 \end{pmatrix} \tag{XX.9}$$

We shall also use the four-vector operator D_μ defined by

$$D_\mu \equiv \partial_\mu + \mathrm{i}eA_\mu \equiv \left(\frac{\partial}{\partial x^0} + \mathrm{i}e\varphi,\, \nabla - \mathrm{i}e\mathbf{A}\right). \tag{XX.10}$$

3. The Lorentz Group

A Lorentz change of referential is a *real*, *linear* transformation of the coordinates *conserving the norm* of the intervals between the different points of space-time. In such a transformation, the new coordinates x'^μ of a space-time point are obtained from the old ones x^μ by the relation

$$x'^\mu = \Omega^\mu{}_\nu x^\nu + a^\mu.$$

The real vector a^μ represents a simple translation of the space-time axes. In what follows, we shall treat the translations separately and give the name of Lorentz transformation to the homogeneous transformations $(a^\mu = 0)$ [1]:

$$x'^\mu = \Omega^\mu{}_\nu\, x^\nu. \tag{XX.11}$$

By raising or lowering the indices, we can obtain the matrices $\Omega_\mu{}^\nu$, $\Omega^{\mu\nu}$, $\Omega_{\mu\nu}$ from the matrix $\Omega^\mu{}_\nu$ (for example: $\Omega^{\mu\nu} = g^{\nu\varrho}\Omega^\mu{}_\varrho$). Specification of any one of these matrices defines the Lorentz trans-

1) The group formed by all of the Lorentz transformations including the translations is commonly called the *inhomogeneous Lorentz group*, or *Poincaré group*.

formation question. The condition of reality and of invariance of the norm are written

$$\Omega_{\mu\nu}{}^* = \Omega_{\mu\nu} \tag{XX.12}$$

$$\Omega_{\mu\nu}\Omega^{\mu\lambda} = \Omega_{\nu\mu}\Omega^{\lambda\mu} = \delta_\nu^{\ \lambda}. \tag{XX.13}$$

It follows that

$$\det |\Omega^\mu{}_\nu| = \pm 1 \tag{XX.14}$$

and the inverse transformation is written

$$x^\mu = x'^\nu \Omega_\nu{}^\mu. \tag{XX.15}$$

These transformations form a group, *the complete Lorentz group.* It is the group of real linear transformations conserving scalar products between four-vectors.

If $\Omega^{00} > 0$, the transformation conserves the sense of time-like vectors, that is, it conserves the sign of the time component of these vectors; it is then called orthochronous, and the set of these particular Lorentz transformations is called *the orthochronous Lorentz group.* If *in addition* $\det |\Omega^\mu{}_\nu| = +1$, the transformation also conserves the sense of Cartesian systems in ordinary space, it is then called a proper Lorentz transformation. The ensemble of these transformation forms a group, *the proper Lorentz group*, which we denote by $\mathscr{L}_0$.

All transformations of the proper group may be considered as a succession of infinitesimal transformations. The matrix $\Omega_{\mu\nu}$ of an *infinitesimal Lorentz transformation* is of the form

$$g_{\mu\nu} + \omega_{\mu\nu},$$

where the quantities $\omega_{\mu\nu}$ are infinitesimals. Conditions (XX.12) and (XX.13) give

$$\omega_{\mu\nu} = \omega_{\mu\nu}{}^*, \qquad \omega_{\mu\nu} + \omega_{\nu\mu} = 0. \tag{XX.16}$$

$\omega_{\mu\nu}$ is therefore a real antisymmetrical tensor.

Put

$$Z^{(\alpha\beta)}_{\mu\nu} = - Z^{(\beta\alpha)}_{\mu\nu} = g_{\mu\alpha} g_{\nu\beta} - g_{\mu\beta} g_{\nu\alpha}. \tag{XX.17}$$

$Z^{(\alpha\beta)}_{\mu\nu}$ is an antisymmetrical tensor whose only non-vanishing elements are the two elements $\mu = \alpha, \nu = \beta$ and $\mu = \beta, \nu = \alpha$; one of which is equal to $+1$, the other to -1. ε being an infinitesimal quantity,

$$g_{\mu\nu} - \varepsilon Z^{(\alpha\beta)}_{\mu\nu}$$

is the matrix of a particular infinitesimal Lorentz transformation, the "rotation" through an angle ε in the $x^\alpha x^\beta$ plane.

There exists in all six infinitesimal transformations of this type. The "rotations" in the planes x^1x^2, x^2x^3 and x^3x^1 are spatial rotations of angle ε about the axes Oz, Ox, Oy respectively, the "rotations" in the planes x^1x^0, x^2x^0, x^3x^0 are special Lorentz transformations of velocity ε in the directions Ox, Oy, Oz respectively [1]).

In addition to infinitesimal transformations, one can define different types of *reflection*, notably the spatial reflection s ($x^0 = x^0$, $x^k = -x^k$) and the time reflection t ($x^0 = -x^0$, $x^k = x^k$). The orthochronous group is made up of the transformations $\mathscr{L}_0$, of the reflection s and of their products $s\mathscr{L}_0$. The complete group is formed of the transformations $\mathscr{L}_0$, $s\mathscr{L}_0$, $t\mathscr{L}_0$, and $st\mathscr{L}_0$. The properties of these four sheets of the complete group are summed up in the following table:

Sheet	Det $\mid \Omega^\mu{}_\nu \mid$	Ω^{00}	group		
$\mathscr{L}_0$	$+1$	> 0	proper	orthochronous	complete
$s\mathscr{L}_0$	-1	> 0			
$t\mathscr{L}_0$	-1	< 0			
$st\mathscr{L}_0$	$+1$	< 0			

1) If the new referential is obtained from the old one by a rotation through a finite angle φ about Oz, one has:

$$x'^1 = x^1 \cos\varphi + x^2 \sin\varphi, \quad x'^2 = x^2 \cos\varphi - x^1 \sin\varphi, \quad x'^3 = x^3, \quad x'^0 = x^0.$$

If it is obtained by a special Lorentz transformation of velocity $v = \tanh\varphi$ directed along Ox, one has

$$x'^1 = x^1 \cosh\varphi - x^0 \sinh\varphi, \quad x'^0 = x^0 \cosh\varphi - x^1 \sinh\varphi, \quad x'^2 = x^2, \quad x'^3 = x^3.$$

The transformations considered above correspond to the case when $\varphi = \varepsilon \equiv$ infinitesimal.

4. Classical Relativistic Dynamics

Let us recall the dynamical properties of a classical particle of rest mass m and charge e in an electromagnetic field $(\varphi, \mathbf{A})$.

Let $\mathbf{v}$ be the velocity of the particle:

$$\mathbf{v} \equiv \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}. \tag{XX.18}$$

We define the relativistic mass M and the mechanical momentum [1] $\boldsymbol{\pi}$ by:

$$M \equiv \frac{m}{\sqrt{1-v^2}}, \qquad \boldsymbol{\pi} \equiv M\mathbf{v} \tag{XX.19}$$

$(M, \boldsymbol{\pi})$ is a certain four-vector π^μ of norm m^2:

$$M^2 - \boldsymbol{\pi}^2 = m^2 \tag{XX.20}$$

and pointing into the future $(M > 0)$.

In the absence of a field, the particle follows a uniform rectilinear motion: $\mathbf{v} = Cst.$

In the presence of an electromagnetic field, the trajectory followed by the particle satisfies the equation

$$\frac{\mathrm{d}\boldsymbol{\pi}}{\mathrm{d}t} = e[\mathscr{E} + \mathbf{v} \times \mathscr{H}] \equiv \mathbf{F}. \tag{XX.21}$$

This is the fundamental equation of the relativistic dynamics of a material point. The vector $\mathbf{F}$ is called the *Lorentz force.*

From (XX.21) we have the equations

$$\frac{\mathrm{d}M}{\mathrm{d}t} = (\mathbf{v}\cdot\mathbf{F}) = e(\mathbf{v}\cdot\mathscr{E}), \tag{XX.21$'$}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{r}\times\boldsymbol{\pi}) = \mathbf{r}\times\mathbf{F} \tag{XX.22}$$

giving respectively the law of motion of the mass and of the moment of the mechanical momentum.

These relations can be put in covariant form by introducing the proper time τ of the particle, in accordance with the definition

$$\begin{aligned}\mathrm{d}\tau &= (\mathrm{d}x^\mu\,\mathrm{d}x_\mu)^{\frac{1}{2}}\\ &= \sqrt{1-v^2}\,\mathrm{d}t.\end{aligned}$$

---

[1]) Not to be confused with the momentum which in this book means the Lagrange canonical conjugate of the coordinates (cf. note, p. 54, vol. I).

One defines the four-velocity

$$u^\mu \equiv \mathrm{d}x^\mu/\mathrm{d}\tau \equiv (\mathrm{d}t/\mathrm{d}\tau, \boldsymbol{v}\,\mathrm{d}t/\mathrm{d}\tau) \qquad (u^\mu u_\mu = 1)$$

whose product with m gives the mechanical four-momentum

$$\pi^\mu \equiv m\,u^\mu \equiv (M, \boldsymbol{\pi}).$$

Equations (XX.21) and (XX.21′) are equivalent to the formally covariant equation

$$\frac{\mathrm{d}\pi^\mu}{\mathrm{d}\tau} = eF^{\mu\nu} u_\nu, \tag{XX.23}$$

or

$$\frac{\mathrm{d}u^\mu}{\mathrm{d}\tau} = \frac{e}{m} F^{\mu\nu} u_\nu$$

$F^{\mu\nu}$ is the electromagnetic tensor [eqs. (XX.8–9)].

These laws of motion can be deduced from a Lagrangian or Hamiltonian formalism (cf. Problem I.5). The momentum $\boldsymbol{p}$ and the energy E form a four-vector p^μ, related to the four-vector π^μ by the relation

$$p^\mu = \pi^\mu + eA^\mu \tag{XX.24}$$

i.e.

$$E = M + e\varphi, \qquad \boldsymbol{p} = \boldsymbol{\pi} + e\boldsymbol{A}.$$

The Hamiltonian function is defined by

$$H \equiv e\varphi + \sqrt{(\boldsymbol{p} - e\boldsymbol{A})^2 + m^2} \tag{XX.25}$$

in accordance with relations (XX.24) and (XX.20). From (XX.25) we obtain Hamilton's canonical equations

$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = \frac{\boldsymbol{\pi}}{M}, \qquad \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -\,e\,\mathrm{grad}\,(\varphi - \boldsymbol{v}\cdot\boldsymbol{A}).$$

The first of these is the definition of velocity. The second is equivalent to (XX.21) as may easily be verified using the definitions of $\mathscr{E}$ and $\mathscr{H}$ [eq. (XX.7)] and the fact that

$$\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}t} = \left(\frac{\partial}{\partial t} + \boldsymbol{v}\cdot\mathrm{grad}\right)\boldsymbol{A}.$$

II. THE DIRAC AND KLEIN–GORDON EQUATIONS

5. The Klein–Gordon Equation

Since the problem of finding a relativistic wave equation for the electron is complicated by the existence of spin, we first look for a relativis quation for a particle of spin 0, a π meson for example. such a particle has no internal degrees of freedom, its wave function Ψ depends only on the variables $\boldsymbol{r}$ and t. Let m be its mass and e its charge, and suppose that it is moving in the electromagnetic potential $A^\mu \equiv (\varphi, \boldsymbol{A})$.

To find the wave equation we proceed empirically using the correspondence principle; this will guarantee that we obtain the classical laws of motion when the classical approximation is valid.

We recall that the Schrödinger correspondence rule is given by

$$E \to \mathrm{i}\frac{\partial}{\partial t}, \qquad \boldsymbol{p} \to -\mathrm{i}\nabla. \tag{XX.26}$$

Putting $p^\mu \equiv (E, \boldsymbol{p})$, this rule can be written more simply:

$$p^\mu \to \mathrm{i}\partial^\mu. \tag{XX.26$'$}$$

From expression (XX.25) for the Hamiltonian we obtain

$$E = e\varphi + \sqrt{(\boldsymbol{p} - e\boldsymbol{A})^2 + m^2} \tag{XX.27}$$

from which we obtain, by rule (XX.26), the wave equation

$$\left(\mathrm{i}\frac{\partial}{\partial t} - e\varphi\right)\Psi = \left[\left(\frac{1}{\mathrm{i}}\nabla - e\boldsymbol{A}\right)^2 + m^2\right]^{\frac{1}{2}}\Psi.$$

This equation has two serious drawbacks. First, the dissymmetry between the space and time coordinates is such that relativistic invariance and its consequences are not clearly exhibited. Second, the operator on the right-hand side is a square root, which is practically untractable except when the field $\boldsymbol{A}$ vanishes.

One avoids these two difficulties by taking relation (XX.20) as the starting point of the correspondence operation, giving

$$(E - e\varphi)^2 - (\boldsymbol{p} - e\boldsymbol{A})^2 = m^2. \tag{XX.28}$$

This relation is not equivalent to (XX.27), but to the more general relation

$$E = e\varphi \pm \sqrt{(\boldsymbol{p} - e\boldsymbol{A})^2 + m^2}. \tag{XX.29}$$

Only the $+$ sign corresponds to real classical solutions; the $-$ sign represents solutions of negative mass without any physical significance. Thus by taking (XX.28) as a starting point we introduce *parasitic solutions of negative mass.*

The correspondence operation applied to (XX.28) gives the *Klein–Gordon equation*:

$$\left[\left(\mathrm{i}\frac{\partial}{\partial t} - e\varphi\right)^2 - \left(\frac{1}{\mathrm{i}}\nabla - e\mathbf{A}\right)^2\right]\Psi = m^2\Psi \qquad \text{(XX.30)}$$

which can also be written in the form

$$(D_\mu D^\mu + m^2)\Psi \equiv [(\partial_\mu + \mathrm{i}eA_\mu)(\partial^\mu + \mathrm{i}eA^\mu) + m^2]\Psi = 0, \qquad \text{(XX.30}')$$

where its relativistic invariance is evident.

Let us briefly consider the interpretation of this equation [1]). To simplify the discussion we limit ourselves to the case when the field vanishes. We then have simply (cf. § II.12):

$$(\Box + m^2)\Psi = 0. \qquad \text{(XX.31)}$$

This is a second-order differential equation with respect to the time, and we must therefore know both Ψ and $\partial\Psi/\partial t$ at the initial time for Ψ to be completely determined at any later time. This difficulty is easily surmounted if we postulate that the dynamical state of the system at a given time is represented not by the single function Ψ but by the set of two functions Ψ and $\partial\Psi/\partial t$ or by the two linear combinations:

$$\Phi = \Psi + \frac{\mathrm{i}}{m}\frac{\partial\Psi}{\partial t}, \qquad \chi = \Psi - \frac{\mathrm{i}}{m}\frac{\partial\Psi}{\partial t}.$$

This is equivalent to postulating that the state of the system is represented by a wave function with two components, Φ and χ. This wave function must obey a differential equation of the first order with respect to time which is easily deduced from the Klein–Gordon equation. In the non-relativistic limit, the energy of the particle is nearly equal to its rest mass m, so that

$$\mathrm{i}\frac{\partial\Psi}{\partial t} \simeq m\Psi$$

and therefore, $\chi \ll \Phi$. One of the two components becoming negligible beside the other, we obtain the non-relativistic Schrödinger theory in which the dynamical state of a particle of spin 0 is represented by a one-component wave function.

[1]) For a more complete account, see H. Feshbach and F. Villars, Rev. Mod. Phys. **30** (1958) 24, where a list of the main references will also be found.

In order to interpret the wave function, we must define a position probability density P and a current probability density $\boldsymbol{j}$ satisfying the equation of continuity (cf. § IV.4):

$$\frac{\partial P}{\partial t} + \nabla \cdot \boldsymbol{j} = 0 \tag{XX.32}$$

or with the notation $j^\mu \equiv (P, \boldsymbol{j})$

$$\partial_\mu j^\mu = 0. \tag{XX.33}$$

Since Ψ and Ψ^* both satisfy equation (XX.31),

$$\Psi^* (\Box \Psi) - (\Box \Psi^*) \Psi = 0$$

which gives, using the definition of the Dalembertian,

$$\partial_\mu [\Psi^* (\partial^\mu \Psi) - (\partial^\mu \Psi^*) \Psi] = 0.$$

The equation of continuity is satisfied if we take j^μ proportional to the bracket on the left-hand side. The proportionality constant is fixed so as to recover the usual definition in the non-relativistic limit:

$$j^\mu = \frac{\mathrm{i}}{2m} [\Psi^* (\partial^\mu \Psi) - (\partial^\mu \Psi^*) \Psi],$$

i.e.

$$\begin{aligned} P(\boldsymbol{r}, t) &= \frac{\mathrm{i}}{2m} \left[\Psi^* \frac{\partial \Psi}{\partial t} - \frac{\partial \Psi^*}{\partial t} \Psi \right] \\ \boldsymbol{j}(\boldsymbol{r}, t) &= \frac{1}{2\mathrm{i}m} [\Psi^* (\nabla \Psi) - (\nabla \Psi^*) \Psi]. \end{aligned} \tag{XX.34}$$

Examining (XX.34) we see that *the density* $P(\boldsymbol{r}, t)$ *is not positive-definite*. Here we have one of the major difficulties with the Klein–Gordon equation.

Another difficulty, related to the preceding one, is due to the possibility of "negative energy solutions". If, for example, we look for the plane wave solutions of the equation in the absence of a field,

$$\Psi = \exp[-\mathrm{i}(Et - \boldsymbol{p} \cdot \boldsymbol{r})]$$

we obtain, substituting this expression in (XX.31), the condition:

$$E = \pm \sqrt{\boldsymbol{p}^2 + m^2}.$$

There therefore exist solutions of negative energy $-\sqrt{\boldsymbol{p}^2 + m^2}$. Their presence is obviously due to the above-mentioned introduction of negative masses into the theory (it would be more correct to call them negative mass solutions; however when the field is null, the distinction between mass and energy is illusory).

Following Pauli and Weisskopf [1]), we deal with these difficulties by modifying the interpretation of the four-vector j^μ and the definition of average values. According to this reinterpretation of the theory, ej^μ denotes the current-density four-vector; in particular $eP(\mathbf{r}, t)$ is the electric charge density. Equation (XX.33) is therefore an equation for the conservation of the charge. On the other hand, the number of particles is not conserved; this is explained by the possibility of annihilation and creation of pairs of particles of opposite charge, phenomena that only Field Theory accounts for in a satisfactory manner. When formulated in this way, *the theory is therefore a one-charge theory and not a one-particle theory*. In the Dirac theory, on the contrary, one is able to define a positive-definite density P, however, we shall see that the difficulty with negative energies remains, and that the Dirac theory cannot be considered in an entirely satisfying fashion as being a one-particle theory either (Section VI).

6. The Dirac Equation

Let us now attempt to form a relativistic wave equation for the electron. Following Dirac, we proceed by analogy with non-relativistic Quantum Mechanics.

Just as the electron of the non-relativistic theory is represented by a two-component spinor which transforms under rotation like an angular momentum of value $\frac{1}{2}$, the electron of the relativistic theory must be represented by a wave function of several components having a certain well-defined variance with respect to the larger group of Lorentz transformations. We denote the s component of the wave Ψ by $\psi_s(\mathbf{r}, t)$. Ψ may be written in the form of a column matrix:

$$\Psi = \begin{vmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{vmatrix}$$

As in the non-relativistic case, one may equally well regard the wave Ψ at a given time as a function of the orbital variables $\mathbf{r}$ and

[1]) W. Pauli and V. Weisskopf, Helv. Phys. Acta **7** (1934) 709. See also H. Feshback and F. Villars *loc. cit.* note p. 886.

the intrinsic, or spin, variables s ($s=1, 2, \ldots, N$). Such a wave represents a certain state vector $|\psi(t)\rangle$; and the space of these states, $\mathscr{E}$, is the tensor product

$$\mathscr{E} = \mathscr{E}^{(0)} \otimes \mathscr{E}^{(s)}$$

of the orbital-variable space $\mathscr{E}^{(0)}$ by the spin-variable space $\mathscr{E}^{(s)}$; the wave Ψ represents this vector in a suitable representation:

$$\Psi(\mathbf{r}, s; t) \equiv \psi_s(\mathbf{r}, t) \equiv \langle \mathbf{r}s|\Psi(t)\rangle.$$

Continuing with the analogy, we define the position probability density by the formula

$$P(\mathbf{r}, t) = \sum_{s=1}^{N} |\psi_s|^2. \tag{XX.35}$$

With these hypotheses, the wave equation is necessarily of the form

$$\mathrm{i}\frac{\partial \Psi}{\partial t} = H_D \Psi, \tag{XX.36}$$

where H_D is a Hermitean operator of state-vector space. To see this, we note, on the one hand that since Ψ completely defines the dynamical state of the electron at each instant the wave equation must be of the first order with respect to time; on the other that H_D must be Hermitean in order to guarantee the self-consistency of our definition of $P(\mathbf{r}, t)$ (cf. § IV.3).

Since we are seeking a relativistic wave equation, we also require that it exhibit a certain formal symmetry between the spatial coordinates and the time namely that it also be of first order with respect to the spatial variables.

Let us first consider the case of an electron in the absence of field. The Hamiltonian must then be invariant under translation, thus independent of $\mathbf{r}$. Taking into account all the preceding hypotheses, it can therefore be written in the form

$$H_D = \boldsymbol{\alpha}\cdot\mathbf{p} + \beta m, \tag{XX.37}$$

where the operator $\mathbf{p}$ has the significance indicated by the correspondence rule (XX.26), i.e. $\mathbf{p} = -\mathrm{i}\nabla$, and where $\boldsymbol{\alpha} \equiv (\alpha_x, \alpha_y, \alpha_z)$ and β denote 4 Hermitean operators acting on the spin variables alone. If we adopt the notation $E \equiv \mathrm{i}\partial/\partial t$ the wave equation reads

$$[E - \boldsymbol{\alpha}\cdot\mathbf{p} - \beta m]\Psi = 0. \tag{XX.38}$$

To determine $\boldsymbol{\alpha}$ and β, we invoke the correspondence principle: we require the solutions of this equation to satisfy the Klein–Gordon equation, i.e. we require that

$$[E^2 - \boldsymbol{p}^2 - m^2]\Psi = 0. \tag{XX.39}$$

Multiplying on the left by the operator $[E + \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m]$, eq. (XX.38) gives the second-order equation

$$[E^2 - \sum_k (\alpha^k)^2 (p^k)^2 - \beta^2 m^2 - \sum_{k<l} (\alpha^k \alpha^l + \alpha^l \alpha^k)\, p^k p^l \\ - \sum_k (\alpha^k \beta + \beta \alpha^k)\, m p^k]\,\Psi = 0.$$

This equation and eq. (XX.39) are identical if the 4 operators β, $\boldsymbol{\alpha}$ anticommute and if their squares are equal to 1:

$$\begin{array}{lll} (\alpha^k)^2 = 1 & \alpha^k\alpha^l + \alpha^l\alpha^k = 0 & (k \neq l) \\ \beta^2 = 1 & \alpha^k\beta + \beta\,\alpha^k = 0 & \end{array} \tag{XX.40}$$

Equation (XX.38), in which the matrices β, $\boldsymbol{\alpha}$ are chosen to be Hermitean and to satisfy relation (XX.40), is called the Dirac equation.

From this equation for the free electron, we pass to the Dirac equation for an electron in the electromagnetic field (φ, $\boldsymbol{A}$) by making the substitution

$$E \to E - e\varphi, \qquad \boldsymbol{p} \to \boldsymbol{p} - e\boldsymbol{A} \tag{XX.41}$$

[e is the charge of the electron ($e < 0$)]. One obtains:

$$[(E - e\varphi) - \boldsymbol{\alpha}\cdot(\boldsymbol{p} - e\boldsymbol{A}) - \beta m]\,\Psi = 0 \tag{XX.42}$$

i.e.

$$\left[\left(\mathrm{i}\frac{\partial}{\partial t} - e\varphi\right) - \boldsymbol{\alpha}\cdot(-\mathrm{i}\nabla - e\boldsymbol{A}) - \beta m\right]\Psi = 0. \tag{XX.43}$$

Comparing this with equation (XX.36) we find the following expression for the Dirac Hamiltonian in the presence of an external field:

$$H_D = e\varphi + \boldsymbol{\alpha}\cdot(\boldsymbol{p} - e\boldsymbol{A}) + \beta m. \tag{XX.44}$$

7. Construction of the Space $\mathscr{E}^{(s)}$. Dirac Representation

It remains to construct $\mathscr{E}^{(s)}$. The operators of this space are the 4 basic operators β, α_x, α_y, α_z and all of the functions that can be formed with them. $\mathscr{E}^{(s)}$ must be irreducible with respect to this set of operators.

To construct $\mathscr{E}^{(s)}$ we shall make use of the Hermitean character of the four basic operators and of relations (XX.40) defining their algebraic properties.

These properties are analogous to those of the three operators $\sigma_1, \sigma_2, \sigma_3$ of the non-relativistic spin $\frac{1}{2}$ theory. In this case, the spin-variable space $\mathscr{E}^{(\sigma)}$ has two dimensions. It can be constructed in the following way. Since σ_3 is Hermitean and $\sigma_3{}^2 = 1$ its only possible eigenvalues are ± 1. Moreover, to each eigenvector of σ_3 one can associate another eigenvector corresponding to the opposite eigenvalue. Consider for example, a vector $|+\rangle$ such that: $\sigma_3 |+\rangle = |+\rangle$. Since σ_3 and σ_1 anticommute, the vector $|-\rangle \equiv \sigma_1 |+\rangle$ has the property $\sigma_3 |-\rangle = (-1) |-\rangle$. One has $\sigma_1 |\pm\rangle = |\mp\rangle$ and $\sigma_3 |\pm\rangle = (\pm 1) |\pm\rangle$. The space spanned by the vectors $|+\rangle$ and $|-\rangle$ is therefore invariant with respect to the operators σ_3 and σ_1 and with respect to functions of these operators (notably $\sigma_2 \equiv \mathrm{i}\sigma_1\sigma_3$). From the very fashion in which it was constructed, it is irreducible. It is therefore the sought-for space $\mathscr{E}^{(\sigma)}$. In the representation with basis vectors $|+\rangle$ and $|-\rangle$ the operators σ_1, σ_2 and σ_3 are represented by the Pauli matrices [cf. § XIII.19 or formula (VII.65)].

To construct $\mathscr{E}^{(s)}$ we reduce the problem to the preceding one. We introduce the operators σ_x, σ_y, σ_z and ϱ_1, ϱ_2, ϱ_3 defined by:

$$\sigma_z = -\mathrm{i}\alpha_x \alpha_y, \quad \sigma_x = -\mathrm{i}\alpha_y \alpha_z, \quad \sigma_y = -\mathrm{i}\alpha_z \alpha_x \qquad \text{(XX.45)}$$

$$\varrho_3 = \beta, \quad \varrho_1 = \sigma_z \alpha_z = -\mathrm{i}\alpha_x \alpha_y \alpha_z, \quad \varrho_2 = \mathrm{i}\varrho_1 \varrho_3 = -\beta \alpha_x \alpha_y \alpha_z; \qquad \text{(XX.46)}$$

the four basic operators are expressed in terms of the ϱ and the σ by the formulas

$$\beta = \varrho_3, \qquad \alpha^k = \varrho_1 \sigma^k. \qquad \text{(XX.47)}$$

The construction of $\mathscr{E}^{(s)}$ therefore consists in the construction of a space irreducible with respect to the ϱ and the σ. Now it is easy to see that:

(*i*) each ϱ commutes with each σ;

(*ii*) the σ are three anticommuting Hermitean operators whose square is unity;

(*iii*) the ϱ are three anticommuting Hermitean operators whose square is unity.

Consequently (cf. § VIII.7):

(*i*) $\mathscr{E}^{(s)}$ is the tensor product

$$\mathscr{E}^{(s)} = \mathscr{E}^{(\varrho)} \otimes \mathscr{E}^{(\sigma)}$$

of a space $\mathscr{E}^{(\varrho)}$ irreducible with respect to the ϱ and a space $\mathscr{E}^{(\sigma)}$ irreducible with respect to the σ;

(*ii*) $\mathscr{E}^{(\sigma)}$ is a 2-dimensional space that can be constructed following the method indicated above;

(*iii*) $\mathscr{E}^{(\varrho)}$ is also a 2-dimensional space that can be constructed by the same method.

The space $\mathscr{E}^{(s)}$ therefore has 4 dimensions.

In the following sections we show that the σ are related to the spin, and the ϱ to the sign of the energy, the Dirac equation having, like the Klein–Gordon — and for the same reasons — negative energy solutions. In particular we shall see that $\boldsymbol{\alpha}$ is a (polar) vector operator and that $\boldsymbol{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ is an (axial) vector operator; in addition one formally has

$$\boldsymbol{\alpha} \times \boldsymbol{\alpha} = 2i\boldsymbol{\sigma}. \qquad \text{(XX.48)}$$

The spin of the electron is $\frac{1}{2}\boldsymbol{\sigma}$. The sign of the energy is roughly given by the eigenvalue of $\beta \equiv \varrho_3$.

The dynamical state of the electron is therefore represented by a function Ψ having 4 components, i.e. twice as many components as the wave of the non-relativistic spin $\frac{1}{2}$ theory. The representation in which the ϱ and the σ are the Pauli matrices [cf. eq. (VII.65–66)] is called the *Dirac representation*; in this representation, each component corresponds to a given orientation of the spin along the axis Oz, and roughly to a given sign of the energy.

8. Covariant Form of the Dirac Equation

Equation (XX.43) is the Dirac equation as originally proposed by Dirac himself. It is in this form that it lends itself most easily to physical interpretation and to the study of the passage to the non-relativistic limit. We now propose to obtain a second form, more symmetrical with respect to the space and time coordinates and therefore more convenient whenever questions of relativistic covariance play a preponderant role.

To this effect, we multiply both sides of (XX.43) on the left by β and put:

$$\begin{gathered} \gamma^\mu \equiv (\gamma^0, \gamma^1, \gamma^2, \gamma^3) \equiv (\gamma^0, \boldsymbol{\gamma}) \\ \gamma^0 \equiv \beta \qquad \boldsymbol{\gamma} \equiv \beta\boldsymbol{\alpha}. \end{gathered} \tag{XX.49}$$

We obtain

$$\boxed{[\mathrm{i}\gamma^\mu D_\mu - m]\,\Psi \equiv [\gamma^\mu(\mathrm{i}\partial_\mu - eA_\mu) - m]\,\Psi = 0} \tag{XX.50}$$

The properties of γ^μ are easily obtained from those of $\boldsymbol{\alpha}$ and β by applying definitions (XX.49). The ten relations (XX.40) give the ten equivalent relations

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu}. \tag{XX.51}$$

The Hermitean conditions on the $\boldsymbol{\alpha}$ and β are equivalent to the conditions

$$\gamma^{0\dagger} = \gamma^0, \qquad \gamma^{k\dagger} = -\gamma^k \tag{XX.52}$$

that may be written in the condensed form

$$\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0. \tag{XX.53}$$

It is convenient to extend the usual rule of raising and lowering of indices to the γ, and to put

$$\gamma_\mu = g_{\mu\nu}\gamma^\nu. \tag{XX.54}$$

Note that:

$$\gamma_0 = \gamma^0, \qquad \gamma_k = -\gamma^k \tag{XX.55}$$

$$\gamma^\mu = \gamma_\mu{}^\dagger = \gamma_\mu{}^{-1}. \tag{XX.56}$$

9. Adjoint Equation. Definition of the Current

We have defined a positive-definite position probability density [eq. (XX.35)]. As indicated above, the Hermitean character of the Dirac Hamiltonian guarantees that this definition is self-consistent. We shall now define a current density and show that the current defined with the solutions of the Dirac equation obeys an equation of continuity. We first give a complete discussion of this problem using the Dirac form, and then repeat the argument with the covariant form.

Suppose that we have chosen a particular representation of the β and $\boldsymbol{\alpha}$. The wave Ψ is then a certain column matrix with four lines

$$\Psi \equiv \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}.$$

Denote its Hermitean conjugate by:

$$\Psi^\dagger \equiv (\psi_1{}^* \psi_2{}^* \psi_3{}^* \psi_4{}^*).$$

The operators of spin space are 4×4 matrices. One can define partial scalar products in which one sums over the spin variables alone. We shall indicate such scalar products by parentheses; thus the density P is written

$$P(\mathbf{r}, t) \equiv (\Psi^\dagger \Psi). \tag{XX.57}$$

As another illustration, denote by β_{st} the element in line s and column t of the matrix β $(s, t=1, 2, 3, 4)$:

$$(\Psi^\dagger \beta \Psi) \equiv \sum_s \sum_t \psi_s{}^* \beta_{st} \psi_t.$$

Now if Ψ is a solution of the Dirac equation, that is, if

$$\begin{aligned} \mathrm{i}\frac{\partial \Psi}{\partial t} &= H_D \Psi \\ &= \left[e\varphi + \sum_k \alpha^k \left(-\mathrm{i}\frac{\partial}{\partial x^k} - eA^k \right) + \beta m \right] \Psi, \end{aligned} \tag{XX.58}$$

then $\Psi^\dagger$ is a solution of the Hermitean conjugate equation, that is of the equation obtained by taking the complex conjugate of (XX.58) and replacing each matrix by its transpose:

$$\begin{aligned} \mathrm{i}\frac{\partial \Psi^\dagger}{\partial t} &= -\Psi^\dagger H_D \\ &= -e\varphi\Psi^\dagger - \sum_k \left(\mathrm{i}\frac{\partial}{\partial x^k} - eA^k \right) \Psi^\dagger \alpha^k - m\Psi^\dagger \beta. \end{aligned} \tag{XX.59}$$

Scalar multiplication of (XX.58) on the left by $\Psi^\dagger$ and (XX.59) on the right by Ψ and then addition gives

$$\mathrm{i}\frac{\partial}{\partial t}(\Psi^\dagger \Psi) = -\mathrm{i}\sum_k \frac{\partial}{\partial x^k} (\Psi^\dagger \alpha^k \Psi). \tag{XX.60}$$

On the left-hand side we recognize the time derivative of the probability density, and on the right-hand side the divergence of a certain vector $\boldsymbol{j}(\boldsymbol{r}, t)$ defined by

$$\boldsymbol{j}(\boldsymbol{r}, t) \equiv (\Psi^\dagger \boldsymbol{\alpha} \Psi). \tag{XX.61}$$

$\boldsymbol{j}(\boldsymbol{r}, t)$ is the sought-for current density and (XX.60) is equivalent to the equation of continuity

$$\frac{\partial}{\partial t} P + \nabla \cdot \boldsymbol{j} = 0.$$

The above may be repeated starting from the covariant form of the Dirac equation [eq. (XX.50)]. The Hermitean conjugate of (XX.50) is

$$(-\mathrm{i}\partial_\mu - eA_\mu)\, \Psi^\dagger \gamma^{\mu\dagger} - m\, \Psi^\dagger = 0. \tag{XX.62}$$

[Here the symbol $\partial_\mu \Psi^\dagger \gamma^{\mu\dagger}$ represents the line matrix with four columns $(\partial \Psi^\dagger / \partial x^\mu)\gamma^{\mu\dagger}$.] It is convenient to put:

$$\overline{\Psi} = \Psi^\dagger \gamma^0, \qquad \Psi^\dagger = \overline{\Psi} \gamma^0. \tag{XX.63}$$

Taking relations (XX.53) into account, equation (XX.62) can then be put after multiplication on the left by γ^0 in the simpler form:

$$\boxed{(-\mathrm{i}\partial_\mu - eA_\mu)\, \overline{\Psi}\, \gamma^\mu - m \overline{\Psi} = 0} \tag{XX.64}$$

This equation is obviously equivalent to (XX.59). $\overline{\Psi}$ is called the *adjoint of* Ψ, and (XX.64) the *adjoint equation.*

Scalar multiplication of (XX.50) on the left by $\overline{\Psi}$ and (XX.64) on the right by Ψ and then subtraction, gives

$$\mathrm{i}\partial_\mu (\overline{\Psi} \gamma^\mu \Psi) = 0.$$

One defines the current density four-vector

$$j^\mu \equiv (\overline{\Psi} \gamma^\mu \Psi). \tag{XX.65}$$

The preceding equation is equivalent to the equation of continuity

$$\partial_\mu j^\mu = 0.$$

One easily verifies that $j^\mu \equiv (P, \boldsymbol{j})$. Thus, as expected, we obtain the equation of continuity written in its covariant form. In the next section, we show that the 4 components of j^μ indeed form a four-vector.

III. INVARIANCE PROPERTIES OF THE DIRAC EQUATION

10. Properties of the Dirac Matrices

As a preliminary to the study of the invariance properties of the Dirac equation we now make a systematic study of the properties of four 4×4 *matrices* $\gamma^\mu \equiv (\gamma^0, \gamma^1, \gamma^2, \gamma^3)$ satisfying the relations

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2 g^{\mu\nu} I, \tag{XX.66}$$

where I is the unit matrix. The matrix relations (XX.66) are analogous to the operator relations (XX.51); however, the matrices introduced here do not necessarily verify the unitarity conditions (XX.53). All of the following properties are consequences of relation (XX.66) alone.

γ^A MATRICES. As the γ^μ anticommute, and as their square is equal to $+I$ or $-I$, any product of several γ^μ is equal, to within a sign, to one of the 16 particular γ^A matrices given in Table 1. These have been grouped in 5 classes denoted by (S), (V), (T), (A) and (P) and containing 1, 4, 6, 4 and 1 elements respectively; the reasons for this classification will become clear at the end of this section (cf. § 14).

TABLE XX.1

The γ^A matrices

Matrix		Explicit form: $(\gamma^A)^2 = I$	Explicit form: $(\gamma^A)^2 = -I$
(S)	$1 \equiv$	I	
(V)	$\gamma^\mu \equiv \{\gamma^0, \gamma^k\} \equiv$	γ^0	$\gamma^1 \quad \gamma^2 \quad \gamma^3$
(T)	$\gamma^{[\lambda\mu]} \equiv \{\gamma^k\gamma^0, \gamma^5\gamma^0\gamma^k\} \equiv$	$\gamma^1\gamma^0 \quad \gamma^2\gamma^0 \quad \gamma^3\gamma^0$	$\gamma^2\gamma^3 \quad \gamma^3\gamma^1 \quad \gamma^1\gamma^2$
(A)	$\gamma^{[\lambda\mu\nu]} \equiv \{\gamma^0\gamma^5, \gamma^k\gamma^5\} \equiv$	$\gamma^1\gamma^2\gamma^3$	$\gamma^0\gamma^2\gamma^3 \quad \gamma^0\gamma^3\gamma^1 \quad \gamma^0\gamma^1\gamma^2$
(P)	$\gamma^{[\lambda\mu\nu\varrho]} \equiv \gamma^5$		$\gamma^0\gamma^1\gamma^2\gamma^3$

It is clear that $(\gamma^A)^2$ is equal, according to the case, to I or to $-I$; the six matrices whose square is equal to I are grouped in the left-hand column; the ten matrices whose square is equal to $-I$ in the right-hand column.

Of all these matrices, only I commutes with all of the others. If

$\gamma^A \neq I$, it anticommutes with 8 of these 16 matrices and commutes with the 8 others.

In particular the matrix γ^5, defined by [1])

$$\gamma^5 \equiv \gamma^0\gamma^1\gamma^2\gamma^3 \tag{XX.67}$$

anticommutes with the γ^μ:

$$\gamma^5\gamma^\mu + \gamma^\mu\gamma^5 = 0 \tag{XX.68}$$

and its square is

$$(\gamma^5)^2 = -I. \tag{XX.69}$$

INVERSE MATRICES (γ_A). We define the γ_μ matrices by the relation:

$$\gamma_\mu = g_{\mu\nu}\gamma^\nu. \tag{XX.70}$$

Obviously:

$$\gamma^\mu = [\gamma_\mu]^{-1}.$$

It follows that the inverse of a γ^A is obtained by reversing the order of the γ^μ involved and replacing each of them by the corresponding γ_μ; we denote the expression thereby obtained by γ_A:

$$\gamma_A\gamma^A = \gamma^A\gamma_A = I. \tag{XX.71}$$

Following this method of constructing the inverse, one finds

$$\gamma_5 = \gamma_3\gamma_2\gamma_1\gamma_0.$$

TRACE AND DETERMINANT

$$\operatorname{Tr}\gamma^A = \begin{cases} 4 & \text{if} \quad \gamma^A = I \\ 0 & \text{if} \quad \gamma^A \neq I. \end{cases} \tag{XX.72}$$

To see this, suppose $\gamma^A \neq I$ and let γ^B be one of the 8 matrices which anticommute with γ^A:

$$\gamma^A = -\gamma^B\gamma^A\gamma_B.$$

We then have:

$$\operatorname{Tr}\gamma^A = -\operatorname{Tr}\gamma^B\gamma^A\gamma_B = -\operatorname{Tr}\gamma_B\gamma^B\gamma^A = -\operatorname{Tr}\gamma^A = 0.$$

We note in passing (Problem XX.3) that:

$$\det\gamma^A = 1.$$

REARRANGEMENT LEMMA. The following property may be verified by simple inspection:

If we multiply each matrix of the set of 16 γ^A matrices on the right

[1]) The index 4 is commonly used to denote the time component, according to the definition: $x^4 = ix^0 = ict$.

(or on the left) by a particular one of them, we obtain the same set of 16 matrices, except for possible changes in order and sign.

LINEAR INDEPENDENCE AND IRREDUCIBILITY. Using the rearrangement lemma and the properties of the trace, it can easily be shown that:

(*i*) The 16 γ^A matrices are linearly independent.

(*ii*) Any 4th order matrix M is a uniquely-defined linear combination of the γ^A:

$$M = \sum_A m_A \gamma^A \qquad m_A = \tfrac{1}{4} \operatorname{Tr} \gamma_A M.$$

(*iii*) Any matrix commuting with every γ^μ, and therefore with every γ^A, is a multiple of the unit matrix:

$$\text{if } [M, \gamma^\mu] = 0 \text{ for any } \mu, \quad M = Cst. \times I.$$

FUNDAMENTAL THEOREM. *Let γ^μ and γ'^μ be two sets of 4 fourth-order matrices satisfying relation* (XX.66). *There exists a matrix S, non-singular* (det $S \neq 0$) *and defined to within a constant, such that*

$$\gamma^\mu = S\gamma'^\mu S^{-1} \qquad (\mu = 0, 1, 2, 3). \tag{XX.73}$$

To demonstrate this theorem we proceed in the following way. To each set γ^μ, γ'^μ there corresponds a set of 16 matrices γ^A, γ'^A whose definition and principle properties were given above; thus to each particular γ^A there corresponds a certain matrix γ'^A, the index A taking all 16 distinct values. Let F be a certain matrix and denote by S the matrix defined by

$$S \equiv \sum_A \gamma'^A F \gamma_A,$$

the sum $\sum_A$ being extended over the 16 possible values of the index A.

Denote a particular matrix by γ^B, its inverse by γ_B and the corresponding matrix in the other system by γ'^B; in virtue of the rearrangement lemma,

$$\gamma'^B S \gamma_B \equiv \sum_A \gamma'^B \gamma'^A F \gamma_A \gamma_B = \sum_A \gamma'^A F \gamma_A \equiv S,$$

therefore

$$\gamma'^B S = S \gamma^B. \tag{XX.74}$$

For relation (XX.73) to be verified by S, it remains to show that S has an inverse. To this effect, we introduce the matrix T, defined by

$$T \equiv \sum_A \gamma^A G \gamma_A',$$

where G is an arbitrary matrix. Reasoning in an analogous way one shows that

$$\gamma^B T = T\gamma'^B.$$

Therefore

$$\gamma^B TS = T\gamma'^B S = TS\gamma^B,$$

whatever γ^B; since TS commutes with any matrix γ^B, it is a multiple of unity: $TS = c \times I$. The multiplication constant is given by the formula:

$$\begin{aligned} c &= \tfrac{1}{4}\operatorname{Tr} TS = \tfrac{1}{4}\sum_A \sum_B \operatorname{Tr} \gamma^A G \gamma'_A \gamma'^B F \gamma_B \\ &= \tfrac{1}{4}\operatorname{Tr} G\,(\sum_A \sum_B \gamma'_A \gamma'^B F \gamma_B \gamma^A) = 4 \operatorname{Tr} GS. \end{aligned}$$

Now F can always be chosen so that S has at least one non-zero element, for clearly the 16 γ^A matrices would not be linearly independent if S vanished for every F. Thus it is always possible to choose G such that

$$\operatorname{Tr} GS \equiv \sum_s \sum_t G_{st} S_{ts} = \tfrac{1}{4};$$

one then has $c = 1$ and therefore $T = S^{-1}$. Thus S does have an inverse and property (XX.73) is obtained by multiplying both sides of (XX.74) on the right by S^{-1}.

If another matrix, S', has the same property, $S^{-1}S'$ commutes with all of the γ^μ and therefore: $S^{-1}S' = Cst \times I$. Conversely, if S has the property (XX.73), then so has any multiple of S. Thus we have shown that the non-singular matrix S exists, and that it is defined to within a constant. Q.E.D.

Unitary γ^μ matrices. If the matrices obeying relations (XX.66) are unitary:

$$\gamma_\mu \equiv \gamma^0 \gamma^\mu \gamma^0 = \gamma^{\mu\dagger}, \qquad \text{(XX.75)}$$

all of the γ^A matrices are unitary and it follows that they are Hermitean or anti-Hermitean according as $(\gamma^A)^2$ is equal to $+I$ or $-I$.

The fundamental theorem is completed by the following corollary, the proof of which is left to the reader:

Let γ^μ and γ'^μ be two systems of 4 fourth-order unitary matrices satisfying relations (XX.66). *There exists a unitary matrix U, defined to within a phase, such that*: $\gamma'^\mu = U\gamma^\mu U^\dagger$ $(\mu = 0, 1, 2, 3)$.

Complex conjugation, B matrix. In particular, if the γ^μ are unitary and obey relations (XX.66), the 4 complex conjugate matrices

$\gamma^{\mu *}$ are also unitary and also obey relations (XX.66). The preceding corollary therefore applies: the γ^μ are obtained from the $\gamma^{\mu *}$ by a unitary transformation. We shall henceforth denote the matrix of that transformation by B (B is defined to within a phase):

$$\gamma^\mu = B\gamma^{\mu *} B^\dagger \qquad \gamma^{\mu *} = B^* \gamma^\mu \widetilde{B}. \tag{XX.76}$$

It can be shown (Problem XX.4) that B is antisymmetrical:

$$B = -\widetilde{B}$$

or, what amounts to the same, that

$$BB^* = B^* B = -I. \tag{XX.77}$$

If the γ matrices are those of the Dirac representation one has

$$B \equiv B_D = \gamma^2 \gamma^5$$
$$= -\mathrm{i}\varrho_3 \sigma_y.$$

Property (XX.77) is easily verified for this particular case.

11. Invariance of the Form of the Dirac Equation in an Orthochronous Change of Referential

In order to satisfy the relativity principle, the Dirac equation and the equation of continuity must have the same form in different Lorentz referentials. In actual fact, the principle requires this invariance of form only with respect to proper Lorentz transformations [1], but it happens that the theory is formally invariant with respect to the complete group. We shall begin with a detailed study of invariance with respect to the orthochronous group. Time-reversal invariance will be examined at the end of this section along with other invariance properties characteristic of the Dirac equation but not directly related to Lorentz transformations.

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[1]) And also with respect to space and time translations. This invariance can easily be demonstrated by an argument analogous to the one given in this paragraph. If the origin of axes is displaced by a four-vector a^μ, that is, if $x'^\mu = x^\mu + a^\mu$, then $A_\mu'(x') = A_\mu(x)$ and the law for the transformation of wave functions [that is, the analogue of (XX.85)] becomes simply:

$$\Psi'(x') = \Psi(x).$$

Let us therefore suppose that the dynamical state of the electron is represented in a referential (R) by a four-component wave function satisfying the Dirac equation:

$$[\gamma^\mu(\mathrm{i}\partial_\mu - eA_\mu(x)) - m]\,\Psi(x) = 0. \qquad \text{(XX.78)}$$

We suppose that a representation has been chosen once and for all for the operators of the space $\mathscr{E}^{(s)}$; the symbols γ^μ therefore denote well-defined matrices and relation (XX.78) represents 4 equations ($s = 1, 2, 3, 4$):

$$\sum_{t=1,2,3,4}\sum_{\mu}(\gamma^\mu)_{st}\left(\mathrm{i}\frac{\partial}{\partial x^\mu} - eA_\mu(x^0x^1x^2x^3)\right)\psi_t(x^0x^1x^2x^3) - m\psi_s(x^0x^1x^2x^3) = 0$$

satisfied by the 4 components $\psi_s(x)$ of the wave function.

Consider this same system in a new referential (R') obtained from the preceding one by a certain orthochronous Lorentz transformation $\mathscr{L}$:

$$(R') = \mathscr{L}(R).$$

$\mathscr{L}$ is characterized by a certain matrix $\Omega^\mu{}_\nu$ having properties (XX.12) and (XX.13) (in addition $\Omega^0{}_0 > 0$) and defining the linear correspondence between the coordinates x^μ of a given point in the referential (R) and the coordinates x'^μ *of the same point* in the referential (R') that is, the law for the transformation of contravariant vectors [eq. (XX.11) and (XX.15)]. We write symbolically

$$x' = \mathscr{L}x, \qquad x = \mathscr{L}^{-1}x'. \qquad \text{(XX.79)}$$

The partial-differentiation operators transform like covariant vectors:

$$\partial_\mu = \partial_\nu{}'\Omega^\nu{}_\mu. \qquad \text{(XX.80)}$$

If we denote the covariant components of the potential in the new referential by $A_\mu{}'(x')$, they too are related to the $A_\mu(x)$ by the law for the transformation of covariant vectors:

$$A_\mu(x) \equiv A_\mu(\mathscr{L}^{-1}x') = A_\nu{}'(x')\Omega^\nu{}_\mu. \qquad \text{(XX.81)}$$

Considered as a function of the new coordinates, $\Psi(x)$ obeys the equation obtained from (XX.78) by substituting into it from (XX.80) and (XX.81):

$$[\hat{\gamma}^\mu(\mathrm{i}\partial_\mu{}' - eA_\mu{}'(x')) - m]\,\Psi(\mathscr{L}^{-1}x') = 0, \qquad \text{(XX.82)}$$

where

$$\hat{\gamma}^\mu \equiv \Omega^\mu{}_\varrho\gamma^\varrho. \qquad \text{(XX.83)}$$

The four γ^μ matrices are unitary and satisfy relations (XX.66). The four $\hat{\gamma}^\mu$ matrices are not necessarily unitary, but, because of the orthogonality of the $\Omega^\mu{}_\nu$ [relations (XX.13)], they also verify relations (XX.66), i.e.

$$\hat{\gamma}^\mu\hat{\gamma}^\nu+\hat{\gamma}^\nu\hat{\gamma}^\mu = \Omega^\mu{}_\varrho\Omega^\nu{}_\sigma(\gamma^\varrho\gamma^\sigma+\gamma^\sigma\gamma^\varrho)$$
$$= 2\Omega^\mu{}_\varrho g^{\varrho\sigma}\Omega^\nu{}_\sigma = 2g^{\mu\nu}.$$

Therefore in virtue of the fundamental theorem of § 10, there exists a non-singular matrix Λ defined to within a constant which transforms the $\hat{\gamma}$ into the γ:

$$\hat{\gamma}^\mu \equiv \Omega^\mu{}_\varrho\gamma^\varrho = \Lambda^{-1}\gamma^\mu\Lambda \qquad (\mu = 0, 1, 2, 3). \tag{XX.84}$$

Substituting this relationship into (XX.82) and putting

$$\Psi'(x') = \Lambda\Psi(x) \equiv \Lambda\Psi(\mathscr{L}^{-1}x') \tag{XX.85}$$

one finds, after multiplying on the left by Λ:

$$[\gamma^\mu(\mathrm{i}\partial_\mu{}' - eA_\mu{}'(x'))]\,\Psi'(x') = 0.$$

This wave equation describes the evolution of the system in the new referential. It is seen to be formally identical with (XX.78). The Dirac equation is therefore formally invariant in an orthochronous change of referential and the law for the transformation of the wave function is given by equation (XX.85).

The matrix Λ, which is defined to within a constant, cannot in general be chosen to be unitary; however it will now be shown that the constant can always be chosen so as to have

$$\Lambda^\dagger = \gamma^0\Lambda^{-1}\gamma^0 \tag{XX.86}$$

Λ is then defined up to an arbitrary phase.

Since the $\Omega^\mu{}_\varrho$ are real and since the γ^μ are unitary and therefore verify (XX.75), the comparison of (XX.83) and its Hermitean conjugate gives

$$\hat{\gamma}^{\mu\dagger} = \gamma^0\hat{\gamma}^\mu\gamma^0.$$

Taking the Hermitean conjugate of (XX.84) and substituting the preceding relation one easily obtains

$$\hat{\gamma}^\mu = (\gamma^0\Lambda^\dagger\gamma^0)\gamma^\mu(\gamma^0\Lambda^\dagger\gamma^0)^{-1}.$$

Comparing with (XX.84), we see that the matrix $\Lambda\gamma^0\Lambda^\dagger\gamma^0$ commutes with the four γ^μ and is therefore a multiple of the unit matrix:

$$\Lambda^\dagger = c\gamma^0\Lambda^{-1}\gamma^0. \qquad \text{(XX.87)}$$

Next we show that the constant c is necessarily real and positive. From (XX.87) and (XX.84),

$$\Lambda^\dagger\Lambda = c\gamma^0(\Lambda^{-1}\gamma^0\Lambda) = c(\Omega^0{}_0 + \sum_k \Omega^0{}_k\gamma^0\gamma^k)$$

whence, taking into account (XX.72), $\mathrm{Tr}\Lambda^\dagger\Lambda = 4c\Omega^0{}_0$. Now since the trace of the Hermitean-definite matrix $\Lambda^\dagger\Lambda$ is necessarily real and positive, and since $\Omega^0{}_0$ is also real and positive, then so also is c. Thus if one multiplies Λ by $\sqrt{c}$, the resulting matrix is also a Λ matrix and verifies equation (XX.86). Q.E.D.

From the law (XX.85) for the transformation of wave functions, we obtain the law for the transformation of the adjoint functions:

$$\overline{\Psi}' \equiv \Psi'^\dagger\gamma^0 = \Psi^\dagger\Lambda^\dagger\gamma^0 = \overline{\Psi}\gamma^0\Lambda^\dagger\gamma^0$$

whence, taking into account (XX.86)

$$\overline{\Psi}'(x') = \overline{\Psi}(x)\Lambda^{-1}. \qquad \text{(XX.88)}$$

Using this transformation law, the reader may easily verify that the adjoint equation (XX.64) is also formally invariant in an orthochronous change of referential.

It remains to show that the equation of continuity is formally invariant or, better, that j^μ [definition (XX.65)] transforms like a contravariant four-vector [1]).

This is easily verified; from (XX.85), (XX.88) and (XX.84),

$$\begin{aligned} j'^\mu(x') &\equiv (\overline{\Psi}'\gamma^\mu\Psi') = (\overline{\Psi}\Lambda^{-1}\gamma^\mu\Lambda\Psi) = \Omega^\mu{}_\varrho(\overline{\Psi}\gamma^\varrho\Psi) \\ &= \Omega^\mu{}_\varrho j^\varrho(x). \end{aligned}$$

For each Lorentz transformation, Λ is defined up to a phase by conditions (XX.84) and (XX.86). *In the present case, this phase has no physical significance.* In so far as possible it is desirable to remove the arbitrary in the phase, while preserving the property of the Λ to form a group homomorphic to the orthochronous Lorentz group (see the discussion of § XV.8).

1) Otherwise, the normalization of the wave function would depend on the reference system and the interpretation of j^0 as a position probability density would not be justified.

Now since the $\Omega^{\mu}{}_{\nu}$ are real, condition (XX.84) gives

$$\Omega^{\mu}{}_{\nu}\gamma^{\nu *} = (\Lambda^*)^{-1}\gamma^{\mu *}\Lambda^*,$$

whence, introducing the unitary matrix B [definition (XX.76)],

$$\Omega^{\mu}{}_{\nu}\gamma^{\nu} = (B\Lambda^* B^{\dagger})^{-1}\gamma^{\mu}(B\Lambda^* B^{\dagger}).$$

Comparing this equation with (XX.84), we see that $B\Lambda^* B^{\dagger}\Lambda^{-1}$ commutes with the four γ^{μ} matrices and is therefore a multiple of the unit matrix; it is easy to see [for example by calculating $\det(B\Lambda^* B^{\dagger}\Lambda^{-1})$] that this multiple is a phase factor; in other words

$$\Lambda^* = e^{i\lambda} B^{\dagger}\Lambda B.$$

since Λ is determined up to a phase factor, one can always choose this phase so as to have $e^{i\lambda} = 1$. In what follows this will always be done; Λ is then defined up to a sign.

In conclusion, to each orthochronous Lorentz transformation there correspond *two* Λ matrices, differing by a sign, defined by the three conditions

$$\Omega^{\mu}{}_{\nu}\gamma^{\nu} = \Lambda^{-1}\gamma^{\mu}\Lambda \qquad \text{(XX.89}a\text{)}$$

$$\Lambda^{\dagger} = \gamma^0\Lambda^{-1}\gamma^0 \qquad \text{(XX.89}b\text{)}$$

$$\Lambda^* = B^{\dagger}\Lambda B. \qquad \text{(XX.89}c\text{)}$$

It is clear that the set of Λ matrices thus defined forms a group and that this group is homomorphic to the orthochronous Lorentz group. We shall see in § 12 that the arbitrary in the sign of the Λ cannot be removed without violating this group property [1]).

[1]) Rather than condition (XX.89*c*), one could just as well take the more general condition: $\Lambda^* = \eta B^{\dagger}\Lambda B$, where η is a constant depending on the particular Lorentz transformation considered. The group property of the Λ is preserved if the η form an Abelian representation of the Lorentz group. Consequently, one necessarily has $\eta = 1$ for the transformations of the proper group $\mathscr{L}_0$, which gives back condition (XX.89*c*). For transformations of the reflection type that is for those of the sheet $s\mathscr{L}_0$, one may choose between the two following possibilities:

(*a*) $\eta = 1$ for any $s\mathscr{L}_0$; we obtain (XX.89*c*);

(*b*) $\eta = -1$ for any $s\mathscr{L}_0$, that is, $\Lambda^* = -B\Lambda B^{\dagger}$.

The physical content of the theory is obviously independent of this choice. The two groups, $G^{(a)}$ and $G^{(b)}$, which correspond respectively to (*a*) and (*b*) above, are both homomorphic to the orthochronous Lorentz group, but they are *not* isomorphic to each other. In particular, the two matrices which correspond to s have their square equal to I in $G^{(a)}$, and to $-I$ in $G^{(b)}$ [Cf. note 1, p. 908 below].

12. Transformation of the Proper Group

We shall now find explicit expressions for the Λ matrices defined by equation (XX.89). In this paragraph we limit ourselves to the transformations of the proper group.

Let us first consider the infinitesimal transformations. To each of the 6 infinitesimal "rotations" $g_{\mu\nu}-\varepsilon Z^{(\alpha\beta)}_{\mu\nu}$ there corresponds a matrix $\Lambda^{(\alpha\beta)}(\varepsilon)$ differing by an infinitesimal from the unit matrix and which may therefore be written in the form

$$\Lambda^{(\alpha\beta)}(\varepsilon) \simeq I+\mathrm{i}\varepsilon S_{\alpha\beta}, \tag{XX.90}$$

where $S_{\alpha\beta}$ is a finite matrix to be determined. One has

$$[\Lambda^{(\alpha\beta)}(\varepsilon)]^{-1} \simeq \Lambda^{(\alpha\beta)}(-\varepsilon) \simeq I-\mathrm{i}\varepsilon S_{\alpha\beta}.$$

Property (XX.89*a*) therefore gives

$$-\varepsilon g^{\mu\nu} Z^{(\alpha\beta)}_{\nu\varrho}\,\gamma^{\varrho} = -\mathrm{i}\varepsilon[S_{\alpha\beta}, \gamma^{\mu}],$$

or, using (XX.17),

$$[S_{\alpha\beta}, \gamma^{\mu}] = \mathrm{i}(\delta^{\mu}{}_{\beta}\gamma_{\alpha}-\delta^{\mu}{}_{\alpha}\gamma_{\beta}).$$

$S_{\alpha\beta}$ satisfies the same commutation relations with the γ^{μ} as the matrix $\frac{1}{2}\mathrm{i}\gamma_{\alpha}\gamma_{\beta}$. The difference therefore commutes with the four γ^{μ} matrices and is thus a constant. One easily sees that conditions (XX.89*b*) and (XX.89*c*) are satisfied if, and only if, this constant vanishes. It is convenient to put

$$\begin{aligned}\sigma_{\mu\nu} &\equiv \tfrac{1}{2}\mathrm{i}[\gamma_{\mu}, \gamma_{\nu}] \\ &\equiv \mathrm{i}\gamma_{\mu}\gamma_{\nu} \qquad (\mu\neq\nu).\end{aligned} \tag{XX.91}$$

One finds therefore:

$$\boxed{S_{\alpha\beta} = \tfrac{1}{2}\sigma_{\alpha\beta}} \tag{XX.92}$$

The symbols $S_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ will also be used for the operators represented by the matrices $S_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ respectively. We shall see further on that $S_{\alpha\beta}$ is an antisymmetrical tensor operator (6 components) representing the intrinsic angular momentum or spin of the particle. To be exact, the spin is the spatial part (3 components) of this operator. $S_{\alpha\beta}$ is related to the operators $\boldsymbol{\sigma}$ and $\boldsymbol{\alpha}$ of § 6 and 7 by the relations

$$S_{10}=\tfrac{1}{2}\mathrm{i}\alpha_x \qquad S_{20}=\tfrac{1}{2}\mathrm{i}\alpha_y \qquad S_{30}=\tfrac{1}{2}\mathrm{i}\alpha_z \tag{XX.93a}$$

$$S_{23}=\tfrac{1}{2}\sigma_x \qquad S_{31}=\tfrac{1}{2}\sigma_y \qquad S_{12}=\tfrac{1}{2}\sigma_z. \tag{XX.93b}$$

Any finite transformation of the proper Lorentz group may be considered as the product of successive infinitesimal transformations. We can therefore construct the Λ matrices corresponding to a finite change of referential by taking the product of matrices for infinitesimal transformations as defined above. If we proceed in this way conditions (XX.89*b*) and (XX.89*c*) are automatically fulfilled and we obtain one of the two possible Λ matrices.

In particular, the "rotation" of angle φ in the plane $x^\alpha x^\beta$ is a product of infinitesimal rotation matrices in this plane, and the matrix $\Lambda^{(\alpha\beta)}(\varphi)$ representing the transformation is therefore

$$\Lambda^{(\alpha\beta)}(\varphi) = \mathrm{e}^{\mathrm{i}\varphi S_{\alpha\beta}} \tag{XX.94}$$

Thus (cf. note, p. 882), if it is a special Lorentz transformation of velocity $v = \tanh\varphi$ directed along the x axis, one finds, taking into account relations (XX.93*a*) and the properties of α_x:

$$\Lambda^{xt}(\varphi) = \mathrm{e}^{-\frac{1}{2}\alpha_x\varphi} = \cosh\tfrac{1}{2}\varphi - \alpha_x \sinh\tfrac{1}{2}\varphi. \tag{XX.95}$$

More generally let $\Lambda_{\mathrm{sp}}(v)$ be the matrix associated with the special Lorentz transformation of velocity $\mathbf{v}$; then

$$\Lambda_{\mathrm{sp}}(\mathbf{v}) = \cosh\tfrac{1}{2}\varphi - (\boldsymbol{\alpha}\cdot\mathbf{u})\sinh\tfrac{1}{2}\varphi,$$

where:

$$\mathbf{u} \equiv \mathbf{v}/v, \qquad \varphi = \tanh^{-1}\mathbf{v}.$$

Let us put

$$b \equiv 1/\sqrt{1-v^2} = \cosh\varphi. \tag{XX.96}$$

After an elementary calculation, the preceding expression takes the form:

$$\Lambda_{\mathrm{sp}}(\mathbf{v}) = \frac{1}{\sqrt{2(1+b)}}\,[1 + b - (\boldsymbol{\alpha}\cdot\mathbf{v})\,b]. \tag{XX.97}$$

Consider now rotations in the ordinary sense of the word. Expression (XX.94) gives for rotations about Oz:

$$\Lambda^{(xy)}(\varphi) = \mathrm{e}^{\mathrm{i}S_{12}\varphi} = \mathrm{e}^{\frac{1}{2}\mathrm{i}\sigma_z\varphi} = \cos\tfrac{1}{2}\varphi + \mathrm{i}\sigma_z \sin\tfrac{1}{2}\varphi. \tag{XX.98}$$

More generally the matrix $\Lambda_{\mathbf{u}}(\varphi)$ associated with a rotation through an angle φ about the axis parallel to the unit vector $\mathbf{u}$ is

$$\Lambda_{\mathbf{u}}(\varphi) = \cos\tfrac{1}{2}\varphi + \mathrm{i}\sigma_u \sin\tfrac{1}{2}\varphi \tag{XX.99}$$

with:

$$\sigma_u \equiv (\boldsymbol{\sigma}\cdot\mathbf{u}).$$

We are now ready to discuss the spin of the particle described by the Dirac equation. The spin is defined by the transformation properties of the internal variables with respect to spatial rotations. Equation (XX.99) gives the general expression for the transformation matrices of the internal variables in a rotation. The only difference between this expression and the one given by equation (XIII.84) is the sign in front of σ_u; one passes from one to the other by changing φ into $-\varphi$; it follows that the two matrices are inverses one of the other. This difference is due to the fact that in Chapter XIII, we considered the rotation of the variables and of the states while keeping the axes fixed; here we have taken the opposite point of view. We now see that the Dirac wave function transforms under rotation like the wave function of *a particle of spin* $\frac{1}{2}$.

Note in particular that a rotation through 2π about any axis does not give back the unit matrix; indeed one finds that

$$\Lambda_{\mathbf{u}}(2n\pi) = (-)^n I, \tag{XX.100}$$

property characteristic of half-integral spins. From this it is clear that the arbitrary in the sign of the Λ cannot be removed without violating their property of forming a group.

We shall henceforth call the wave functions of the Dirac theory *spinors.*

13. Spatial Reflection and the Orthochronous Group

Once the law of transformation of spinors in proper changes of referential has been determined, we need only to know the law of transformation in the reflection s to be able to determine the law of transformation in any orthochronous change of referential.

Denote by Λ_s the matrix corresponding to the reflection s of the referential. In this case (XX.85) becomes

$$\Psi'(t, \mathbf{r}) = \Lambda_s \Psi(t, -\mathbf{r}). \tag{XX.101}$$

Condition (XX.89*a*) gives

$$\Lambda_s^{-1} \gamma^0 \Lambda_s = \gamma^0 \qquad \Lambda_s^{-1} \gamma^k \Lambda_s = -\gamma^k,$$

whence

$$\Lambda_s = c_s \gamma^0.$$

The constant c_s is fixed by (XX.89*b*) and (XX.89*c*); one finds

$$c_s = \pm 1.$$

Therefore:

$$\Lambda_s = \pm \gamma^0 \tag{XX.102}$$

Λ_s is defined up to a sign in accordance with what was said above [1]).

14. Construction of Covariant Quantities

From the components of the spinor $\Psi(x)$ and those of its adjoint $\overline{\Psi}(x)$, one can form in all 16 linearly independent functions of x^0, x^1, x^2, x^3 that are bilinear in Ψ and $\overline{\Psi}$. They can be grouped into 5 fields of well-defined tensorial character, namely: a scalar S, a vector V^μ, an antisymmetrical tensor with two indices $T^{[\mu\nu]}$, an antisymmetrical tensor with three indices, or pseudovector $A^{[\lambda\mu\nu]}$ and an antisymmetrical tensor with four indices, or pseudoscalar P. These are given in Table XX.2.

The indicated tensorial characters can easily be demonstrated using the law for the transformation of the spinors Ψ and $\overline{\Psi}$ [eq. (XX.85) and (XX.88)] and relation (XX.89*a*) between the matrix Λ and the coefficients $\Omega^\mu{}_\nu$ of the corresponding Lorentz transformation.

Recall that the law for the transformation of a pseudoscalar differs from that of a scalar only by the presence of the additional factor det $|\Omega^\mu{}_\nu|$:

$$P(x') = \det |\Omega^\mu{}_\nu| \, P(x).$$

TABLE XX.2

Tensors bilinear in Ψ and $\overline{\Psi}$

Tensor	Number of Components	Nature
$S(x) \equiv (\overline{\Psi}\Psi)$	1	Scalar
$V^\mu(x) \equiv (\overline{\Psi}\gamma^\mu\Psi)$	4	Vector
$T^{[\mu\nu]}(x) \equiv (\overline{\Psi}\gamma^\mu\gamma^\nu\Psi) \quad (\mu \neq \nu)$	6	Tensor of rank 2
$A^{[\lambda\mu\nu]}(x) \equiv (\overline{\Psi}\gamma^\lambda\gamma^\mu\gamma^\nu\Psi) \quad (\lambda \neq \mu,\ \mu \neq \nu,\ \nu \neq \lambda)$	4	Pseudovector
$P(x) \equiv (\overline{\Psi}\gamma^5\Psi)$	1	Pseudoscalar

[1]) Expression (XX.102) corresponds to choice (*a*) defined in note, p. 904. Choice (*b*) leads to:

$$\Lambda_s = \pm \mathrm{i}\gamma^0.$$

Thus a pseudoscalar field transforms like a scalar field in a proper Lorentz transformation, but changes sign in a reflection s. Similarly, the law for the transformation of a pseudovector differs from that of a vector only by the presence of the additional factor $\det |\Omega^{\mu}{}_{\nu}|$.

The vector $V^{\mu}(x)$ has already been interpreted as the current-density four-vector:

$$V^{\mu}(x) \equiv j^{\mu}(x).$$

The other covariants are also capable of interpretation. Thus $T^{[\mu\nu]}$ is, to within a constant, equal to a tensor $S^{\mu\nu}$, which can be interpreted as a spin density:

$$T^{[\mu\nu]} = -2\mathrm{i}S^{\mu\nu}(x) \equiv -2\mathrm{i}(\overline{\Psi}S^{\mu\nu}\Psi).$$

15. A Second Formulation of the Invariance of Form: Transformation of States

In the preceding paragraph, each transformation is considered as an operation on the reference axes, and the physical system is not modified. Inversely, one may effect the transformation on the physical system and leave the axes fixed; this second point of view was systematically adopted in the third part (cf. in particular the remarks of § XIII.11). Although the results are expressed in different language, it is clear that the two points of view are equivalent.

In order to clarify this equivalence, let (S) be the state of the physical system represented in the referential (R) by the spinor $\Psi(x)$. Let (S') be the state obtained by effecting the transformation $\mathscr{L}$ on (S), and $(\hat{R})$ the referential which is taken into (R) by the same transformation (cf. Fig. (XX.1):

$$(S') = \mathscr{L}(S), \qquad (\hat{R}) = \mathscr{L}^{-1}(R).$$

We consider the following three spinors:

$\Psi(x)$	representing	(S)	in referential	(R)
$\hat{\Psi}(\hat{x})$	,,	(S)	,, ,,	$(\hat{R})$
$\Psi'(x)$	,,	(S')	,, ,,	(R)

It is clear that $\hat{\Psi}$ and Ψ' are equal for equal values of their arguments:

$$\Psi'(x) = \hat{\Psi}(x). \qquad \text{(XX.103)}$$

The correspondence between $\hat{\Psi}$ and Ψ was established in § 11. Since one passes from $(\hat{R})$ to (R) by the transformation $\mathscr{L}$, one has, applying

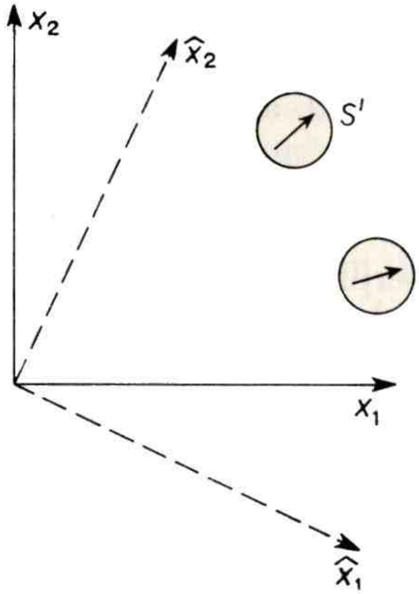

Fig. XX.1. The two ways of looking at a Lorentz transformation: change of referential ($\hat{x} \rightarrow x$) and transformation of the system ($S \rightarrow S'$).

(XX.85) and denoting the matrix associated with $\mathscr{L}$ by Λ:

$$\Psi(\hat{x}) = \Lambda \hat{\Psi}(\mathscr{L}^{-1}\hat{x}).$$

Therefore:

$$\Psi'(x) = \Lambda^{-1}\Psi(\mathscr{L}x). \tag{XX.104}$$

Comparing with equation (XX.85), one sees that the transformation of states is realized by the inverse of the operator corresponding to the change of referential.

These remarks also apply to the electromagnetic field in which the Dirac particle moves. Denote this field by (A) and the field obtained by the transformation $\mathscr{L}$ by (A'):

$$(A') = \mathscr{L}(A).$$

We consider the following three (covariant) four-vectors:

$A_\mu(x)$	representing	(A)	in	referential	(R),
$\hat{A}_\mu(\hat{x})$	,,	(A)	,,	,,	$(\hat{R})$,
$A_\mu'(x)$	,,	(A')	,,	,,	(R).

We can repeat the argument given above for the spinors. One obviously has:

$$A_\mu'(x) = \hat{A}_\mu(x). \tag{XX.105}$$

But, according to (XX.81):

$$\hat{A}_\mu(\mathscr{L}^{-1}x) = A_\nu(x)\Omega^\nu{}_\mu$$

whence

$$A_\mu'(x) = A_\nu(\mathscr{L}x)\Omega^\nu{}_\mu. \tag{XX.106}$$

Suppose now that $\Psi(x)$ satisfies the Dirac equation in the potential $A_\mu(x)$:

$$[\gamma^\mu(\mathrm{i}\partial_\mu - eA_\mu) - m]\Psi = 0. \tag{XX.107}$$

Taking into account equalities (XX.103) and (XX.105), the invariance of the form of the Dirac equation in the change of referential $(R) \to (\hat{R})$ gives

$$[\gamma^\mu(\mathrm{i}\partial_\mu - eA_\mu') - m]\Psi' = 0. \tag{XX.108}$$

The invariance of form can therefore be expressed in the following way:

If $\Psi(x)$ satisfies the Dirac equation in a potential $A_\mu(x)$, the state $\Psi'(x)$ obtained by the transformation $\mathscr{L}$ satisfies the Dirac equation in the transformed potential $A_\mu'(x)$.

16. Invariance of the Law of Motion

Equations (XX.107) and (XX.108) are in general different. They are identical when the external potential (A) is invariant in the transformation $\mathscr{L}$, that is, when

$$A_\mu'(x) = A_\mu(x).$$

In this case, Ψ and Ψ' obey the *same* wave equation. Thus, *the law of motion of the dynamical states is invariant in any transformation $\mathscr{L}$ that conserves the external potential.*

In all of the preceding work $\mathscr{L}$ was any orthochronous Lorentz transformation. However, all that has been said can be repeated for space-time *translations* [cf. note, p. 900].

The two properties mentioned above – invariance of form and invariance of the law of motion – remain valid when $\mathscr{L}$ represents a space or time translation.

17. Transformation Operators. Momentum, Angular Momentum, Parity

To continue this analysis in accordance with the general scheme set forth in Chapter XV we write the transformation law (XX.104) in the form

$$\Psi' = T\Psi, \tag{XX.109}$$

where T is an appropriate linear operator. The invariance of the Dirac equation in the transformation can then be expressed by the operator relation

$$T\,\mathscr{D}(A)\,T^{-1} = \mathscr{D}(A'), \qquad \text{(XX.110)}$$

in which $\mathscr{D}(A)$ and $\mathscr{D}(A')$ denote the Dirac operators in the potentials A and A' respectively:

$$\mathscr{D}(A) \equiv \gamma^\mu(\mathrm{i}\partial_\mu - eA_\mu). \qquad \text{(XX.111)}$$

The condition for the invariance of the law of motion under the transformation $\mathscr{L}$ is then expressed by the commutation relation

$$[T, \mathscr{D}(A)] = 0. \qquad \text{(XX.112)}$$

The operator T is easily constructed. It is the product of an operator $T^{(s)}$ acting on the spin variables alone, and an operator $T^{(0)}$ acting on the orbital variables alone:

$$T = T^{(s)} \otimes T^{(0)}.$$

Comparing (XX.109) and (XX.104), one sees that

$$T^{(s)} = \Lambda^{-1}, \qquad \text{(XX.113)}$$

where Λ denotes the *operator* represented by the matrix Λ defined in § 11.

Let us derive the explicit form of T for the infinitesimal Lorentz translations and "rotations", and for the reflection s.

For the translations one has $T^{(s)} = 1$. Let us introduce the differential operator

$$\boxed{p_\mu \equiv \mathrm{i}\partial_\mu} \qquad \text{(XX.114)}$$

p_μ represents the *energy-momentum four-vector* (more precisely, the covariant components of the energy-momentum four-vector). For an infinitesimal translation ε along the direction of the axis x^α, one finds

$$T = 1 + \mathrm{i}\varepsilon p_\alpha.$$

Consider now an "infinitesimal rotation" of angle ε in the plane $x^\alpha x^\beta$. In this case one has

$$\begin{aligned}(\mathscr{L}x)^\mu &= x^\mu - \varepsilon Z^{(\alpha\beta)\mu}{}_\nu x^\nu \\ &= x^\mu - \varepsilon\,(\delta^\mu{}_\alpha x_\beta - \delta^\mu{}_\beta x_\alpha).\end{aligned}$$

If $\psi_s(x)$ is a particular component of the spinor $\Psi(x)$, then to the first order in ε:

$$\psi_s(\mathscr{L}x) \simeq \psi_s(x) + \varepsilon\left(x_\alpha \frac{\partial \psi_s}{\partial x^\beta} - x_\beta \frac{\partial \psi_s}{\partial x^\alpha}\right).$$

If we introduce the differential operator

$$L_{\alpha\beta} \equiv x_\alpha p_\beta - x_\beta p_\alpha \qquad \text{(XX.115)}$$

the preceding equation takes the form

$$\psi_s(\mathscr{L}x) \simeq (1 - \mathrm{i}\varepsilon L_{\alpha\beta})\psi_s(x).$$

On the other hand, from (XX.90) and (XX.113),

$$T^{(s)} \simeq (1 - \mathrm{i}\varepsilon S_{\alpha\beta}),$$

where $S_{\alpha\beta}$ is defined by equation (XX.92). Finally, formula (XX.109) giving the law for the transformation of a spinor becomes in the "infinitesimal rotation" case

$$\begin{aligned} \Psi'(x) &\simeq (1 - \mathrm{i}\varepsilon S_{\alpha\beta})(1 - \mathrm{i}\varepsilon L_{\alpha\beta})\Psi(x) \\ &\simeq (1 - \mathrm{i}\varepsilon J_{\alpha\beta})\Psi(x), \end{aligned}$$

where

$$\boxed{J_{\alpha\beta} \equiv L_{\alpha\beta} + S_{\alpha\beta} \equiv x_\alpha p_\beta - x_\beta p_\alpha + \tfrac{1}{2}\sigma_{\alpha\beta}} \qquad \text{(XX.116)}$$

The three spatial components J_{23}, J_{31} and J_{12} of $J_{\alpha\beta}$ are associated with infinitesimal rotations about the axes Ox, Oy and Oz respectively; they are the components of the total angular momentum $\boldsymbol{J}$ and one has

$$\begin{gathered} \boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S} \\ \boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}, \qquad \boldsymbol{S} = \tfrac{1}{2}\boldsymbol{\sigma}. \end{gathered} \qquad \text{(XX.117)}$$

The components of $\boldsymbol{L}$ act on the orbital variables alone: $\boldsymbol{L}$ is the orbital angular momentum. The components of $\boldsymbol{S}$ act on the internal variables alone: $\boldsymbol{S}$ is the spin vector of the particle.

The reader will verify that $\boldsymbol{J}$, $\boldsymbol{L}$ and $\boldsymbol{S}$ satisfy the commutation relations characteristic of angular momenta and that $\boldsymbol{S}$ has the property

$$\boldsymbol{S}^2 = \tfrac{3}{4}$$

characteristic of a particle of spin $\frac{1}{2}$.

The operator associated with spatial reflection [1]) will be called the

[1]) See *Note added in proof*, p. 956.

parity operator and denoted by P. Let us denote by $P^{(0)}$ the "orbital parity" operator

$$P^{(0)}\Psi(t, \boldsymbol{r}) = \Psi(t, -\boldsymbol{r}).$$

According to (XX.113) we have for P the choice between two expressions differing by a sign, expressions easily obtained from the study of § 13 [cf. relation (XX.102)]. We adopt the most convenient one:

$$\boxed{P = \gamma^0 P^{(0)}} \qquad \text{(XX.118)}$$

Note that P is Hermitean and that $P^2 = 1$.

18. Conservation Laws and Constants of the Motion

If the transformation depends on the time, the associated operator T explicitly brings in the time dependence of Ψ. This occurs notably in the case of the time translations and the special Lorentz transformations.

On the other hand, *for any transformation independent of the time, the action of T is defined independently of the law of motion of the state vector to which it is applied.* T can then be defined as a transformation operator acting on the state-vectors and observables of the system as was done in Chapter XV (Section II); the invariance properties of the law of motion of the states may then be expressed in the form of conservation laws.

For example, if $\mathscr{L}$ is a spatial transformation, T is a certain function of the operators of reflection, infinitesimal translation and infinitesimal rotation, that is, a certain function of P, $\boldsymbol{J}$ and $\boldsymbol{p}$; T therefore commutes with γ^0. And since

$$\gamma^0\left(\mathrm{i}\frac{\partial}{\partial t} - H_D\right) \equiv \mathscr{D}(A) - m,$$

the commutation relation (XX.112) is equivalent, in this case, to

$$[T, H_D] = 0.$$

This condition is the same as the one studied in § XV.12, and what was said there concerning the connection between the symmetries of the Hamiltonian and the laws of conservation may be applied here.

Thus, if $A_\mu(x)$ is invariant under translation, one obtains the commutation relations

$$[\boldsymbol{p}, H_D] = 0$$

and the conservation of momentum. If $A_\mu(x)$ is spherically symmetrical,

$$[\boldsymbol{J}, H_D] = 0$$

and the total angular momentum is conserved. If $A_\mu(x)$ is invariant under reflection in the origin,

$$[P, H_D] = 0$$

and the parity is conserved.

19. Time Reversal and Charge Conjugation

In this paragraph, we shall demonstrate the invariance of the form of the Dirac equation under two antilinear operations, time reversal and charge conjugation. It is convenient, for this, to introduce an antiunitary operator K [1]) of state-vector space having certain particularly simple general properties.

THE ANTIUNITARY OPERATOR K. K is by definition the antiunitary operator which transforms $\boldsymbol{p}$ into $-\boldsymbol{p}$ and conserves $\boldsymbol{r}$ and γ^μ:

$$K\boldsymbol{r}K^\dagger = \boldsymbol{r}, \qquad K\boldsymbol{p}K^\dagger = -\boldsymbol{p}. \tag{XX.119}$$

$$K\gamma^\mu K^\dagger = \gamma^\mu \qquad (\mu = 0, 1, 2, 3). \tag{XX.120}$$

It will be shown that such an operator exists, is defined to within a phase, and has the property

$$K^2 = -1. \tag{XX.121}$$

That K, if it exists, is defined to within a phase follows from relations (XX.119–120) and the fact that state-vector space is irreducible with respect to the basic operators $\boldsymbol{r}$, $\boldsymbol{p}$ and γ^μ. Let us now choose a particular representation, the Dirac representation for example. Each *operator* γ^μ is then represented by a certain matrix $\gamma_D{}^\mu$. Denote the operator represented by the "B matrix" which transforms the $\gamma_D{}^\mu$ into their respective complex conjugates by B_D. Here, B_D will be considered as a (unitary) operator of the total space and not as an operator of spin space alone; it is a unitary operator commuting with $\boldsymbol{r}$ and $\boldsymbol{p}$. Let K_D be the complex-conjugation operator associated with the representation (definition of § XV.5). Relations (XX.76) give:

$$\gamma^\mu = B_D(K_D\gamma^\mu K_D{}^\dagger)B_D{}^\dagger.$$

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[1]) This operator *is not* the time reversal operator. The latter is denoted below by K_T.

Therefore, the antiunitary operator

$$K \equiv B_D K_D$$

satisfies relations (XX.120). Since B_D commutes with $\boldsymbol{r}$ and $\boldsymbol{p}$, and since from the definition of K_D,

$$K_D \boldsymbol{r} K_D = \boldsymbol{r}, \qquad K_D \boldsymbol{p} K_D = -\boldsymbol{p},$$

K also satisfies relations (XX.119). Finally, since $K_D = K_D^\dagger$, (XX.77) gives:

$$B_D(K_D B_D K_D) \equiv K^2 = -1.$$

This is just (XX.121); it obviously remains true if K is multiplied by any phase factor. Q.E.D.

Charge-conjugation. Multiplying both sides of equation (XX.107) on the left by K and using the fact that K is antilinear and commutes with γ^μ, ∂_μ and $A_\mu(x)$, one finds:

$$[\gamma^\mu(-\mathrm{i}\partial_\mu - eA_\mu(x)) - m]\, K\Psi(x) = 0. \qquad \text{(XX.122)}$$

$K\Psi$ therefore satisfies a wave equation differing from the Dirac equation only by the substitution of $-\mathrm{i}$ for $+\mathrm{i}$. Let us multiply both sides by γ^5. Since γ^5 anticommutes with γ^μ and commutes with all of the other operators in the bracket on the left-hand side, we obtain

$$[\gamma^\mu(\mathrm{i}\partial_\mu + eA_\mu(x)) - m]\, \gamma^5 K\Psi(x) = 0. \qquad \text{(XX.123)}$$

Put:

$$\boxed{K_C \equiv \gamma^5 K} \qquad \text{(XX.124)}$$

$$\Psi^C(x) \equiv K_C \Psi(x). \qquad \text{(XX.125)}$$

Equation (XX.123) now becomes:

$$[\gamma^\mu(\mathrm{i}\partial_\mu + eA_\mu(x)) - m]\, \Psi^C(x) = 0. \qquad \text{(XX.126)}$$

The equation satisfied by $\Psi^C(x)$ differs from the one satisfied by $\Psi(x)$ only in the sign of the charge. Thus, *if $\Psi(x)$ represents the motion of a Dirac particle of mass m and charge e in the potential $A_\mu(x)$, $\Psi^C(x)$ represents the motion of a Dirac particle of the same mass m and of opposite charge $(-e)$ in the same potential $A_\mu(x)$.*

The spinors Ψ and Ψ^C are called charge conjugates one of the other, and the transformation K_C is called *charge conjugation.*

It follows from the properties of K and γ^5 that

$$K_C^2 = 1. \tag{XX.127}$$

Thus the correspondence between Ψ and Ψ^C is reciprocal. It is easy to show that charge conjugation commutes with translations and orthochronous Lorentz transformations. More precisely, if $L\Psi$ is the transform of Ψ in one of these transformations, its charge-conjugate is $L\Psi^C$ in the case of a translation or a proper Lorentz transformation, and $-L\Psi^C$ in the case of a reflection (cf. Problem XX.5).

Time reversal. The time reversal invariance of the Dirac equation can be demonstrated directly, but it is just as simple to start from the preceding results on charge conjugation.

A given potential $A_\mu(t, \mathbf{r})$ is created by a certain number of charges in motion. The time-reversed potential $A_\mu'(t, \mathbf{r})$, is obtained by reversing the motion of these charges. In this operation the currents, and therefore the magnetic field, change their sign while electric charges, and therefore the electric field, remain unchanged

$$\mathscr{H}'(t, \mathbf{r}) = -\mathscr{H}(-t, \mathbf{r}), \qquad \mathscr{E}'(t, \mathbf{r}) = \mathscr{E}(-t, \mathbf{r}).$$

It follows that A_μ "transforms like a pseudovector":

$$\mathbf{A}'(t, \mathbf{r}) = -\mathbf{A}(-t, \mathbf{r}) \qquad A_0'(t, \mathbf{r}) = A_0(-t, \mathbf{r}).$$

If we change t into $-t$ in equation (XX.126), we therefore have

$$[-\gamma^0(\mathrm{i}\partial_0 - eA_0'(t, \mathbf{r})) + \sum_k \gamma^k(\mathrm{i}\partial_k - eA_k'(t, \mathbf{r})) - m]\,\Psi^C(-t, \mathbf{r}) = 0.$$

Let us multiply both sides by $\gamma^5\gamma^0$. Since this operator anticommutes with γ^0 and commutes with γ^k, we obtain:

$$[\gamma^\mu(\mathrm{i}\partial_\mu - eA_\mu'(t, \mathbf{r})) - m]\,\Psi'(t, \mathbf{r}) = 0 \tag{XX.128}$$

if we put:

$$\Psi'(t, \mathbf{r}) \equiv \gamma^5\gamma^0\Psi^C(-t, \mathbf{r}) \tag{XX.129}$$
$$= \gamma^0 K\Psi(-t, \mathbf{r}).$$

Let us introduce the (antiunitary) time-reversal operator:

$$\boxed{K_T \equiv \gamma^0 K} \tag{XX.130}$$

$\Psi'(t, \mathbf{r})$ is by definition the time-reversal transform of $\Psi(-t, \mathbf{r})$. It satisfies equation (XX.128). Therefore, if Ψ satisfies the Dirac equation in the potential A_μ, its time-reversal transform Ψ' satisfies the Dirac equation in the potential A_μ' obtained from A_μ by time reversal.

In particular, if A_μ is invariant under time reversal (for example, if the particle is in a stationary electric field: $\mathbf{A}=0$, $\partial A_0/\partial t=0$), Ψ and Ψ' both obey the same Dirac equation.

From the properties of γ^0 and K, one obtains:

$$K_T{}^2 = -1. \tag{XX.131}$$

This result, characteristic of systems of half-integral angular momenta, has already been obtained in the non-relativistic case [eq. (XV.88)]. The consequences, in particular Kramers degeneracy, are also valid here.

Expressing B_D in terms of the ϱ and σ (cf. end of § 10), we easily obtain from definitions (XX.124) and (XX.130) the equivalent relations

$$K_C = \mathrm{i}\varrho_2\,\sigma_y\,K_D$$
$$K_T = \mathrm{i}\sigma_y\,K_D.$$

These are useful when manipulating the operators K_C and K_T in the Dirac representation.

20. Gauge Invariance

For completeness, we shall mention here the property of gauge invariance (cf. § XXI.20).

Changing the gauge of the electromagnetic potential means replacing the components $A_\mu(x)$ by

$$A_\mu'(x) \equiv A_\mu(x) - \partial_\mu G(x), \tag{XX.132}$$

where $G(x)$ is an arbitrary function of the space-time coordinates. This gives

$$A_0' = A_0 - \frac{\partial G}{\partial t}, \qquad \mathbf{A}' = \mathbf{A} + \nabla G.$$

The electric and magnetic fields are invariant in such a transformation.

If $\Psi(x)$ is a solution of the Dirac equation in the potential A_μ, then clearly

$$\Psi'(x) \equiv \mathrm{e}^{\mathrm{i}eG(x)}\Psi(x) \tag{XX.133}$$

is a solution of the Dirac equation in the potential A_μ'. This is called the gauge-invariance property of the Dirac equation.

IV. INTERPRETATION OF THE OPERATORS AND SIMPLE SOLUTIONS

21. The Dirac Equation and the Correspondence Principle

When the electromagnetic field is not zero, the solutions of the Dirac equation satisfy a second-order equation different to the Klein–Gordon equation but conforming with the correspondence principle.

To obtain this equation, one can start from the covariant form (XX.50) and write that the action of the operator $(-i\gamma^\lambda D_\lambda - m)$ on the left-hand side gives zero:

$$[\gamma^\lambda\gamma^\mu D_\lambda D_\mu + m^2]\Psi = 0. \qquad \text{(XX.134)}$$

From the algebraic properties of the γ^μ operators, one obtains

$$\gamma^\lambda\gamma^\mu \equiv g^{\lambda\mu} + \tfrac{1}{2}[\gamma^\lambda, \gamma^\mu]. \qquad \text{(XX.135)}$$

By renaming the dummy indices, we have

$$[\gamma^\lambda, \gamma^\mu] D_\lambda D_\mu \equiv -[\gamma^\lambda, \gamma^\mu] D_\mu D_\lambda = \tfrac{1}{2}\,[\gamma^\lambda, \gamma^\mu]\,[D_\lambda, D_\mu]. \qquad \text{(XX.136)}$$

and, from the definition of the operator D_μ [eq. (XX.10)]

$$\begin{aligned}[D_\lambda, D_\mu] &\equiv ie[\partial_\lambda, A_\mu] + ie[A_\lambda, \partial_\mu] \\ &\equiv ie\left(\frac{\partial A_\mu}{\partial x^\lambda} - \frac{\partial A_\lambda}{\partial x^\mu}\right) \equiv ieF_{\lambda\mu}.\end{aligned} \qquad \text{(XX.137)}$$

Equations (XX.135–137) give

$$\gamma^\lambda\gamma^\mu D_\lambda D_\mu \equiv D_\mu D^\mu + eS^{\lambda\mu}F_{\lambda\mu}, \qquad \text{(XX.138)}$$

where $S^{\lambda\mu}$ represents the spin of the particle [definition (XX.92)]. Equation (XX.134) can therefore be put in the form

$$[D_\mu D^\mu + eS^{\lambda\mu}F_{\lambda\mu} + m^2]\Psi = 0. \qquad \text{(XX.139)}$$

Comparing (XX.139) with the form (XX.30′) of the Klein–Gordon equation, it is seen that it differs by the presence of the term

$$eS^{\lambda\mu}F_{\lambda\mu}, \qquad \text{(XX.140)}$$

which is a term coupling the spin of the particle to the electromagnetic field. This term has no classical analogue and its contribution is negligible when the classical approximation is valid. The motion of a Dirac wave packet is then the same as the motion of a Klein–Gordon wave packet.

22. Dynamical Variables of a Dirac Particle

From time to time we have given the physical interpretation of a certain number of dynamical variables of the Dirac theory. We shall now take up this question in a more systematic way, and indicate, in particular, the variables of the Quantum Theory which correspond to the different classical quantities of § 4.

The relativistic invariance of the theory plays no essential role in this discussion. We adopt the same point of view as in non-relativistic Quantum Mechanics: the system is defined by giving a certain number of dynamical variables obeying a well-defined algebra, and the Dirac equation – in the Dirac form [eqs. (XX.36) and (XX.44)] – describes the evolution of the dynamical states in the Schrödinger "representation".

In what follows time is therefore treated as a simple parameter, while the spatial coordinates are included among the dynamical variables of the system. The fundamental variables are $\mathbf{r}$ and $\mathbf{p}$ together with the internal variables $\boldsymbol{\alpha}$ and β. The whole of representation theory applies here without change. In particular, in the Dirac representation, the state-vectors $|\Psi\rangle$, $|\Phi\rangle$, ..., are represented by four-component wave functions, $\Psi(\mathbf{r})$, $\Phi(\mathbf{r})$, ... of the coordinates x, y, z. In this representation the scalar product $\langle\Phi|\Psi\rangle$ is defined as a summation over the 4 possible values of the index representing the internal degree of freedom and an integration over the coordinates x, y, z:

$$\langle\Phi|\Psi\rangle = \sum_{s=1}^{4} \int \varphi_s^*(\mathbf{r})\, \psi_s(\mathbf{r})\, \mathrm{d}\mathbf{r}.$$

This definition of the scalar product is consistent with the definition of the position probability density given in § 6 [formula (XX.35)]. More generally, we shall adopt here without change the statistical interpretation of the theory as set forth in the first part of this book; in particular, the average value of an operator Q for a given state of the system is given by

$$\langle Q\rangle = \langle u|Q|u\rangle,$$

where $|u\rangle$ is the normalized ket representing that state.

The observables of the theory that do not act on the internal degree of freedom have an obvious interpretation; in particular we have:

$\boldsymbol{r}$, the position vector,

$\boldsymbol{p}$, the (Lagrange canonical) momentum, called the momentum in this book.

$\boldsymbol{\pi} \equiv \boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r}, t)$, the mechanical momentum.

Among the functions of $\boldsymbol{r}$ we have the operator

$$\delta(\boldsymbol{r} - \boldsymbol{r}_0),$$

which is the projector onto the subspace of the eigenvalue $\boldsymbol{r}_0$; it represents the position probability density at the point $\boldsymbol{r}_0$.

Among the observables depending on the internal degree of freedom we define [1]):

the energy:

$$H \equiv e\varphi + \boldsymbol{\alpha} \cdot \boldsymbol{\pi} + \beta m; \tag{XX.141}$$

the relativistic mass:

$$M \equiv H - e\varphi \equiv \boldsymbol{\alpha} \cdot \boldsymbol{\pi} + \beta m; \tag{XX.142}$$

the current density at $\boldsymbol{r}$:

$$\boldsymbol{j}(\boldsymbol{r}_0) \equiv \boldsymbol{\alpha}\delta(\boldsymbol{r} - \boldsymbol{r}_0); \tag{XX.143}$$

the total angular momentum:

$$\boldsymbol{J} \equiv (\boldsymbol{r} \times \boldsymbol{p}) + \tfrac{1}{2}\boldsymbol{\sigma}; \tag{XX.144}$$

the spin:

$$\boldsymbol{S} \equiv \tfrac{1}{2}\boldsymbol{\sigma}; \tag{XX.145}$$

the parity:

$$P \equiv \beta P^{(0)}. \tag{XX.146}$$

The definitions of H and M are based on the correspondence with classical mechanics; that of $\boldsymbol{j}(\boldsymbol{r}_0)$ follows from the equation of continuity; those of $\boldsymbol{J}$ and $\boldsymbol{S}$ are related to the transformations of the states under rotation and that of P to the transformations under reflection.

Finally, *the correspondence principle leads to the interpretation of* $\boldsymbol{\alpha}$ *as the velocity of the particle*. This interpretation is also suggested by the expression for the current density. To establish it, we compare the classical equations (XX.18), (XX.19) and (XX.21) with the corresponding quantum equations, and to do this we must obviously pass

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[1]) Note that $\boldsymbol{p}$ depends on the choice of gauge; only the momentum of the total system (particle + electromagnetic field) is independent of this choice. The same remarks apply to the energy H and to the angular momentum $\boldsymbol{J}$ (cf. § XXI.23).

over to the Heisenberg "representation". The Heisenberg equations for the variables $\boldsymbol{r}$ and $\boldsymbol{\pi}$ (in the Heisenberg "representation") are written:

$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = -\,\mathrm{i}[\boldsymbol{r}, H]$$

$$\frac{\mathrm{d}\boldsymbol{\pi}}{\mathrm{d}t} = -\,\mathrm{i}[\boldsymbol{\pi}, H] + \frac{\partial \boldsymbol{\pi}}{\partial t}.$$

Replacing H and $\boldsymbol{\pi}$ on the right-hand side by the expressions given above and using the commutation or anti-commutation relations for the operators $\boldsymbol{r}$, $\boldsymbol{p}$, $\boldsymbol{\alpha}$ and β, one finds, after a rather long but straightforward calculation (Problem XX.6),

$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = \boldsymbol{\alpha} \tag{XX.147}$$

$$\frac{\mathrm{d}\boldsymbol{\pi}}{\mathrm{d}t} = e(\mathscr{E} + \boldsymbol{\alpha} \times \mathscr{H}). \tag{XX.148}$$

Also, from (XX.142) and the properties of $\boldsymbol{\alpha}$, one has the identity

$$\boldsymbol{\pi} = \tfrac{1}{2}(M\boldsymbol{\alpha} + \boldsymbol{\alpha} M). \tag{XX.149}$$

Equations (XX.147–149) between dynamical variables in the Heisenberg "representation" may be identified respectively with equations (XX.18), (XX.21) and (XX.19) between the classical dynamical variables if one treats $\boldsymbol{\alpha}$ as the classical velocity $\boldsymbol{v}$.

Note that the components of the velocity $\boldsymbol{\alpha}$ do not commute, and that each of them has in all two eigenvalues, $+c$ and $-c$ ($+1$ and -1 in the units used here). Here we have no difficulty of principle, but simply an additional indication that the classical picture of the phenomena should not be taken too seriously. We shall return to this question in § 37.

23. The Free Electron. Plane Waves

In the rest of this section we examine the solutions of the Dirac equation, first in the absence of a field, then in a static central potential. Solving the Dirac equation is then equivalent to finding the eigensolutions of the Hamiltonian H_D. Unless otherwise indicated, the calculations will be made in the Dirac representation, and we shall frequently make use of the operators ϱ_1, ϱ_2, ϱ_3 and σ_x, σ_y, σ_z introduced in § 7.

We first suppose the field null. The Hamiltonian H_D then commutes with the three components of the momentum. We therefore wish to find the eigensolutions of H_D corresponding to a well-defined value $\boldsymbol{p}$ for the momentum. Such solutions are plane waves, that is, functions of the form

$$u(\boldsymbol{p})\, e^{i\boldsymbol{p}\cdot\boldsymbol{r}},$$

where $u(\boldsymbol{p})$ is a four-component spinor independent of $\boldsymbol{r}$. It is determined by the eigenvalue equation

$$Hu(\boldsymbol{p}) = Eu(\boldsymbol{p}), \qquad \text{(XX.150)}$$

where H is the following operator of $\mathscr{E}^{(s)}$ space:

$$H \equiv \boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m \equiv \varrho_1(\boldsymbol{\sigma}\cdot\boldsymbol{p})+\varrho_3 m. \qquad \text{(XX.151)}$$

A simple calculation gives:

$$H^2 = p^2+m^2.$$

The only possible eigenvalues of H are therefore the two values $\pm\sqrt{p^2+m^2}$, i.e.:

$$\begin{aligned} E &= \varepsilon E_p \qquad (\varepsilon = \pm 1) \\ E_p &= \sqrt{p^2+m^2}. \end{aligned} \qquad \text{(XX.152)}$$

It is easy to show – for example by using the fact that ϱ_2 anticommutes with H – that these two values are doubly degenerate.

The *component* $\boldsymbol{\sigma}\cdot\boldsymbol{p}/2p$ *of the spin in the direction of* $\boldsymbol{p}$ *commutes with* H. This can be seen from the last of expressions (XX.151); (the other spin components do not commute with H). We are therefore led to look for the common eigensolutions of H and $\boldsymbol{\sigma}\cdot\boldsymbol{p}/2p$. We obtain the following 4 pairs of eigenvalues:

$$(+E_p,+\tfrac{1}{2}) \quad (+E_p,-\tfrac{1}{2}) \quad (-E_p,+\tfrac{1}{2}) \quad (-E_p,-\tfrac{1}{2}).$$

To each of these pairs there corresponds a single eigenstate. The corresponding eigenspinor is easily determined from the two eigenvalue equations. An alternative method for finding this spinor will be given in the following paragraph.

The components of the 4 eigenspinors (normalized to unity) are given in Table XX.3 for the particularly simple case when $\boldsymbol{p}$ is directed along the z axis. Recall that, in the Dirac representation, β and σ_z are represented by diagonal matrices.

TABLE XX.3

Components of the spinors corresponding to the wave of momentum $\boldsymbol{p} \equiv (0, 0, p)$ *in the Dirac representation* ($E_p = \sqrt{m^2 + p^2}$).

Energy $E =$	Positive $+E_p$		Negative $-E_p$	
Spin $\boldsymbol{\sigma}\cdot\boldsymbol{p}/2p \equiv \frac{1}{2}\sigma_z$	↺ $+\frac{1}{2}$	↷ $-\frac{1}{2}$	↺ $+\frac{1}{2}$	↷ $-\frac{1}{2}$
$\left(\frac{2E_p}{E_p+m}\right)^{\frac{1}{2}} \times$ $u_1 =$	1	0	$-\frac{p}{E_p+m}$	0
$u_2 =$	0	1	0	$\frac{p}{E_p+m}$
$u_3 =$	$\frac{p}{E_p+m}$	0	1	0
$u_4 =$	0	$-\frac{p}{E_p+m}$	0	1

The 4 spinors are normalized to unity: $u^\dagger u = 1$.

24. Construction of the Plane Waves by a Lorentz Transformation

When $A_\mu = 0$, any Lorentz transform of a solution of the Dirac equation is another solution of the Dirac equation. In particular, any plane wave of momentum $\boldsymbol{p}$ can be obtained by a Lorentz transformation from a plane wave of momentum zero. We shall now describe a method based on this remark for constructing the spinors $u(\boldsymbol{p})$ of the preceding paragraph.

For a zero momentum, equation (XX.150) becomes

$$\beta m u(0) = E u(0).$$

The two possible eigenvalues are $+m$ and $-m$. To the eigenvalue $\varepsilon m (\varepsilon = \pm 1)$ there corresponds the spinor $u^{(\varepsilon)}(0)$; it is an eigenvector of the operator β. We shall suppose it normalized to unity, and we fix the direction of the spin in an arbitrary way; $u^{(\varepsilon)}(0)$ is then defined up to a phase.

The plane wave

$$\Psi_0^{(\varepsilon)} = u^{(\varepsilon)}(0) \mathrm{e}^{-\mathrm{i}\varepsilon m t}$$

is a solution of the Dirac equation corresponding to a momentum zero and an energy εm, that is, to the energy-momentum four-vector $(\varepsilon m, 0)$.

Consider the same solution in a new referential having a velocity

$\mathbf{v} = -\mathbf{p}/\varepsilon\sqrt{m^2+p^2} = -\mathbf{p}/\varepsilon E_p$ with respect to the preceding one. In this new referential, the energy-momentum of the particle is

$$p^\mu \equiv (\varepsilon E_p, \mathbf{p}). \tag{XX.153}$$

The solution is there represented by the plane wave:

$$\begin{aligned}\Psi_{\mathbf{p}}^{(\varepsilon)} &= \Lambda_{\text{sp}}(\mathbf{v})\, u^{(\varepsilon)}(0) \exp(-\mathrm{i}p^\mu x_\mu) \\ &= [\Lambda_{\text{sp}}(\mathbf{v})\, u^{(\varepsilon)}(0)] \exp[-\mathrm{i}(\varepsilon E_p t - \mathbf{p}\cdot\mathbf{r})].\end{aligned}$$

The term in brackets is therefore proportional to one of the sought-for spinors $u(\mathbf{p})$ which we shall henceforth denote by $u^{(\varepsilon)}(\mathbf{p})$. Its norm is the time component of the associated current four-vector; it may be obtained from the current four-vector associated with $u^{(\varepsilon)}(0)$ by a Lorentz transformation; it is therefore equal to:

$$b \equiv (1-v^2)^{-\frac{1}{2}} = E_p/m.$$

We therefore adopt the definition:

$$u^{(\varepsilon)}(\mathbf{p}) \equiv b^{-\frac{1}{2}} \Lambda_{\text{sp}}(\mathbf{v})\, u^{(\varepsilon)}(0).$$

Substituting (XX.97) into this definition with the values of $\mathbf{v}$ and b given above, one finds

$$u^{(\varepsilon)}(\mathbf{p}) = [2E_p(m+E_p)]^{-\frac{1}{2}}[m+E_p+\varepsilon\boldsymbol{\alpha}\cdot\mathbf{p}]u^{(\varepsilon)}(0), \tag{XX.154}$$

which is the required expression. In particular if $u^{(\varepsilon)}(0)$ is an eigenstate of $(\boldsymbol{\sigma}\cdot\mathbf{p})$, then so is $u^{(\varepsilon)}(\mathbf{p})$, which is therefore in this case one of the spinors defined in the preceding paragraph. In particular one obtains the results of Table 3 when $\mathbf{p}$ is directed along the z axis.

Expression (XX.154) may also be put in the form

$$u^{(\varepsilon)}(\mathbf{p}) = [2E_p(m+E_p)]^{-\frac{1}{2}}[m+\gamma^\mu p_\mu]u^{(\varepsilon)}(0), \tag{XX.155}$$

in which p_μ represents the energy-momentum four-vector defined by equation (XX.153).

25. Central Potential

We now look for the eigensolutions of a Dirac particle in a static central potential $V(r)$. The Dirac Hamiltonian is then

$$H_D \equiv \boldsymbol{\alpha}\cdot\mathbf{p}+\beta m+V(r). \tag{XX.156}$$

It is invariant under rotation and reflection:

$$[H_D, \mathbf{J}] = 0, \qquad [H_D, P] = 0.$$

We therefore look for eigensolutions of well-defined angular momentum and parity.

It is convenient to write the solutions Ψ in the form

$$\Psi = \begin{pmatrix} \Phi \\ \chi \end{pmatrix}, \tag{XX.157}$$

where

$$\Phi \equiv \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \qquad \chi \equiv \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix}. \tag{XX.158}$$

Projecting Ψ onto the subspaces $\beta = +1$ and $\beta = -1$, one finds

$$\tfrac{1}{2}(1+\beta)\,\Psi = \begin{pmatrix} \Phi \\ 0 \end{pmatrix}, \qquad \tfrac{1}{2}(1-\beta)\,\Psi = \begin{pmatrix} 0 \\ \chi \end{pmatrix}. \tag{XX.159}$$

Φ and χ are functions of $\boldsymbol{r}$ and of the spin component μ along the z axis; they may also be considered as functions of the radial variable r and of the "angular variables" (θ, φ, μ): in this they are entirely analogous to the wave functions of the Pauli theory.

Let us now suppose that Ψ is a simultaneous eigenfunction of $\boldsymbol{J}^2$, J_z and P. We denote the angular momentum quantum numbers by (JM). For convenience, we indicate the parity with the aid of the quantum number ϖ such that:

$$\varpi = \begin{cases} +1 \text{ for states of parity } (-)^{J+\frac{1}{2}} \\ -1 \text{ for states of parity } (-)^{J-\frac{1}{2}} \end{cases} \tag{XX.160}$$

Thus, by hypothesis:

$$\begin{gathered} \boldsymbol{J}^2 \begin{pmatrix} \Phi \\ \chi \end{pmatrix} = J(J+1) \begin{pmatrix} \Phi \\ \chi \end{pmatrix}, \qquad J_z \begin{pmatrix} \Phi \\ \chi \end{pmatrix} = M \begin{pmatrix} \Phi \\ \chi \end{pmatrix} \\ P^{(0)} \begin{pmatrix} \Phi \\ \chi \end{pmatrix} = (-)^{J+\frac{1}{2}\varpi} \begin{pmatrix} \Phi \\ -\chi \end{pmatrix}. \end{gathered} \tag{XX.161}$$

Let $\mathscr{Y}_{LJ}^{M}(\theta, \varphi, \mu)$ be the function of total angular momentum (JM) formed by the composition of a spin $\frac{1}{2}$ with the spherical harmonics of order L. The parity of this function is $(-)^L$. Also, according to the rules for the composition of angular momenta, L can take only the two values

$$L = l \equiv J + \tfrac{1}{2}\varpi \qquad L = l' \equiv J - \tfrac{1}{2}\varpi \tag{XX.162}$$

and the two functions $\mathscr{Y}_{lJ}^{M}$ and $\mathscr{Y}_{l'J}^{M}$ are of opposite parity, that of the first being $(-)^{J+\frac{1}{2}\varpi}$ and that of the second $(-)^{J-\frac{1}{2}\varpi}$. According to equations (XX.161), Φ is a function of $(r, \theta, \varphi, \mu)$ of angular momentum (JM) and of parity $(-)^{J+\frac{1}{2}\varpi}$; it is therefore necessarily equal to the product of a function of r by $\mathscr{Y}_{lJ}^{M}$. A similar argument shows that χ is equal to the product of a function of r by $\mathscr{Y}_{l'J}^{M}$.

In conclusion, if $\Psi_{\varpi J}^{M}$ represents a state of angular momentum (JM) and of parity $(-)^{J+\frac{1}{2}\varpi}$, it can be written in the form

$$\Psi_{\varpi J}^{M} = \frac{1}{r}\begin{pmatrix} F\ \mathscr{Y}_{lJ}^{M} \\ \mathrm{i}G\ \mathscr{Y}_{l'J}^{M} \end{pmatrix}, \tag{XX.163}$$

where l and l' are given by equations (XX.162), and F and G are arbitrary functions of r.

Consider now the eigenvalue problem

$$H_D \Psi_{\varpi J}^{M} = E \Psi_{\varpi J}^{M}. \tag{XX.164}$$

To solve this equation we separate the "angular" variables from the radial variables in the operator H_D. The method to be followed is wholly analogous to the one of Chapter IX.

We introduce the radial momentum p_r and the "radial velocity" α_r:

$$p_r \equiv -\mathrm{i}\frac{1}{r}\frac{\partial}{\partial r} r \tag{XX.165}$$

$$\alpha_r \equiv \boldsymbol{\alpha}\cdot\hat{\boldsymbol{r}} = \varrho_1 (\boldsymbol{\sigma}\cdot\boldsymbol{r})/r. \tag{XX.166}$$

From identity (XIII.83), one obtains

$$\begin{aligned}(\boldsymbol{\alpha}\cdot\boldsymbol{r})(\boldsymbol{\alpha}\cdot\boldsymbol{p}) = (\boldsymbol{\sigma}\cdot\boldsymbol{r})(\boldsymbol{\sigma}\cdot\boldsymbol{p}) &= \boldsymbol{r}\cdot\boldsymbol{p}+\mathrm{i}\boldsymbol{\sigma}\cdot\boldsymbol{L} \\ &= rp_r+\mathrm{i}(1+\boldsymbol{\sigma}\cdot\boldsymbol{L}).\end{aligned}$$

Whence, multiplying on the left by α_r/r and using the obvious property $\alpha_r^2=1$, the identity:

$$\boldsymbol{\alpha}\cdot\boldsymbol{p} \equiv \alpha_r\left(p_r+\frac{\mathrm{i}}{r}(1+\boldsymbol{\sigma}\cdot\boldsymbol{L})\right). \tag{XX.167}$$

Let us examine the operator $1+\boldsymbol{\sigma}\cdot\boldsymbol{L}$. One easily shows that

$$1+\boldsymbol{\sigma}\cdot\boldsymbol{L} = \boldsymbol{J}^2+\tfrac{1}{4}-\boldsymbol{L}^2.$$

Further, from (XX.163), it is clear that the action of $\mathbf{L}^2$ on $\Psi_{\varpi J}^{M}$ is equivalent to that of the operator

$$(J+\tfrac{1}{2}\varpi\beta)(J+\tfrac{1}{2}\varpi\beta+1) \equiv J(J+1)+\tfrac{1}{4}+\tfrac{1}{2}\varpi\beta(2J+1).$$

Therefore:

$$(1+\boldsymbol{\sigma}\cdot\mathbf{L})\Psi_{\varpi J}^{M} = -\tfrac{1}{2}\varpi(2J+1)\beta\Psi_{\varpi J}^{M}. \qquad \text{(XX.168)}$$

Substituting relations (XX.167) and (XX.168) into equation (XX.164), one obtains

$$\left[\alpha_r\left(p_r - \frac{\mathrm{i}\varpi(J+\frac{1}{2})}{r}\,\beta\right) + m\beta + V(r)\right]\Psi_{\varpi J}^{M} = E\Psi_{\varpi J}^{M}.$$

By replacing the eigenfunction by expression (XX.163), the operators p_r and α_r by their definitions (XX.165) and (XX.166) and using the identites (cf. Problem XX.8):

$$\begin{aligned}(\boldsymbol{\sigma}\cdot\hat{\mathbf{r}})\,\mathscr{Y}_{lJ}^{M} &= -\,\mathscr{Y}_{l'J}^{M}\\ (\boldsymbol{\sigma}\cdot\hat{\mathbf{r}})\,\mathscr{Y}_{l'J}^{M} &= -\,\mathscr{Y}_{lJ}^{M}\end{aligned} \qquad \text{(XX.169)}$$

this equation leads to two coupled differential equations for the radial functions $F(r)$ and $G(r)$, namely

$$\left[-\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\varpi(J+\frac{1}{2})}{r}\right]G = (E-m-V)\,F \qquad \text{(XX.170}a\text{)}$$

$$\left[\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\varpi(J+\frac{1}{2})}{r}\right]F = (E+m-V)\,G. \qquad \text{(XX.170}b\text{)}$$

These equations here play the role of equation (IX.20) in the non-relativistic theory.

After integration over the angles, the norm of $\Psi_{\varpi J}^{M}$ is given by the expression:

$$\langle\Psi_{\varpi J}^{M}|\Psi_{\varpi J}^{M}\rangle = \int_0^\infty (|F|^2+|G|^2)\,\mathrm{d}r \qquad \text{(XX.171)}$$

to be compared with expression (IX.21).

The discussion of the regularity of F and G is in all ways analogous to the discussion of the regularity of $y_l(r)$ in the non-relativistic theory. We shall not go into the details here.

26. Free Spherical Waves

For $V=0$, the method of the preceding paragraph gives the stationary solutions of the Dirac equation of the free electron which correspond to well-defined angular momentum and parity; these are the Dirac free spherical waves.

In this case, eq. (XX.170b) gives,

$$G = \frac{1}{E+m}\left[\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\varpi(J+\frac{1}{2})}{r}\right] F. \qquad \text{(XX.172)}$$

Substituting this expression into (XX.170a), one finds:

$$(E^2-m^2)\,F = \left[-\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\varpi(J+\frac{1}{2})}{r}\right]\left[\frac{\mathrm{d}}{\mathrm{d}r} + \varpi\frac{(J+\frac{1}{2})}{r}\right] F$$
$$= \left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{(J+\frac{1}{2})\,(J+\varpi+\frac{1}{2})}{r^2}\right] F.$$

It can easily be shown that

$$(J+\tfrac{1}{2})(J+\varpi+\tfrac{1}{2}) = l(l+1),$$

where l is the integer defined by equation (XX.162). The preceding equation is therefore identical with the free wave radial equation of the non-relativistic theory if one substitutes for (E^2-m^2) the product of $2m$ by the non-relativistic energy. It has one and only one regular solution for any positive value of (E^2-m^2). If one puts

$$k = \sqrt{E^2-m^2} \qquad (|E| \geqslant m)$$

it becomes

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + k^2\right] F = 0.$$

Its regular solution (defined up to a constant) is given by

$$F = r j_l(kr).$$

The corresponding G function is obtained by applying relation (XX.172). Using the recursion relations (B.42) and (B.43) [the first for $\varpi=1$, the second for $\varpi=-1$, both being written with $\gamma=0$], one finds

$$G = \frac{\varpi k}{E+m}\, r j_{l'}(kr).$$

In conclusion, for any value of the energy E situated outside the interval $(-m, +m)$, there exists a free spherical wave of angular momentum (JM) and parity $(-)^{J+\frac{1}{2}\varpi}$. In the form (XX.163), it is written

$$Cst. \times \begin{pmatrix} |E+m|^{\frac{1}{2}}\, j_l(\sqrt{E^2-m^2}\,r)\, \mathscr{Y}_{lJ}^{M} \\ \mathrm{i}\varpi\varepsilon|E-m|^{\frac{1}{2}}\, j_{l'}(\sqrt{E^2-m^2}\,r)\, \mathscr{Y}_{l'J}^{M} \end{pmatrix} \tag{XX.173}$$

where: $\varepsilon = E/|E|$.

27. The Hydrogen Atom

As a second example, let us look for the bound states of an electron in the Coulomb field of an atomic nucleus. The nucleus will be treated as a point charge equal to $(-Z)$ times the charge of the electron, and fixed at the origin [1]). We must therefore find *the bound states* of a Dirac particle in the central potential

$$V = -\frac{Ze^2}{r}.$$

This eigenvalue problem can be exactly solved. Here we shall give only the broad outline of the method, which is a simple extension of the one set forth in § XI.4.

It is clear from an examination of the asymptotic behavior of the solutions of the set of radial equations (XX.170) that E must be contained in the interval $(-m, +m)$. The desired eigenvalues are those for which the solutions that are regular at the origin behave asymptotically like $\exp(-\sqrt{m^2-E^2}\,r)$.

Put:

$$\varkappa = \sqrt{m^2-E^2} \qquad \nu = \sqrt{\frac{m-E}{m+E}} \tag{XX.174}$$

$$\zeta = Ze^2 \qquad \tau = \varpi(J+\tfrac{1}{2}) \tag{XX.175}$$

and introduce the variable

$$\varrho \equiv \varkappa r. \tag{XX.176}$$

The set (XX.170) is equivalent to

$$\left(-\frac{\mathrm{d}}{\mathrm{d}\varrho} + \frac{\tau}{\varrho}\right) G = \left(-\nu + \frac{\zeta}{\varrho}\right) F \tag{XX.177a}$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}\varrho} + \frac{\tau}{\varrho}\right) F = \left(\nu^{-1} + \frac{\zeta}{\varrho}\right) G. \tag{XX.177b}$$

---

1) This supposes the nucleus infinitely heavy. The error thus made cannot be neglected, for it is of the order of magnitude of the relativistic effects. It is largely compensated for if the mass of the electron m is everywhere replaced by the reduced mass.

We look for solutions of the form

$$F(\varrho) = \varrho^s e^{-\varrho}(a_0 + a_1\varrho + a_2\varrho^2 + \dots) \quad (a_0 \neq 0) \qquad \text{(XX.178}a\text{)}$$

$$G(\varrho) = \varrho^s e^{-\varrho}(b_0 + b_1\varrho + b_2\varrho^2 + \dots) \quad (b_0 \neq 0). \qquad \text{(XX.178}b\text{)}$$

Substituting these expansions into equations (XX.177) and equating terms of successive orders one obtains a series of equations of which the first fixes s and the subsequent ones permit the determination of the coefficients $a_0, b_0, a_1, b_1, \dots, a_n, b_n \dots$ by recurrence. The equation in s has the two roots $\pm \sqrt{\tau^2 - \zeta^2}$. A necessary and sufficient condition for F and G to fulfil the conditions of regularity at the origin $F(0) = G(0) = 0$, is that $s > 0$. Thus only the positive root is to be kept [1]):

$$s = \sqrt{\tau^2 - \zeta^2}.$$

Thus for each value of E there is one solution that is regular at the origin. In general it behaves like $\varrho^s e^{\varrho}$ at infinity unless the two expansions (XX.178) have only a finite number of terms. This can only happen for certain particular values of E; these are the required energy levels. The calculation shows that they are given by the expression

$$m\left[1 + \frac{\zeta^2}{(n' + s)^2}\right]^{-\frac{1}{2}},$$

where n', the radial quantum number, is the degree of the polynomials figuring in expressions (XX.178). For each positive value of n' there exists a regular solution for each of the two values of ϖ; for $n' = 0$ there exists a regular solution for $\varpi = -1$, but no solution for $\varpi = +1$.

Let us introduce the principal quantum number

$$n = J + \tfrac{1}{2} + n'.$$

The preceding results may then be reformulated in the following way. The levels of the discrete spectrum depend on the two quantum numbers n and J according to the formula

$$E_{nJ} = m\left[1 + \frac{Z^2e^4}{(n - \varepsilon_J)^2}\right]^{-\frac{1}{2}} \qquad \text{(XX.179)}$$

$$\varepsilon_J = J + \tfrac{1}{2} - \sqrt{(J + \tfrac{1}{2})^2 - Z^2e^4}, \qquad \text{(XX.179')}$$

---

[1]) We suppose $\zeta < |\tau|$, i.e. $Ze^2 < (J + \frac{1}{2})$. This condition is always fulfilled if $Z < 137$, which is always the case in practice. If it were not, the discussion of the regularity conditions at the origin would be much more delicate.

where n can take all positive integral values and J all half-integral values in the interval $(0, n)$:

$$n = 1, 2, \ldots, \infty; \qquad J = \tfrac{1}{2}, \tfrac{3}{2}, \ldots, n - \tfrac{1}{2}.$$

To each value of J there correspond two series of $(2J+1)$ solutions of opposite parities, except for the value $J = n - \frac{1}{2}$ to which there corresponds a single series of $(2J+1)$ solutions of parity $(-)^{n-1}$. Rather than specify the parities, one may instead specify the values of l, the orbital angular momentum of the first two components of the spinor; recall that the parity of the spinor is $(-)^l$.

The spectroscopic notation nl_J is generally used to distinguish these different series of solutions one from another. The following table lists the first few levels in increasing order, with the corresponding spectroscopic terms [each term has a degeneracy of order $2J+1$]:

$n=1$	$J=\frac{1}{2}$	$1s_{1/2}$			$(n'=0)$
$n=2$	$J=\frac{1}{2}$	$2s_{1/2}$	$2p_{1/2}$		$(n'=1)$
	$J=\frac{3}{2}$		$2p_{3/2}$		$(n'=0)$
$n=3$	$J=\frac{1}{2}$	$3s_{1/2}$	$3p_{1/2}$		$(n'=2)$
	$J=\frac{3}{2}$		$3p_{3/2}$	$3d_{3/2}$	$(n'=1)$
	$J=\frac{5}{2}$			$3d_{5/2}$	$(n'=0)$.

If expression (XX.179) is expanded into a power series in Z^2e^4 one finds

$$E_{nJ} = m\left[1 - \frac{Z^2e^4}{2n^2} - \frac{(Z^2e^4)^2}{2n^4}\left(\frac{n}{J+\frac{1}{2}} - \frac{3}{4}\right) + \ldots\right].$$

The first term is the mass term. The second, $-Z^2e^4/2n^2$, is exactly equal to the quantity given by the non-relativistic theory. The third and following terms give the relativistic corrections. These corrections partially remove the "accidental degeneracy" of the non-relativistic levels: for n fixed, the binding energy $m-E$ of each term is slightly increased; the increase depends only on J, and is larger for smaller J.

The experimental results on the fine structure of the hydrogen atom and hydrogen-like atoms (notably He^+) are in broad agreement with these predictions.

However, the agreement is not perfect. The largest discrepancy is observed in the fine structure of the $n=2$ levels of the hydrogen atom [1]). In the non-relativistic approximation, the three levels $2s_{1/2}$,

[1]) W. E. Lamb and R. C. Retherford, Phys. Rev. **72** (1947) 241.

$2p_{1/2}$ and $2p_{3/2}$ are equal. In the Dirac theory, the levels $2s_{1/2}$ and $2p_{1/2}$ are still equal, while the $2p_{3/2}$ level is slightly lower (the separation is of the order of 10^{-4}eV). The level distance $2p_{3/2}-2p_{1/2}$ agrees with the theory but the level $2s_{1/2}$ is lower than the level $2p_{1/2}$ and the distance $2s_{1/2}-2p_{1/2}$ is equal to about a tenth of the distance $2p_{3/2}-2p_{1/2}$. This effect is known as the Lamb shift. To explain it, we need a rigorous treatment of the interaction between the electron, the proton and the quantized electromagnetic field; in the Dirac theory one retains only the Coulomb potential which is the main term in that interaction; the Lamb shift represents "radiative corrections" to this approximation [1]).

V. NON-RELATIVISTIC LIMIT OF THE DIRAC EQUATION

28. Large and Small Components

Consider the positive energy plane waves whose components are given in Table XX.3. Let us suppose that the energy E_p differs little from the rest energy:

$$W \equiv E_p - m \ll m.$$

The non-relativistic approximation is then valid, for the kinetic energy W is nearly equal to $\frac{1}{2}mv^2$ and we have

$$\frac{W}{m} \simeq \tfrac{1}{2}v^2 \ll 1.$$

It will be seen that the non-vanishing component corresponding to $\beta = +1$ is then much larger than the one corresponding to $\beta = -1$:

$$\sigma_z = +1 \qquad \frac{u_3}{u_1} = \left(\frac{W}{W+2m}\right)^{\frac{1}{2}} \simeq \mathrm{O}\left(\frac{v}{c}\right) \ll 1$$

$$\sigma_z = -1 \qquad \frac{u_4}{u_2} = -\left(\frac{W}{W+2m}\right)^{\frac{1}{2}} \simeq \mathrm{O}\left(\frac{v}{c}\right) \ll 1.$$

A similar observation applies for the free spherical waves [cf. expression (XX.173)] or for the eigenfunctions of the hydrogen atom (cf.

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[1]) The most recent measurements give 1057.77 ± 0.70 Mc/s (Mc/s $\equiv$ Megacycle per second) for the separation $2s_{1/2} - 2p_{1/2}$; the theoretical value obtained when the "radiative corrections" predicted by Quantum Electrodynamics are taken into account is 1057.99 ± 0.2 Mc/s [C. M. Sommerfield, Phys. Rev. **107** (1957) 328].

notably the particular eigensolutions defined in Problem XX.10). This suggests that in the non-relativistic approximation two of the components of the spinor Ψ, the components Ψ_3 and Ψ_4 corresponding to the eigenvalue -1 of β, are very small and may be neglected, and that the Dirac theory is then equivalent to a two-component theory.

In order to put this point properly in evidence, we write the Dirac spinor Ψ in the form (XX.157), Φ and χ being defined by equations (XX.158) or (XX.159). As has already been noted in § 25, Φ and χ may be regarded as vectors of the state-vector space of the two component non-relativistic theory.

With these notations the Dirac equation relative to a stationary state of energy E is written, in the Dirac form and representation:

$$(\boldsymbol{\sigma}\cdot(\boldsymbol{p}-e\boldsymbol{A}))\,\chi+(e\varphi+m)\,\Phi = E\Phi \tag{XX.180a}$$

$$(\boldsymbol{\sigma}\cdot(\boldsymbol{p}-e\boldsymbol{A}))\,\Phi+(e\varphi-m)\,\chi = E\chi. \tag{XX.180b}$$

Let us put:

$$\begin{gathered} \boldsymbol{\pi} = \boldsymbol{p}-e\boldsymbol{A}, \qquad M = E-e\varphi \\ W = E-m, \qquad M' = \tfrac{1}{2}(m+M) = m+\tfrac{1}{2}(W-e\varphi). \end{gathered} \tag{XX.181}$$

Solving equation (XX.180*b*) for χ and then substituting into equation (XX.180*a*), we obtain

$$\chi = \frac{1}{2M'}\,(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\,\Phi \tag{XX.182}$$

$$\left[(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\,\frac{1}{2M'}\,(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})+e\varphi\right]\Phi = W\Phi. \tag{XX.183}$$

The set of equations (XX.182–183) is *exactly equivalent* to the Dirac equation.

In the non-relativistic limit

$$W,\ e\varphi,\ \boldsymbol{p},\ e\boldsymbol{A} \ll m, \qquad M' \simeq m. \tag{XX.184}$$

It is clear from equation (XX.182) that

$$\chi \ll \Phi$$

and that the ratio of these two quantities is of the order of p/m, i.e. v/c. χ and Φ are known as the *small and large* components respectively.

In the rest of this section, we shall make use of the concept of "*even*" and "*odd*" operators. By definition:

(*i*) an operator $\mathscr{P}$ is "even" if it has no matrix element linking small and large components (examples: $\boldsymbol{p}$, $\boldsymbol{r}$, $\boldsymbol{L}$, $\boldsymbol{\sigma}$, $\boldsymbol{J}$, $P(\boldsymbol{r}_0)$, β);

(*ii*) an operator $\mathscr{I}$ is "odd" if its non-vanishing matrix elements link small and large components (examples: $\boldsymbol{\alpha}$, $\beta\boldsymbol{\alpha}$, γ^5, $\mathbf{j}(\mathbf{r}_0)$).

It is equivalent to say that $\mathscr{P}$ is an operator that commutes with β, $\mathscr{I}$ an operator that anticommutes with β:

$$\mathscr{P} = \beta\mathscr{P}\beta, \qquad \mathscr{I} = -\beta\mathscr{I}\beta. \tag{XX.185}$$

Any operator Q is the sum of an "even" and an "odd" operator, and furthermore this decomposition is unique:

$$Q = \tfrac{1}{2}[Q+\beta Q\beta]+\tfrac{1}{2}[Q-\beta Q\beta].$$

The product of two "even" or of two "odd" operators is an "even" operator; the product of an "even" operator by an "odd" operator is an "odd" operator.

29. The Pauli Theory as the Non-relativistic Limit of the Dirac Theory

We now return to the system of equations (XX.182–183). In neglecting the small components, one makes an error of order v^2/c^2 in the normalization of the wave function. An error of the same order is made in replacing the operator M' in equation (XX.183) by the mass m. In this approximation equation (XX.183) takes the form of an eigenvalue equation [1]:

$$H_{n.r.}\Phi = W\Phi \tag{XX.186}$$

of a certain Hamiltonian

$$H_{n.r.} \equiv \frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) + e\varphi \tag{XX.187}$$

acting on the two-component wave function Φ. Equation (XX.186) defines the energy W to within v^2/c^2.

In order to put $H_{n.r.}$ in a more familiar form we apply identity (XIII.83), noting that the components of $\boldsymbol{\pi}$ do not commute, and that therefore:

$$\boldsymbol{\pi}\times\boldsymbol{\pi} = \mathrm{i}e \operatorname{curl} \mathbf{A} = \mathrm{i}e\mathscr{H}.$$

One then obtains

$$H_{n.r.} \equiv \frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2 - \frac{e}{2m}(\boldsymbol{\sigma}\cdot\mathscr{H}) + e\varphi. \tag{XX.188}$$

---

[1] Equation (XX.183) is not a true eigenvalue equation since the operator in brackets on the left-hand side depends on the "eigenvalue" W through M'.

This will be recognized as the Hamiltonian of the Pauli theory corresponding to a particle of mass m, charge e and intrinsic angular momentum:

$$\boldsymbol{\mu} = \mu_B \boldsymbol{\sigma} \qquad (\mu_B \equiv \text{Bohr magneton} \equiv e/2m).$$

Not only does the Dirac theory predict the existence of an intrinsic magnetic moment for the electron, but it gives its correct value (§ XIII.18). This is one of the major successes of the theory [1]).

In order to prove that the Dirac theory in the approximation considered here is equivalent to the two-component Pauli theory, we must be able to find operators corresponding to the operators in the Dirac theory but acting only on the large components.

This can actually be done provided that the said operators enter into the calculations only through their matrix elements between states Ψ', Ψ'' whose energy is positive and sufficiently close to that of the rest mass for the non-relativistic approximation to be valid.

If we are concerned with an even operator $\mathscr{P}$, the matrix element $\langle \Psi'' | \mathscr{P} | \Psi' \rangle$ takes the form

$$\langle \Phi'' | \mathscr{P} | \Phi' \rangle + \langle \chi'' | \mathscr{P} | \chi' \rangle.$$

The second term is $(v/c)^2$ times smaller than the first, and may be neglected in the approximation discussed here. $\mathscr{P}$ may then be replaced by its projection on the space of the large components: this projection represents in the non-relativistic Pauli theory the physical quantity represented by $\mathscr{P}$ in the Dirac theory.

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[1]) In actual fact, the experimental value μ_{exp} differs slightly from this theoretical value for the magnetic moment of the electron [P. Kusch and H. M. Foley, Phys. Rev. **72** (1947) 1256]. More recent measurements give

$$\Delta\mu_{\text{exp}} \equiv \mu_{\text{exp}} - \mu_B = (1.165 \pm 0.011) \times 10^{-3}\, \mu_B.$$

The "radiative corrections" of Quantum Electrodynamics account for the existence of this anomalous magnetic moment; they give (Sommerfield, *loc. cit.*):

$$\Delta\mu_{\text{th}} = 1.163 \times 10^{-3}\, \mu_B.$$

Note in passing that the equation obtained by adding the term $\varkappa \mu_B \sigma_{\mu\nu} F^{\mu\nu}$ to the Dirac operator has all the invariance properties of the Dirac equation, and this for any given value of the numerical constant $\varkappa$; such an equation describes a particle of mass m, of charge e and of intrinsic magnetic moment $(1 + \varkappa)\, \mu_B$.

If we are concerned with an odd operator, $\mathscr{I}$, one has

$$\langle \Psi''|\mathscr{I}|\Psi'\rangle = \langle \Phi''|\mathscr{I}|\chi'\rangle + \langle \chi''|\mathscr{I}|\Phi'\rangle.$$

Here the small components are involved explicitly in each term on the right-hand side. In the approximation in question however equation (XX.182) gives

$$|\chi\rangle = \varrho_1 \frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2m}\, |\Phi\rangle$$

from which

$$\langle \Psi''|\mathscr{I}|\Psi'\rangle = \frac{1}{2m}\, \langle \Phi''|[\mathscr{I}\, \varrho_1(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) + (\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\, \varrho_1 \mathscr{I}]\,|\Phi'\rangle.$$

$\mathscr{I}$ may therefore be replaced by the projection on the space of the large components of the operator

$$\frac{1}{2m}\, [\mathscr{I}\, \varrho_1(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) + (\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\, \varrho_1 \mathscr{I}].$$

Thus the "velocity" $\boldsymbol{\alpha} = \varrho_1 \boldsymbol{\sigma}$ may be replaced by the operator in the space of the large components

$$\frac{\boldsymbol{\pi}}{m} \equiv \frac{\boldsymbol{\sigma}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) + (\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\, \boldsymbol{\sigma}}{2m}.$$

Similarly, the current density at the point $\boldsymbol{r}_0$:

$$\boldsymbol{j}(\boldsymbol{r}_0) \equiv \varrho_1 \boldsymbol{\sigma} \delta(\boldsymbol{r}-\boldsymbol{r}_0)$$

may be replaced by the operator in the space of the large components:

$$(\boldsymbol{j}(\boldsymbol{r}_0))_{n.r.} \equiv \delta(\boldsymbol{r}-\boldsymbol{r}_0)\, \boldsymbol{\sigma} \left(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2m}\right) + \left(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2m}\right) \boldsymbol{\sigma}\, \delta(\boldsymbol{r}-\boldsymbol{r}_0)$$

or again, applying identity (XIII.83):

$$(\boldsymbol{j}(\boldsymbol{r}_0))_{n.r.} \equiv \boldsymbol{j}^{(\mathrm{I})} + \boldsymbol{j}^{(\mathrm{II})} \tag{XX.189}$$

$$\boldsymbol{j}^{(\mathrm{I})} \equiv \frac{\delta(\boldsymbol{r}-\boldsymbol{r}_0)\, \boldsymbol{\pi} + \boldsymbol{\pi}\, \delta(\boldsymbol{r}-\boldsymbol{r}_0)}{2m} \tag{XX.190a}$$

$$\boldsymbol{j}^{(\mathrm{II})} \equiv \mathrm{i}\, \frac{\delta(\boldsymbol{r}-\boldsymbol{r}_0)\, (\boldsymbol{p}\times\boldsymbol{\sigma}) - (\boldsymbol{p}\times\boldsymbol{\sigma})\, \delta(\boldsymbol{r}-\boldsymbol{r}_0)}{2m}. \tag{XX.190b}$$

In this limit, the Dirac electric current $e\boldsymbol{j}$ is therefore made up of two terms. The first, $e\boldsymbol{j}^{(\mathrm{I})}$, is identical with the current of the Schrödinger theory (cf. Problem IV.1). In order to interpret the second we consider its matrix element between the large components Φ' and Φ''. The calculation shows that

$$\langle \Phi'' | e\boldsymbol{j}^{(\mathrm{II})} | \Phi' \rangle = \frac{e}{2m} \operatorname{curl} \langle \Phi'' | \delta(\mathbf{r} - \mathbf{r}_0)\, \boldsymbol{\sigma} | \Phi' \rangle.$$

This is a magnetic current term, and the quantity

$$\frac{e}{2m} \langle \Phi'' | \delta(\mathbf{r} - \mathbf{r}_0)\, \boldsymbol{\sigma} | \Phi' \rangle \equiv \langle \Phi'' | \delta(\mathbf{r} - \mathbf{r}_0)\, \boldsymbol{\mu} | \Phi' \rangle$$

may be interpreted as a magnetic moment density. It will be seen that the divergence of this magnetic current vanishes, and therefore that it gives no contribution to the equation of continuity.

30. Application: Hyperfine Structure and Dipole-Dipole Coupling

We now consider an electron in the electric field of an atom, described by a certain electrostatic potential $\varphi(r)$, and examine the effect of the field created by the magnetic moment $\boldsymbol{M}$ of the nucleus. The field created by a magnetic dipole $\boldsymbol{M}$ situated at the origin of coordinates may be represented by the vector potential:

$$\boldsymbol{A} \equiv \frac{\boldsymbol{M} \times \mathbf{r}}{r^3} \qquad \text{(XX.191)}$$

$$\equiv \operatorname{curl} (\boldsymbol{M}/r). \qquad \text{(XX.191')}$$

The presence of this field leads to an additional term $-e\boldsymbol{\alpha} \cdot \boldsymbol{A}$ in the Dirac Hamiltonian.

To determine the effect of this field in the non-relativistic approximation we can calculate the non-relativistic limit of the operator $-e\boldsymbol{\alpha} \cdot \boldsymbol{A}$ by the method of the preceding paragraph. We can equally well directly examine the modifications of the Pauli Hamiltonian (XX.188) due to the presence of $\boldsymbol{M}$. These two methods are equivalent. We shall adopt the second one here.

If we retain only terms linear in $\boldsymbol{M}$, the Pauli Hamiltonian contains the two supplementary terms:

$$I_a = -\frac{e}{2m} (\boldsymbol{p} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{p})$$

$$I_b = -\frac{e}{2m} (\boldsymbol{\sigma} \cdot \mathscr{H}) = -\boldsymbol{\mu} \cdot \mathscr{H};$$

where $\mathscr{H}$ is the field created by the dipole $\boldsymbol{M}$.

I_a is a spin-orbit coupling term (spin of the nucleus, orbit of the electron). Clearly, [cf. eq. (XX.191′)] div $\boldsymbol{A}=0$ whence:

$$I_a = -\frac{e}{m}\,\boldsymbol{A}\cdot\boldsymbol{p}$$

Substituting expression (XX.191) onto the right-hand side, and introducing the orbital angular momentum of the electron $\boldsymbol{L} \equiv \boldsymbol{r}\times\boldsymbol{p}$, one finds:

$$I_a = -\frac{e\boldsymbol{M}\cdot\boldsymbol{L}}{mr^3}. \qquad \text{(XX.192)}$$

I_b is the spin-spin or dipole-dipole coupling term. It can be calculated with the aid of (XX.191′):

$$\begin{aligned} I_b &= -\,\boldsymbol{\mu}\cdot(\nabla\times\boldsymbol{A}) = -\,\boldsymbol{\mu}\cdot\left[\nabla\times\left(\nabla\times\frac{\boldsymbol{M}}{r}\right)\right] \\ &= (\boldsymbol{\mu}\cdot\boldsymbol{M})\,\triangle\left(\frac{1}{r}\right) - [(\boldsymbol{\mu}\cdot\nabla)\,(\boldsymbol{M}\cdot\nabla)]\left(\frac{1}{r}\right). \end{aligned} \qquad \text{(XX.193)}$$

When $r\neq 0$, I_b can easily be calculated by performing the differentiation, which gives:

$$-\,\frac{3(\boldsymbol{M}\cdot\boldsymbol{r})\,(\boldsymbol{\mu}\cdot\boldsymbol{r}) - (\boldsymbol{M}\cdot\boldsymbol{\mu})\,r^2}{r^5}.$$

Considered as a simple function, expression (XX.193) has a singularity in $1/r^3$ at the origin. To determine the action of the operator I_b, it is convenient to examine the result of integration of the product of this quantity by a regular function $f(\boldsymbol{r})$ in a small domain about the point $r=0$. To this effect, we write I_b in the form

$$I_b = \tfrac{2}{3}\,(\boldsymbol{\mu}\cdot\boldsymbol{M})\,\triangle\left(\frac{1}{r}\right) - [(\boldsymbol{\mu}\cdot\nabla)\,(\boldsymbol{M}\cdot\nabla) - \tfrac{1}{3}\,(\boldsymbol{\mu}\cdot\boldsymbol{M})\,\triangle]\left(\frac{1}{r}\right). \qquad \text{(XX.193′)}$$

The second term in this expression is a second order tensor operator in the space of functions of $\boldsymbol{r}$; if, to effect the integration mentioned above, $f(\boldsymbol{r})$ is expanded into spherical harmonics. Only coefficients of spherical harmonics of order 2 will contribute to the integration over the angles; these vanish at the origin at least as rapidly as r^2; the contribution of the second term of (XX.193′) also vanishes at the origin in spite of the singularity in $1/r^3$. With the aid of identity

(A.12), the first term may be put in the form $-(\frac{8}{3}\pi)\,(\boldsymbol{\mu}\cdot\boldsymbol{M})\delta(\boldsymbol{r})$. Thus, for any $\boldsymbol{r}$, including the origin:

$$I_b = -\frac{8\pi}{3}\,(\boldsymbol{M}\cdot\boldsymbol{\mu})\,\delta(\boldsymbol{r}) - \frac{1}{r^3}\left[3\left(\boldsymbol{M}\cdot\frac{\boldsymbol{r}}{r}\right)\left(\boldsymbol{\mu}\cdot\frac{\boldsymbol{r}}{r}\right) - (\boldsymbol{M}\cdot\boldsymbol{\mu})\right]. \quad \text{(XX.194)}$$

Expressions (XX.192) and (XX.194) are valid in the non-relativistic imit and allow the determination of the hyperfine structure of atomic levels to within v^2/c^2. In particular, the contribution of the s-electrons to the hyperfine structure is given by the contact term $-(\frac{8}{3}\pi)\,(\boldsymbol{\mu}\cdot\boldsymbol{M})\delta(\boldsymbol{r})$.

31. Higher-order Corrections and the Foldy–Wouthuysen Transformation

To the lowest order in v/c, the Dirac theory is equivalent to the two-component Pauli theory. It is possible to obtain higher-order relativistic corrections by starting as before from equations (XX.182–183). To this effect, one replaces $1/M'$ by its expansion in powers of $[(W-e\varphi)/2m]$:

$$\frac{1}{M'} = \frac{1}{m}\left[1 - \frac{W-e\varphi}{2m} + \left(\frac{W-e\varphi}{2m}\right)^2 - \dots\right].$$

Since:

$$\left\langle\frac{W-e\varphi}{2m}\right\rangle \simeq \left\langle\frac{\boldsymbol{\pi}^2}{4m^2}\right\rangle \simeq \mathrm{O}\left(\frac{v^2}{c^2}\right),$$

this is essentially a power series expansion in v^2/c^2. If this expansion is stopped at the first term one obtains the Pauli theory, as in § 29. Higher-order relativistic corrections are obtained by taking the expansion beyond the first term. However, once corrections of the order of v^2/c^2 are taken into account, the Dirac theory in the form (XX.182–183) ceases to be formally equivalent to a two-component theory. This is because:

(*i*) the contribution from the small components can no longer be neglected, neither in the normalization, nor in the calculation of matrix elements of even operators;

(*ii*) equation (XX.183) is properly speaking no longer an eigenvalue equation (cf. note, p. 935).

Although the method is not thereby absolutely condemned, its application and the interpretation of the results becomes rather delicate. Foldy and Wouthuysen [1]) have proposed another method which allows one to approximate to the Dirac theory by a two-component theory to any given order in v/c. It essentially consists in effecting a suitably chosen unitary transformation on the wave functions and operators of the Dirac theory. In the new "representation" – which we shall call the FW "representation" – the Dirac Hamiltonian is an "even" operator to the given order in v/c, so that in this approximation the small and the large components are completely decoupled in the wave equation. One may therefore simply ignore the small components, thereby obtaining the desired two-component theory. The operators of the two-component theory are then obtained from the "even" operators of the FW "representation" and not from the operators of the old "representation". One is thus led to a new interpretation of the operators of non-relativistic mechanics, notably of the position operator, an interpretation in many ways more satisfying than the old one.

The rest of this section is devoted to the FW transformation and to its application to the non-relativistic approximation of the Dirac equation.

32. FW Transformation for a Free Particle

In the case of a free particle, the small and large components can be completely decoupled in all orders of v/c.

We consider the Dirac Hamiltonian

$$H_0 \equiv \boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m.$$

Let Γ_+ and Γ_- be the projectors onto the positive and negative energy solutions respectively:

$$\Gamma_\pm \equiv \frac{1}{2}\left[1 \pm \frac{H_0}{E_p}\right] = \frac{1}{2}\left[1 \pm \frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m}{E_p}\right]. \qquad \text{(XX.195)}$$

$$E_p \equiv \sqrt{m^2+\boldsymbol{p}^2}.$$

[1]) L. L. Foldy and S. A. Wouthuysen, Phys. Rev. **78** (1958) 29.

Denote by B_+ and B_- the projectors onto the spaces of the large and small components respectively:

$$B_\pm \equiv \tfrac{1}{2}(1 \pm \beta).$$

By definition, the operator U, which takes us over to the FW "representation", transforms Γ_+ into B_+ and Γ_- into B_-. With primes denoting the vectors and operators of the FW "representation", we therefore have:

$$U^\dagger U = UU^\dagger = 1$$

$$\Gamma'_\pm \equiv U\Gamma_\pm U^\dagger = B_\pm.$$

We also require that U be invariant under translation, rotation and reflection. It is left to the reader to show that U is then defined to within a phase factor. Fixing this phase one obtains

$$U = \sqrt{\frac{2E_p}{m+E_p}}\,\frac{1}{2}\left[1+\beta\,\frac{H_0}{E_p}\right] \qquad \text{(XX 196)}$$

$$= \sqrt{\frac{m+E_p}{2E_p}} + \beta\,\frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{\sqrt{2E_p(m+E_p)}}. \qquad \text{(XX.196')}$$

It will easily be verified that this expression has all the desired properties.

Since U is time-independent, the Hamiltonian H_{F} which governs the evolution of the states in the FW "representation" is given by the equation

$$H_{\mathrm{F}} = UH_DU^\dagger,$$

which gives, with the aid of (XX.196),

$$H_{\mathrm{F}} = \beta E_p \equiv \beta(m^2+\boldsymbol{p}^2)^{\frac{1}{2}}. \qquad \text{(XX.197)}$$

Since H_{F} is an even operator, the large components Φ' and the small components χ' are completely decoupled in the equation of motion:

$$\mathrm{i}\,\frac{\partial\Phi'}{\partial t} = E_p\,\Phi' \qquad \text{(XX.198}a\text{)}$$

$$\mathrm{i}\,\frac{\partial\chi'}{\partial t} = -\,E_p\,\chi'. \qquad \text{(XX.198}b\text{)}$$

If we limit ourselves to positive energy solutions – *a fortiori* to non-relativistic energies — the Dirac theory is exactly equivalent to the two-component theory represented by equation (XX.198a) to all orders in v/c.

The operator U commutes with $\boldsymbol{p}$, $\boldsymbol{J}$ and the parity operator P, but not with $\boldsymbol{r}$. In a representation with $\boldsymbol{r}$ diagonal, it is an integral operator with matrix element:

$$\langle \boldsymbol{r}|U|\boldsymbol{r}'\rangle = \int\int \langle \boldsymbol{r}|\boldsymbol{p}\rangle\, \mathrm{d}\boldsymbol{p}\, \langle \boldsymbol{p}|U|\boldsymbol{p}'\rangle\, \mathrm{d}\boldsymbol{p}'\, \langle \boldsymbol{p}'|\boldsymbol{r}'\rangle,$$

whence, with use of (XX.196′),

$$\langle \boldsymbol{r}|U|\boldsymbol{r}'\rangle = (2\pi)^{-3} \int \left[\sqrt{\frac{m+E_p}{2E_p}} + \beta\, \frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{\sqrt{2E_p(m+E_p)}}\right] \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\, \mathrm{d}\boldsymbol{p}$$

$\langle \boldsymbol{r}|U|\boldsymbol{r}'\rangle$ is a function of $(\boldsymbol{r}-\boldsymbol{r}')$ that practically vanishes for $|\boldsymbol{r}-\boldsymbol{r}'| \gg 1/m$, but which takes non-negligible values when $|\boldsymbol{r}-\boldsymbol{r}'|$ is smaller or of the order of $1/m$. The FW transformation is therefore a non-local transformation in which the spinor $\Psi'(\boldsymbol{r})$, the transform of $\Psi(\boldsymbol{r})$, is obtained by taking a certain average over the values taken by Ψ in a volume about $\boldsymbol{r}$ whose linear dimensions are of the order of $1/m$, the Compton wavelength of the particle.

The position of the particle is represented in the FW "representation" by the operator

$$\boldsymbol{r}' \equiv U\boldsymbol{r}U^{\dagger}.$$

This operator is different to $\boldsymbol{r}$. Following Foldy and Wouthuysen, we shall call the quantity represented by $\boldsymbol{r}$ in the FW "representation" the *average position*. In the ordinary "representation", it is represented by a certain operator $\boldsymbol{R}$ and one has $\boldsymbol{R}' \equiv \boldsymbol{r}$, therefore:

$$\boldsymbol{R} \equiv U^{\dagger}\boldsymbol{r}U.$$

In the Dirac representation, $\boldsymbol{R}$ is a non-local operator whose action on the spinor $\Psi(\boldsymbol{r})$ consists, roughly, in multiplying by $\boldsymbol{r}$ and replacing the value at each point by a certain average over the values of the spinor in a domain of order $1/m$ about the point, whence the name of average position given above.

If Q' is an "even" operator of the FW "representation", the corresponding observable $Q_{n.r.}$ in the above-defined two-component theory is obtained by keeping only the matrix elements of Q' between vectors of the space of the large components: $Q_{n.r.} \equiv B_+ Q' B_+$. In particular, the observable $\boldsymbol{r}$ representing the position in the two-component theory corresponds to the "average position" $\boldsymbol{R}$ and not to the position operator of the Dirac theory proper [1]).

33. FW Transformation for a Particle in a Field

In the presence of a field the Dirac Hamiltonian takes the form:

$$H = \beta m + \mathscr{I} + \mathscr{P}$$
$$\mathscr{I} \equiv \boldsymbol{\alpha}\cdot\boldsymbol{\pi} = \boldsymbol{\alpha}\cdot(\boldsymbol{p} - e\boldsymbol{A}), \qquad \mathscr{P} \equiv e\varphi.$$

In general, there exists no "representation" in which the Hamiltonian is exactly "even" but by applying successive unitary transformations one may obtain "representations" in which the respective Hamiltonians have an "odd" part of higher and higher order in v/c.

To see this, let us make the unitary transformation

$$U = \exp\,(\beta\mathscr{I}/2m).$$

The Hamiltonian H_1 which governs the evolution of states in the new representation is given by the equation

$$H_1 = UHU^\dagger - \mathrm{i}U\,\partial U^\dagger/\partial t.$$

By making use of the fact that $\beta\mathscr{I}$ anticommutes with $(\beta m + \mathscr{I})$ and that $U^\dagger = \exp\,(-\beta\mathscr{I}/2m)$, one obtains:

$$\begin{aligned} U(\beta m+\mathscr{I})U^\dagger &= U^2(\beta m+\mathscr{I}) \\ &= \beta m[\cos\,(\mathscr{I}/m) + (\mathscr{I}/m)\sin\,(\mathscr{I}/m)] \\ &\qquad + m[(\mathscr{I}/m)\cos\,(\mathscr{I}/m) - \sin\,(\mathscr{I}/m)]. \end{aligned}$$

The terms $U\mathscr{P}U^\dagger$ and $\mathrm{i}U\,\partial U^\dagger/\partial t$ may be expanded into a power series

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1) In accordance with the interpretation given here, the orbital angular momentum $\boldsymbol{r}\times\boldsymbol{p}$ and the spin $\boldsymbol{\sigma}$ of the two-component theory do not correspond to the orbital angular momentum and spin of the Dirac theory, but to the "average angular momentum" $\boldsymbol{R}\times\boldsymbol{p}$ and the "average spin" $\boldsymbol{\Sigma}$. Here $\boldsymbol{\Sigma}$ is the operator whose correspondent in the FW "representation" is $\boldsymbol{\sigma}$; $\boldsymbol{\Sigma}' \equiv \boldsymbol{\sigma}$. The reader may verify that each of the components of the average spin and each of the components of the average angular momentum commutes with the free particle Hamiltonian; the spin and the orbital angular momentum proper do not have this property. Note also that:

$$\boldsymbol{J} \equiv (\boldsymbol{r}\times\boldsymbol{p}) + \tfrac{1}{2}\boldsymbol{\sigma} = (\boldsymbol{R}\times\boldsymbol{p}) + \tfrac{1}{2}\boldsymbol{\Sigma}.$$

in $\mathscr{I}/m$ by using the following operator identity, valid for any two operators A and B (cf. Problem VIII.4):

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2}[A, [A, B]] + \ldots + \frac{1}{n!}\overbrace{[A, [A, \ldots [A, [A, B]] \ldots]]}^{n \text{ brackets}} + \ldots$$

We shall only give the result of the calculation of H' when $\mathscr{I}$ is time-independent. Since we are concerned with a first approximation, we put: $H' = H_1$. One finds:

$$H_1 = \beta m + \mathscr{P}_1 + \mathscr{I}_1$$

$$\mathscr{P}_1 = \mathscr{P} + \beta \frac{\mathscr{I}^2}{2m} - \frac{1}{8} m \left[\frac{\mathscr{I}}{m}, \left[\frac{\mathscr{I}}{m}, \frac{\mathscr{P}}{m}\right]\right] - \frac{1}{8}\beta m \left(\frac{\mathscr{I}}{m}\right)^4 + \ldots$$

$$\mathscr{I}_1 = m\left(\frac{1}{2}\beta\left[\frac{\mathscr{I}}{m}, \frac{\mathscr{P}}{m}\right] - \frac{1}{3}\left(\frac{\mathscr{I}}{m}\right)^3\right) + \ldots$$

The terms given in these expansions of the "even" and "odd" parts of H_1 allow the determination of $\mathscr{P}_1$ to within $(\mathscr{I}/m)^6$ or $(\mathscr{P}/m)\,(\mathscr{I}/m)^4$ whichever is the larger and the determination of $\mathscr{I}_1$ to within $(\mathscr{I}/m)^5$ or $(\mathscr{P}/m)\,(\mathscr{I}/m)^3$ whichever is the larger. The "odd" part of H_1 is therefore smaller than that of H by a factor of the order of the larger of $\mathscr{P}/m$ or $(\mathscr{I}/m)^2$; in the non-relativistic limit, $\mathscr{P}/m$ and $\mathscr{I}/m$ are of the order of $(v/c)^2$ and v/c respectively: $\mathscr{I}_1$ is therefore of the order of $(v/c)^3$.

We now effect upon H_1 the operation that we have effected upon H; i.e. we make a new unitary transformation with the operator

$$U_1 = \exp\,(\beta\mathscr{I}_1/2m),$$

and denote the new Hamiltonian by H_2. Its "odd" part $\mathscr{I}_2$ is smaller than that of H_1 by a factor of the order of $\mathscr{P}_1/m$ or $(\mathscr{I}_1/m)^2$, whichever is the larger: in the non-relativistic limit, $\mathscr{P}_1/m$ is of the order of $(v/c)^2$, $(\mathscr{I}_1/m)^2$ of the order of $(v/c)^6$ and $\mathscr{I}_2$ is therefore of the order of $(v/c)^5$. If one neglects terms of this order, H_2 is an "even" operator given by the formula:

$$H_2 \simeq \beta m + \mathscr{P}_2 + \mathrm{O}(v^5)$$

$$\simeq \beta m + \mathscr{P} + \beta\frac{\mathscr{I}^2}{2m} - \frac{1}{8} m\left[\frac{\mathscr{I}}{m}, \left[\frac{\mathscr{I}}{m}, \frac{\mathscr{P}}{m}\right]\right] - \frac{1}{8}\beta m\left(\frac{\mathscr{I}}{m}\right)^4 + \mathrm{O}(v^5)$$

$$\simeq \beta m + e\varphi + \frac{1}{2m}\beta(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2 - \frac{e}{8m^2}[(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}), [(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}), \varphi]] - \frac{1}{8m^3}\beta(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^4 + \mathrm{O}(v^5).$$

Similarly, if one neglects terms of order $(v/c)^3$, H_1 is the "even" operator given by

$$H_1 \simeq \beta m + e\varphi + \frac{1}{2m}\,\beta(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2 + \mathrm{O}(v^3).$$

We may now pass over to the two-component theory as in the case of the free particle. To within $(v/c)^5$, the positive energy solutions are represented by the wave functions Φ' of the space of the large components which obey the equation

$$\mathrm{i}\,\frac{\partial \Phi'}{\partial t} = (m + H'_{n.r.})\,\Phi',$$

where $(m+H'_{n.r.})$ is the projection of the above approximate expression for H_2 onto the space of the large components; i.e.

$$H'_{n.r.} = e\varphi + \frac{1}{2m}\,(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2 - \frac{e}{8m^2}\,[(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}),\,[(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}),\,\varphi]] - \frac{1}{8m^3}\,(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^4. \quad \text{(XX.199)}$$

The first two terms are the Hamiltonain $H_{n.r.}$ of Pauli theory. The last two terms are relativistic corrections of order $(v/c)^2$ to the non-relativistic energy $H_{n.r.}$.

A simple calculation gives

$$(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^4 = (\boldsymbol{\pi}^2 - e(\boldsymbol{\sigma}\cdot\mathscr{H}))^2 \qquad \text{(XX.200)}$$

$$[(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}),\,[(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}),\,\varphi]] = \operatorname{div}\mathscr{E} + 2\boldsymbol{\sigma}\cdot(\mathscr{E}\times\boldsymbol{\pi}), \qquad \text{(XX.201)}$$

which allows $H'_{n.r.}$ to be put in a more familiar form.

By successive application of a sufficient number of these unitary transformations, one may thus construct a two-component theory giving the positive energy states to any desired order in v/c. Each new transformation reduces the error by a factor of $(v/c)^2$. The study of the convergence of the series is rather delicate; it is very likely that it is an asymptotic expansion in most cases. Roughly speaking, it is a power series expansion in the operators $\boldsymbol{p}/m$, that is $(\hbar/mc)$ grad [and in $\partial/m\partial t$, that is, $(\hbar/mc^2)\partial/\partial t$]. The rate of convergence of the series therefore depends on the smallness of the variation of the potential $(\boldsymbol{A}, \varphi)$ over a distance of the order of $\hbar/mc$ [and over a time interval of the order of $\hbar/mc^2$, the interval necessary to travel one Compton wave length at the velocity of light].

34. Electron in a Central Electrostatic Potential

As an application of the technique described in the preceding paragraph, consider an electron in a central electrostatic potential $V(r) \equiv e\varphi(r)$. In this case, $A(\boldsymbol{r})=0$ and the Hamiltonian of the Pauli theory is just the Hamiltonian of the ordinary Schrödinger theory:

$$H_{n.r.} = \frac{\boldsymbol{p}^2}{2m} + V(r).$$

If one wishes to continue the calculations to the order immediately above v^2/c^2, one must replace $H_{n.r.}$ by $H'_{n.r.}$. This amounts to adding the last two terms of (XX.199) to $H_{n.r.}$. In the present case

$$e\mathscr{E} = -\operatorname{grad} V = -\frac{\boldsymbol{r}}{r}\frac{\mathrm{d}V}{\mathrm{d}r}$$

$$e \operatorname{div} \mathscr{E} = -\triangle V$$

which gives, taking into account relation (XX.200) and (XX.201),

$$H'_{n.r.} = H_{n.r.} - \frac{p^4}{8m^3c^2} + \frac{\hbar^2}{4m^2c^2}\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r}(\boldsymbol{\sigma}\cdot\boldsymbol{L}) + \frac{\hbar^2}{8m^2c^2}\triangle V. \quad \text{(XX.202)}$$

The first correction term, $-p^4/8m^3c^2$, is the relativistic correction to the kinetic energy $p^2/2m$. The second is a spin-orbit coupling term [cf. formula (XIII.95)]. The third term, $\hbar^2\triangle V/8m^2c^2$, is a correction to the central potential known as the Darwin term; if $V(r) = -Ze^2/r$ (pure Coulomb potential), the Darwin term is equal to

$$(\pi Z e^2\hbar^2/2m^2c^2)\,\delta(\boldsymbol{r})$$

and affects only the s-states.

35. Discussions and Conclusions

In the presence, as in the absence, of a field, the operators of the two component non-relativistic theory are the projections of operators of the FW "representation" on the space of the large components. In particular, the operator $\boldsymbol{r}$ of the non-relativistic theory can be identified with what we have called the "average position" $\boldsymbol{R}$. In the Dirac theory, the interaction of the particle with the electromagnetic potential is a local interaction, in other words the particle interacts with the electromagnetic potential at its position $\boldsymbol{r}$. When we pass to the "FW representation", where $\boldsymbol{r}$ represents the "average position", this interaction is transformed into a non-local interaction which has contributions from the values taken by the electromagnetic potential in a domain about the particle of approximate dimensions $\hbar/mc$; if the potential $(\boldsymbol{A}, \varphi)$ varies little in this domain, this interaction can be represented by a Taylor expansion involving the value of the potential and its successive derivatives at the point $\boldsymbol{r}$. A Hamiltonian such as $H'_{n.r.}$ [eqs. (XX.199) or (XX.202)] contains the first terms of this expansion.

Thus in the non-relativistic limit, the Dirac electron appears not as a point charge, but as a distribution of charge and current extending over a domain of linear dimensions $\hbar/mc$. This explains the appearance of interaction terms characteristic of the presence of a magnetic moment (interaction $-\boldsymbol{\mu}\cdot\mathscr{H}$, spin-orbit interaction) and of an extended charge distribution (Darwin term).

Finally, we note that the application of the non-relativistic approximation to potentials that are singular at the origin such as $\boldsymbol{A} = \boldsymbol{M} \times \boldsymbol{r}/r^3$ or $\varphi = -Ze/r$ is not rigorously justified since in the neighborhood of the point $r=0$ the quantities $e\boldsymbol{A}/m$ and $e\varphi/m$ cease to be small. If the method of successive approximations described in this section was continued sufficiently far, terms sufficiently singular in the origin to give an infinite contribution to the energy would make their appearance in the non-relativistic Hamiltonian. The solution to this difficulty is suggested by the preceding discussion. In the non-relativistic Hamiltonian, $\boldsymbol{A}$ and φ are replaced by a certain average of these quantities over a domain of linear dimensions of the order of $\hbar/mc$. If the non-relativistic approximation is really justified, this amounts to effecting a cut-off of the singularity at a distance $\hbar/mc$ from the origin in all the singular expressions encountered in the calculation. In order for the non-relativistic approximation to be applicable to the two cases mentioned above, it suffices that [1]):

$$e|\boldsymbol{A}| \ll mc^2, \qquad e\varphi \ll mc^2$$

at the point $r = \hbar/mc$.

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[1]) If m_N is the mass of the atomic nucleus $|\boldsymbol{M}| \simeq Ze\hbar/m_N c$; the quantity eA/mc^3 is of the order of $(e^2/\hbar c)(Zm/m_N)$ at the point $r = \hbar/mc$, i.e. 10^{-5} to 10^{-6}; our calculation of the hyperfine coupling is therefore entirely justified. With regard to the example of § 34, the quantity $e\varphi/mc^2$ being of the order of $Ze^2/\hbar c$, the calculation is valid if $Z \ll 137$.

VI. NEGATIVE ENERGY SOLUTIONS AND POSITRON THEORY

Θαλασσα! θαλασσα! (Anabasis, IV.8).

36. Properties of Charge Conjugate Solutions

The concept of charge conjugation defined in § 19 will be useful to us in the following discussion. Charge conjugation is an antilinear and reciprocal correspondence between wave functions representing the evolution of two different particles in the same electromagnetic potential $(\mathbf{A}, \varphi)$: these particles have the same mass m but opposite charges $+e$ and $-e$.

If a physical quantity associated with the first particle is represented by $Q(e)$ the same quantity associated with the second particle is represented by $Q(-e)$. Thus the momentum is represented in both cases by $\boldsymbol{p} \equiv -\mathrm{i}\nabla$, and the energy is represented by

$$H(e) \equiv \boldsymbol{\alpha}\cdot(\boldsymbol{p}-e\mathbf{A})+\beta m+e\varphi$$

in the one case and by

$$H(-e) \equiv \boldsymbol{\alpha}\cdot(\boldsymbol{p}+e\mathbf{A})+\beta m-e\varphi$$

in the other.

Consider a solution $\Psi(\mathbf{r}, t)$ and the charge-conjugate solution $\Psi^C(\mathbf{r}, t)$. We wish to compare the physical properties of the states represented by these solutions. One knows that

$$\Psi^C = K_C \Psi, \tag{XX.203}$$

where K_C is the antilinear operator defined by equation (XX.124). The notation $\langle Q\rangle$ will be used to denote the average value of Q in the state Ψ and the notation $\langle Q\rangle_C$ to denote the average value of the same operator in the state Ψ^C. Ψ and Ψ^C being supposed normalized to unity, we have

$$\langle Q\rangle = \langle\Psi|Q|\Psi\rangle$$
$$\langle Q\rangle_C = \langle\Psi^C|Q|\Psi^C\rangle.$$

From relation (XX.203),

$$\langle Q\rangle_C = (\langle\Psi|K_C{}^{\dagger})(QK_C|\Psi\rangle)$$
$$= \langle\Psi|(K_C{}^{\dagger}QK_C)|\Psi\rangle^* = \langle\Psi|(K_C{}^{\dagger}Q^{\dagger}K_C)|\Psi\rangle$$

from which we obtain the relation between average values

$$\langle Q\rangle_C = \langle(K_C{}^{\dagger}Q^{\dagger}K_C)\rangle. \tag{XX.204}$$

By applying this relation and making use of the properties of the antiunitary transformation K_C, one finds the following relations between average values in the state Ψ and in the charge conjugate state:

$$\begin{array}{lll} \langle\beta\rangle_C = -\langle\beta\rangle & \langle\boldsymbol{\alpha}\rangle_C = \langle\boldsymbol{\alpha}\rangle & \langle\boldsymbol{\sigma}\rangle_C = -\langle\boldsymbol{\sigma}\rangle \\ \langle\mathbf{r}\rangle_C = \langle\mathbf{r}\rangle & \langle\mathbf{p}\rangle_C = -\langle\mathbf{p}\rangle & \langle\mathbf{L}\rangle_C = -\langle\mathbf{L}\rangle \\ \langle P(\mathbf{r}_0)\rangle_C = \langle P(\mathbf{r}_0)\rangle & \langle\mathbf{j}(\mathbf{r}_0)\rangle_C = \langle\mathbf{j}(\mathbf{r}_0)\rangle & \langle\mathbf{J}\rangle_C = -\langle\mathbf{J}\rangle \end{array} \tag{XX.205}$$
$$\langle H(-e)\rangle_C = -\langle H(e)\rangle.$$

It is seen that the two charge-conjugate solutions have the *same probability density and the same current density at all points* — thus opposite charge densities and electric-current densities — *but opposite energies*: charge conjugation changes the sign of the energy.

37. Abnormal Behavior of the Negative Energy Solutions

After these preliminaries, we are in a position to discuss the question of negative energies in detail.

We first consider the free particle case. The solutions of the Dirac equation were given in § 23. The energy spectrum is made up of two continuous bands $(-\infty, -mc^2)$ and $(mc^2, +\infty)$ separated by an interval of $2mc^2$ (Fig. XX.2a). The first of these bands corresponds to negative energy states: $E = -E_p = -\sqrt{m^2+p^2}$, and the second to positive energy states.

We propose to study the motion of a packet of free waves. It will be shown that in general it is only in the average that the center of the packet follows the classical trajectory. To this effect, we integrate the equations of motion in the Heisenberg "representation" which in this case are:

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathrm{i}[H, \mathbf{r}] = \boldsymbol{\alpha} \tag{XX.206}$$

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{\alpha}}{\mathrm{d}t} &= \mathrm{i}[H, \boldsymbol{\alpha}] = \mathrm{i}(H\boldsymbol{\alpha} + \boldsymbol{\alpha}H) - 2\mathrm{i}\boldsymbol{\alpha}H \\ &= 2\mathrm{i}\mathbf{p} - 2\mathrm{i}\boldsymbol{\alpha}H, \end{aligned} \tag{XX.207}$$

$\mathbf{p}$ and H being constant in time, equation (XX.207) is easily integrated to give

$$\boldsymbol{\alpha}(t) = \left(\boldsymbol{\alpha}(0) - \frac{\mathbf{p}}{H}\right) \mathrm{e}^{-2\mathrm{i}Ht} + \frac{\mathbf{p}}{H}.$$

The dependence of $d\boldsymbol{r}/dt$ on t being thus explicitly given, equation (XX.206) can easily be integrated to give:

$$\boldsymbol{r}(t) = \boldsymbol{r}(0) + \frac{\boldsymbol{p}}{H}\,t + \mathrm{i}\left(\boldsymbol{\alpha}(0) - \frac{\boldsymbol{p}}{H}\right)\frac{\mathrm{e}^{-2\mathrm{i}Ht}}{2H}. \qquad \text{(XX.208)}$$

Equation (XX.208) gives the operator $\boldsymbol{r}$ of the Heisenberg "representation" at time t as a function of the values taken by the operators $\boldsymbol{r}$ and $\boldsymbol{\alpha}$ at the initial time $t=0$. From it we can obtain the law of motion of the center $\langle \boldsymbol{r} \rangle$ of any wave packet, which it will be instructive to compare with the classical law:

$$\boldsymbol{r}_{\mathrm{cl}}(t) = \boldsymbol{r}_{\mathrm{cl}}(0) + \left(\frac{\boldsymbol{p}}{H}\right)_{\mathrm{cl}} t.$$

Instead of the classical uniform rectilinear motion, the free wave packet follows a complicated motion resulting from the addition of a uniform rectilinear motion of velocity $\langle \boldsymbol{p}/H \rangle$ and a rapidly oscillatory motion,

$$\left\langle \mathrm{i}\left(\boldsymbol{\alpha}(0) - \frac{\boldsymbol{p}}{H}\right)\frac{\mathrm{e}^{-2\mathrm{i}Ht}}{2H}\right\rangle,$$

whose amplitude and period are of the order of $\hbar/2mc$ and $\hbar/2mc^2$ respectively. This oscillatory motion is called "Zitterbewegung".

The "Zitterbewegung" term vanishes if the packet is a superposition of only positive or only negative energy waves. To see this it suffices to show that

$$\Gamma_\pm\left(\boldsymbol{\alpha} - \frac{\boldsymbol{p}}{H}\right)\frac{\mathrm{e}^{-2\mathrm{i}Ht}}{2H}\,\Gamma_\pm = 0;$$

where Γ_+ and Γ_- are the projectors onto the states of positive and negative energies respectively [definition (XX.195)]. One finds successively

$$[H, \boldsymbol{\alpha}] = 2\boldsymbol{p} - 2\boldsymbol{\alpha}H$$

$$[\Gamma_\pm, \boldsymbol{\alpha}] = \pm\frac{\boldsymbol{p}}{E_p} \mp \boldsymbol{\alpha}\frac{H}{E_p},$$

and since $H\Gamma_\pm = \pm E_p\Gamma_\pm$, it can be deduced that

$$0 \equiv \Gamma_\pm[\Gamma_\pm, \boldsymbol{\alpha}]\,\Gamma_\pm = \Gamma_\pm\left(\frac{\boldsymbol{p}}{H} - \boldsymbol{\alpha}\right)\Gamma_\pm,$$

from which we obtain the enunciated property by using the fact that H commutes with Γ_+ and Γ_-. "The Zitterbewegung" is therefore caused by interference between the positive and negative energy components of the wave packet.

The "Zitterbewegung" is a curious effect related to negative energies but does not, in itself, constitute a difficulty. The difficulty appears when one studies the motion of a wave packet formed exclusively of negative energy states. In this case, the "Zitterbewegung" disappears; the center of the packet describes a uniform rectilinear motion of velocity:

$$\mathbf{v} = \left\langle \frac{\mathbf{p}}{H} \right\rangle = - \left\langle \frac{\mathbf{p}}{E_p} \right\rangle$$

in the opposite direction to its momentum $\langle \mathbf{p} \rangle$. In particular, in a non-relativistic limit ($H \simeq -mc^2$), one has the relation $\mathbf{v} = -\langle \mathbf{p} \rangle / m$, i.e. the particle behaves as if it had a negative mass $-m$.

This type of difficulty is even more apparent when one studies the motion of wave packets in a static field.

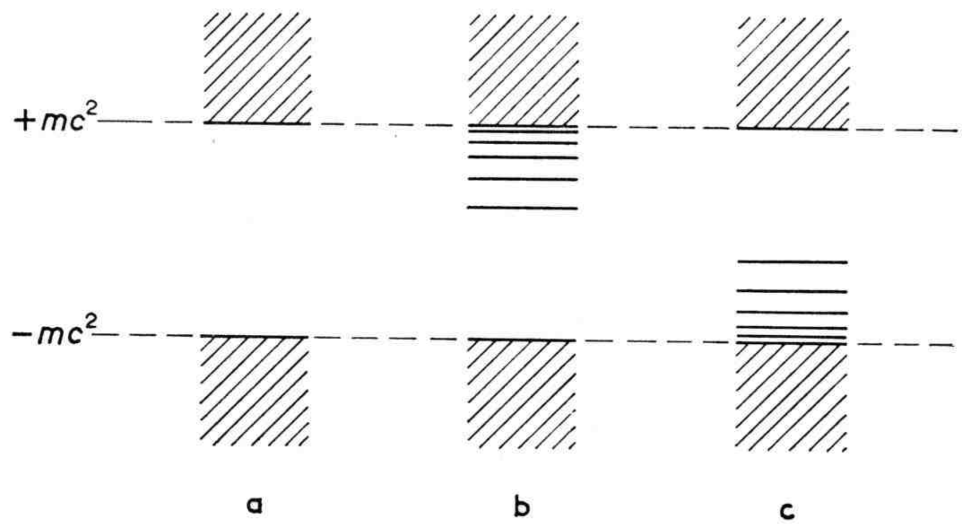

Fig. XX.2. Energy spectrum of a Dirac electron: (a) free; (b) in the attractive potential $-Ze^2/r$; (c) in the repulsive potential Ze^2/r.

Consider, for example, an electron in the attractive Coulomb potential $-Ze^2/r$. The spectrum (cf. Fig. XX.2b) is made up of a continuous positive energy band from mc^2 to ∞, a series of positive energy levels smaller than mc^2 and a continuous negative energy band from $-mc^2$ to $-\infty$. To picture the negative energy states, recall that they correspond by charge conjugation to the states of a particle of the same mass and of opposite charge (that is, a positron) in the same potential or, what amounts to the same, to the states of an electron in the repulsive potential Ze^2/r. In this correspondence the energy changes sign and the small and large components are interchanged, but the densities and the current densities remain the same [cf. eq. (XX.205)]. The spectrum of the electron in the repulsive potential Ze^2/r is shown in Figure XX.2*c*. The positive energy continuum in the repulsive potential corresponds to the negative energy continuum in the attractive potential.

Let us consider the motion of a packet of negative energy waves in the potential $-Ze^2/r$, assuming that the non-relativistic approximation is valid ($Ze^2 \ll 1$, energies near $-mc^2$); the motion is the same as that of the packet of positive energy waves that corresponds by charge conjugation. In particular, in the limit of very small velocities, the classical approximation may be applied (cf. § VI.5) and the motion at the center of the packet is essentially that of a classical electron in the potential with the opposite sign, that is, of *a particle of negative mass* $-m$ in the potential $-Ze^2/r$: the velocity points in the opposite direction to the momentum, the acceleration in the opposite direction to the force. Such a situation has never been observed experimentally.

38. Reinterpretation of the Negative Energy States. Theory of "Holes" and Positrons

As they stand, the negative energy solutions have no physical significance. If it were possible to completely decouple the positive and negative energy states the latter could simply be ignored. Such, however, is not the case.

Consider, for example, a free electron in a positive energy state E_+, and subject it during a time interval $(0, t)$ to a radio-frequency field of frequency ω. If t is sufficiently long and the intensity of the field not too strong, the resulting effect can be calculated by the method of § XVII.6; one finds a non-vanishing probability for the electron to make a transition to a state of energy $E_+ + \hbar\omega$ or $E_+ - \hbar\omega$. In particular if

$$\hbar\omega > E_+ + mc^2,$$

the second transition is made to a state of negative energy.

As another example, consider the complete spectrum of the hydrogen atom (Fig. XX.2*b*). Owing to the coupling of the electron with the electromagnetic field, there is always a certain probability of a radiative transition from a given state of the atom to a state of lower energy. Consequently an electron in one of the bound states of the hydrogen atom can, even if isolated, make quantum jumps to states of negative energy with emission of one or several photons; further, since the spectrum has no lower bound, the hydrogen atom has no stable state [1]).

In order to avoid these difficulties Dirac has made the following suggestion. In what one calls the "vacuum", all of the states of negative energy are occupied by an electron. If an electron is added to this "vacuum", it will necessarily be in a positive energy state since all of the negative energy states are occupied and electrons obey Fermi–Dirac statistics.

The "vacuum" therefore appears as a completely degenerate Fermi gas of infinite density. In addition, it is supposed that it is completely unobservable, giving rise to no gravitational or electromagnetic effects. The observable physical properties of a given state will be the deviations of that state from this "vacuum". Thus the observable charge of the system (electron+"vacuum") is the difference between the total charge of the system and the charge of the "vacuum", i.e. the charge of the electron. Similarly the observable energy of this system is the difference between its total energy and the energy of the "vacuum", and is therefore the energy of the electron. Up to the present, therefore, the only effect of redefining the vacuum in this way, and reinterpreting measurable quantities accordingly, is to forbid transitions to the negative energies, owing to the exclusion principle [2]).

Let us now consider what will be observed when an electron of the negative energy "sea" is missing. Applying the above convention concerning observable physical properties, we can conclude that this "hole" will have a charge opposite to that of the missing electron. It will also have an energy of opposite sign, that is a positive energy, and a momentum in the opposite direction. These considerations are valid whether or not the missing electron is in an eigenstate of the Hamiltonian. If, in particular, the missing electron forms a wave packet moving with velocity $\mathbf{v}$, the "hole" moves with the same

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[1]) O. Klein has formulated a celebrated paradox which exhibits in another way the existence of a non-vanishing probability of transition to negative energy states. Klein's paradox is expounded in many treatises, for example, in M. Born, *loc. cit.*, note 1, p. 4, Vol. I.

[2]) In particular, the Zitterbewegung effect is automatically eliminated.

velocity but opposite momentum: the "hole" therefore acts like a particle of positive mass $+m$ and charge $-e$. Such particles have been observed in nature: they are called *positrons*.

Under the action of an electromagnetic field or any other suitable perturbation, an electron from the negative energy "sea" can make a transition to a state of positive energy. The "hole" of negative energy appears as a positron. In such a transformation, a pair of particles of opposite sign is thus formed. The creation of positron-electron pairs has been observed experimentally.

Similarly, if there is a "hole" in the negative energy "sea", an electron in a positive energy state can make a transition to this unoccupied negative energy state with emission of photons. This phenomenon of annihilation of an electron-positron pair with emission of photons has also been observed experimentally.

39. Difficulties with the "Hole" Theory

The "hole" theory which was briefly outlined above, permits the reconciliation of the Dirac theory with the experimental facts: non-existence of negative energy states, existence of positrons, creation and annihilation of pairs. It therefore constitutes a considerable step forward. However, it has a number of limitations and difficulties.

First of all, it is incomplete. By postulating the occupation of the quasi-totality of negative energy states, *the theory ceases to be a one-particle theory*, even when it sets out to describe a single electron. The formalism of the Dirac theory of a single particle, as set forth in this chapter, is therefore insufficient for describing such a situation, and it is only in the framework of Field Theory that one can hope to obtain a self-consistent description.

The hole theory is only a first step in the direction of a correct theory of the quantized electron field. It has the merit of providing simple pictures and can therefore serve as a guide in the elaboration of the correct theory. But pitfalls and contradictions appear when it is pushed too far.

For example, having defined the "vacuum" as composed of an infinite number of electrons, it is inconsistent to assume that these electrons do not interact.

Another weak point of the theory is the apparently very unsymmetrical role played by the electrons and the positrons. One can also construct a corresponding charge-conjugate theory where the positrons play the role of the particles and the electrons that of the holes without any of the physical consequences being changed. All of these difficulties can be avoided in the Field Theory formalism by starting from equations invariant with respect to charge conjugation.

Finally, we note that even the definition of the negative energy states depends on the applied electromagnetic potential. In the two cases considered in § 37, namely the free particle and the particle in a Coulomb field, the space of the negative energy states is not the same. If, for example, the ground-state wave function for the hydrogen atom is expanded in a series of plane waves, one finds a weak but non-vanishing contribution from plane waves of negative energy. In the above definition of the "vacuum", the states of negative energy considered are those of the free particle; indeed it is natural to define the vacuum in the absence of a field. The introduction of an external electromagnetic field modifies this state of the "vacuum" (pair creation), the latter acting like a polarizable medium, in such a way that an electric charge in the "vacuum" seems smaller than it really is. Such effects are also found in field theory. Hole theory predicts these effects but gives no reliable and self-consistent method for their calculation.

Note Added in Proof (cf. p. 913).

To be entirely correct, one should state the parity question as follows. To the transformation s of the orthochronous Lorentz group, there correspond two transformations, s' and s'', of the group $G^{(a)}$ of Lorentz transformation operators. These are respectively represented by the *two* parity operators P' and P'' given by $P' = c'\gamma^0 P^{(0)}$ and $P'' = c''\gamma^0 P^{(0)}$, with $c' = -c''$. The set (c', c'') defines the *intrinsic parity* of the particle. According to the discussion of § 13, there are two possible intrinsic parities, $(+1, -1)$ and $(-1, +1)$. They correspond to two inequivalent irreducible representations of the group $G^{(a)}$. Since we are dealing here with a single particle, this notion of intrinsic parity is academic. However, it is relevant in Quantum Field Theory when the interaction between several different particles is considered.

A similar treatment applies if $G^{(b)}$ instead of $G^{(a)}$ is chosen as the group of Lorentz transformation operators (cf. notes, p. 904 and p. 908). One again finds two possible values of the intrinsic parity, namely $(+i, -i)$ and $(-i, +i)$.

It should be noted that, contrary to what is often stated in the literature, the number of possible intrinsic parities for spinors *is not four but two.*

EXERCISES AND PROBLEMS

1. Show that if Ψ satisfies the Klein–Gordon equation with a field A^μ, the equation of continuity is satisfied by the four-current:

$$j^\mu = \frac{\mathrm{i}}{2m}[\Psi^*(D^\mu\Psi) - \Psi(D^\mu\Psi)^*] \equiv \frac{\mathrm{i}}{2m}[\Psi^*(\partial^\mu\Psi) - \Psi(\partial^\mu\Psi^*)] - \frac{e}{m}A^\mu\Psi^*\Psi$$

(cf. Problem IV.1).

2. Consider a hydrogen atom in which the electron is replaced by a particle of the same mass and the same charge obeying the Klein–Gordon equation. The levels E of the discrete spectrum are then given by the eigenvalue equation:

$$\left[\Delta + m^2 - \left(E - \frac{e^2}{r}\right)^2\right]\Psi(\mathbf{r}) = 0.$$

Show that this equation can be solved exactly by separating the angular and radial variables, and that the levels of the discrete spectrum depend on the quantum numbers n and l according to the formula:

$$E^{nl} = m\left(1 + \frac{e^4}{(n-\varepsilon_l)^2}\right)^{-\frac{1}{2}} \qquad \varepsilon_l = l + \tfrac{1}{2} - [(l+\tfrac{1}{2})^2 - e^4]^{\frac{1}{2}}$$

$$[n = 1, 2, \ldots, \infty; \qquad l = 0, 1, \ldots, n-1].$$

Compare this spectrum with that given by the non-relativistic Schrödinger theory.

3. Show that all of the (not necessarily unitary) γ^A matrices defined in Table 1 (§ 10), have a determinant equal to 1.

4. If B is the matrix defined at the end of § 10, show that $BB^* = B^*B = -I$. [Show first that

(*i*) BB^* is a multiple of the unit element, and therefore that $BB^* = B^*B = \pm I$;

(*ii*) the matrix BB^* is the same whatever the system of 4 unitary matrices γ^μ used to define B.]

5. Prove the following properties of the (antiunitary) charge conjugation operator K_C defined in § 19

$$K_C\, p_\mu\, K_C{}^\dagger = -\,p_\mu, \qquad K_C\, J_{\alpha\beta}\, K_C{}^\dagger = -\,J_{\alpha\beta}$$
$$K_C\, P\, K_C{}^\dagger = -\,P, \qquad K_C\, K_T\, K_C{}^\dagger = -\,K_T.$$

From these, deduce that with the choice made for the phase of the transformation operators in § 17, K_C commutes with the operators of translation and of the proper Lorentz transformations and that it anticommutes with the spatial reflections and time reversal. How must the choice of phases be modified in order to have K_C commute with all of these transformations.

6. From the Dirac Hamiltonian deduce the equation of motion (XX.147) and (XX.148) for the operators $\boldsymbol{r}$ and $\boldsymbol{\pi}$ in the Heisenberg representation. Similarly deduce the equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[(\boldsymbol{r}\times\boldsymbol{\pi})+\frac{1}{2}\boldsymbol{\sigma}\right]=\boldsymbol{r}\times\boldsymbol{F}, \qquad \frac{\mathrm{d}M}{\mathrm{d}t}=\boldsymbol{\alpha}\cdot\boldsymbol{F}\equiv e\boldsymbol{\alpha}\cdot\mathscr{E},$$

where $\boldsymbol{F}$ is the "Lorentz force": $\boldsymbol{F}\equiv e(\mathscr{E}+\boldsymbol{\alpha}\times\mathscr{H})$; compare these with equations (XX.22) and (XX.21′) from classical dynamics.

7. In the absence of a field, any solution of the Dirac equation is a solution of the Klein–Gordon equation. Show by giving a counter example that the converse is not true.

8. Prove identities (XX.169).

9. Expand a Dirac plane wave of momentum $\boldsymbol{p}$ directed along the z axis into free spherical waves.

10. Make a systematic search for the wave functions of the hydrogen atom such that the radial functions F and G are multiples of each other. Verify that the levels found correspond to $n'=0$ (therefore $J=n-\frac{1}{2}$) and $l=n-1$. One finds (notations of § 27):

$$E_{n,n-\frac{1}{2}}=m\left(1-\frac{e^4}{n^2}\right)^{\frac{1}{2}}$$

$$F=Cst.\times\varrho^s\,\mathrm{e}^{-\varrho}, \qquad G=-\,\nu F$$

with

$$s=\sqrt{n^2-e^4}, \qquad \varkappa=me^2/n, \qquad \varrho=\varkappa r, \qquad \nu=\varkappa/(E+m)\simeq e^2/2n.$$

11. Following the method described in § 27, calculate the levels of the hydrogen atom predicted by the Dirac theory.

12. Compare the fine structure of the levels of the hydrogen atom as given by the Dirac theory and as given by the Klein–Gordon theory of a particle of the same mass and same charge in the same Coulomb field (cf. Problem XX.2).

13. Calculate the relativistic corrections of order v^2/c^2 given by expression (XX.202) for the levels $2s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$ of the hydrogen atom. Verify that in this approximation the states $2s_{1/2}$ and $2p_{1/2}$ remain at the same level and compare the results with those given by the exact treatment of § 27.