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## The Dirac Electron Theory

E. L. HILL AND R. LANDSHOFF\*  
*University of Minnesota, Minneapolis, Minnesota*

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### §1. INTRODUCTION

OF the many perennial problems absorbing the attention of the physicist, one of the most appealing is certainly that of the nature of the elementary particles of matter. The rapid extension of our experimental knowledge of their

properties has been accompanied by an equally rapid alteration in the ideas and methods used by theoretical physicists in the attempt to weave a comprehensive mathematical theory which will accurately picture the results of the experimentalist. The discoveries of the neutron and of the positron, as well as the rapidly expanding field of nuclear physics have already opened up many fascinating avenues for speculation. At the same time, the imminent probability of further

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discoveries of new particles<sup>1</sup> in the cosmic rays which bombard the earth and the possibility of the appearance of entities such as the neutrino in nuclear disintegration processes make it abundantly clear that the time is not yet ripe for the crystallization of a fundamental theory of matter. The theorist can only approach these problems in the spirit of the experimentalist who must learn not only the nature of the problem which he wishes to study, but also the characteristics of the tools with which he must work.

The most fundamental theoretical advance in the field in recent years has been the discovery of the relativistic wave equation of Dirac. Since its publication<sup>2</sup> in 1928 it has occupied a central position in quantum-mechanical theory, and has been the starting point for theories of the positron,<sup>3</sup> the photon,<sup>4</sup>  $\beta$ -ray disintegrations,<sup>5</sup> nuclear forces,<sup>6</sup> "heavy particles,"<sup>7</sup> etc.

In this article we propose to review the principal properties of the Dirac equation and of its solutions. In order not to expand our discussion out of all bounds, we must assume that our readers have a reasonable familiarity with the Schrödinger theory and the general principles of quantum mechanics.

As a preliminary to the discussion of the Dirac equation, we have given a rather lengthy treatment of the nonrelativistic theory of Pauli. It has been our aim to develop this more familiar

theory in a manner which would bring out the transition from the Schrödinger to the Dirac equations more clearly than is done by the customary procedure of simply "tacking on" the spin to the Schrödinger theory. We have attempted to minimize the use of formal symbolic techniques insofar as it seems reasonable to do so, but naturally a compromise must be struck, since the clarity of straightforward computations may well be undermined by their laboriousness. From similar considerations we have not made explicit use of the spinor notation (cf. Appendix H).

The question of notation is always a worrisome one, and a word of justification may be offered for our choice. The point of departure has been the explicit use of symbols for the vectors in "spin space," with  $\psi$  written as a linear sum in terms of them. This avoids the writing of  $\psi$  as a one-column matrix. For the components of  $\psi$ , which are the Pauli functions, or the four Dirac functions as the case may be, we have ventured to use the symbol  $\chi$ , instead of  $\psi$ . The reason for this decision is, that after the *matrices* have been explicitly chosen for the spin operators, the results of operations with these matrices are slightly different depending on whether the matrices are defined as operators on the "unit vectors" or on the components. We have here chosen to consider them as operators on the unit reference vectors rather than as operators on the components. It is hoped that this choice will not be considered merely as an irritating deviation from the literature.

## §2. THE ELECTRON SPIN HYPOTHESIS

The modern phase of the theory of the elementary particles of matter may be said to have begun in 1925–26 with the discovery of Uhlenbeck and Goudsmit<sup>8</sup> that the electron should be considered not purely as a point particle, but also as possessing an intrinsic angular momentum, now universally referred to as the *electron spin*. The development of this idea in the succeeding years has produced incontrovertible evidence for its validity, so that today we take it as axiomatic in our discussions.

Since it is an angular momentum, the spin

<sup>1</sup> S. H. Neddermeyer and C. D. Anderson, *Phys. Rev.* **51**, 884 (1937). J. C. Street and E. C. Stevenson, *Phys. Rev.* **51**, 1005 (1937); **52**, 1003 (1937). Y. Nishina, M. Takeuchi, and T. Ichimiya, *Phys. Rev.* **52**, 1198 (1937). D. R. Corson and R. B. Brode, *Phys. Rev.* **53**, 215 (1938). A. J. Ruhlig and H. R. Crane, *Phys. Rev.* **53**, 266 (1938). L. Nordheim, *Phys. Rev.* **53**, 694 (1938).

<sup>2</sup> P. A. M. Dirac, *Proc. Roy. Soc.* **A117**, 610 (1928); **A118**, 351 (1928).

<sup>3</sup> P. A. M. Dirac, *Proc. Roy. Soc.* **A126**, 360 (1931). Cf. §23.

<sup>4</sup> L. de Broglie, "Une Nouvelle Conception de la Lumière," *Actualités Scientifiques et Industrielles*, No. 181 (1934); "Nouvelles Recherches sur la Lumière," No. 411 (1936). Cf. also P. Jordan, *Zeits. f. Physik* **93**, 464 (1935). R. de L. Kronig, *Annales de l'Institut Henri Poincaré* **6**, 213 (1936). P. Jordan, *Zeits. f. Physik* **105**, 114 and 229 (1937).

<sup>5</sup> E. Fermi, *Zeits. f. Physik* **88**, 161 (1934). E. Konopinski and G. E. Uhlenbeck, *Phys. Rev.* **48**, 7 (1935). I. Tamm, *Physik. Zeits. Sowjetunion* **10**, 567 (1936). H. A. Bethe and R. Bacher, *Rev. Mod. Phys.* **8**, 82 (1936).

<sup>6</sup> G. Breit, *Phys. Rev.* **53**, 153 (1938) and the references in footnotes 5 and 7.

<sup>7</sup> H. Yukawa, *Proc. Phys. Math. Soc. Japan* **17**, 48 (1935). H. Yukawa and S. Sakata, *Proc. Phys. Math. Soc. Japan* **19**, 1084 (1937). H. Yukawa, S. Sakata, and M. Taketani, *Proc. Phys. Math. Soc. Japan* **20**, April (1938). R. Serber, *Phys. Rev.* **53**, 211 (1938). W. E. Lamb, Jr. and L. I. Schiff, *Phys. Rev.* **53**, 651 (1938).

<sup>8</sup> G. E. Uhlenbeck and S. Goudsmit, *Naturwiss.* **13**, 953 (1925); *Nature* **117**, 264 (1926). Cf. also F. R. Bichowsky and H. C. Urey, *Proc. Nat. Acad. Sci.* **12**, 80 (1926).

exhibits the characteristics of a vector quantity.<sup>9</sup> We shall designate it by the symbol  $\mathbf{s}$ ; its cartesian components in any convenient set of axes by  $s_x, s_y, s_z$ . The electron also has a magnetic moment which, according to the hypothesis of Uhlenbeck and Goudsmit, is related to the spin angular momentum, by the equation<sup>10</sup>

$$\mathbf{u} = (\epsilon/m_0c)\mathbf{s}, \quad (1)$$

where  $\epsilon$  is the (algebraic) value of the charge, and  $m_0$  is the rest mass of the electron.

The absolute magnitude of the spin is supposed to be a constant, independent of the external fields in which the electron may be moving, and for this reason is one of the most characteristic properties of the electron. Its numerical value is found to be<sup>10a</sup>

$$\left[\frac{1}{2}\left(\frac{1}{2}+1\right)\right]^{\frac{1}{2}}\hbar = \left(\frac{3}{4}\right)^{\frac{1}{2}}\hbar,$$

where  $\hbar = h/2\pi (= 1.05 \times 10^{-27} \text{ g cm}^2 \text{ sec.}^{-1})$  and  $h$  is Planck's constant.

During the last several years, it has been found that the other "elementary" particles of matter, the proton, the neutron, and the positron also have intrinsic spin angular momenta of the same magnitude as that of the electron. On the other hand, for the proton and the neutron, the simple relation (1) connecting magnetic moment and spin is not valid. On the basis of present experimental evidence for the proton, the factor is approximately.<sup>11</sup>

$$+2.85(\epsilon_p/M_p c),$$

where  $\epsilon_p$  and  $M_p$  are the charge and mass of the

<sup>9</sup> More properly, the angular momentum in Newtonian mechanics is an antisymmetrical tensor of rank 2, but it behaves like a vector under rotations of the coordinate axes.

<sup>10</sup> Throughout this article we treat the electrical charge as an algebraic quantity. For the electron  $\epsilon = -e = -4.80 \times 10^{-10}$  e.s.u.

<sup>10a</sup> Ordinarily one makes the rough statement that "the spin of the electron is  $\frac{1}{2}\hbar$ ." The correct formulation is that the projection of the spin along any fixed axis can take the values  $\pm\frac{1}{2}\hbar$ . The determination of the square of the magnitude of the spin from the projections depends on quantum mechanical theory as given here. We assume the reader to have a preliminary acquaintance with calculations of this type. Cf. Kemble, *The Fundamental Principles of Quantum Mechanics* (McGraw-Hill, 1937).

<sup>11</sup> This value is that found by I. I. Rabi, J. B. M. Kellogg, and J. R. Zacharias, *Phys. Rev.* **50**, 472 (1936) who used atomic beams. The value obtained by I. Estermann, O. C. Simpson, and O. Stern, *Phys. Rev.* **52**, 535 (1937) who used molecular beams is 2.46 ( $\epsilon_p/M_p c$ ). The exact origin of the discrepancy is not clear. Cf. also L. A. Young, *Phys. Rev.* **52**, 138 (1937).

proton. For the neutron<sup>11a</sup> the present experimental evidence sets the factor at about

$$-2.0(\epsilon_p/M_p c)$$

even though the neutron has no resultant electric charge.

These facts point very strongly to the possibility that the proton and the neutron are not elementary particles, but are probably complex structures of some sort. Other lines of evidence based on the theory of the  $\beta$ -ray disintegration of nuclei lead to the same conclusion, though at the present time no satisfactory picture of the nature of these structures has been found.

For this reason it is scarcely possible, in the present state of our knowledge, to present any definitive considerations on the proton and the neutron as fundamental particles, and most of our discussion will be confined to the electron, and its counterpart, the positron.

### §3. THE NONRELATIVISTIC THEORY OF PAULI

After the preliminary discussion of Uhlenbeck and Goudsmit, the first treatment of the electron spin was given by Heisenberg and Jordan,<sup>12</sup> who employed the formal methods of the then newly discovered matrix mechanics.

The first systematic attempts to develop a technique applicable to wave mechanical methods were made by Darwin<sup>13</sup> and Pauli.<sup>14</sup>

The method proposed by Pauli soon became standard for the discussion of all ordinary problems of atomic and molecular structure, and has been employed almost without change in the treatment of nuclear problems involving only protons and neutrons. None of these authors pretended to offer a theory of the origin of the electron spin, but tried only to find a suitable procedure for the mathematical description of the physical ideas proposed by Uhlenbeck and Goudsmit. Since their methods do not conform to the requirements of the special theory of rela-

<sup>11a</sup> O. R. Frisch, H. von Halban, Jr., and J. Koch, *Phys. Rev.* **53**, 719 (1936). The magnetic moment of the deuteron which was determined by I. I. Rabi, J. B. M. Kellogg, and J. R. Zacharias, *Phys. Rev.* **46**, 163 (1934), and by Farkas and Farkas, *Proc. Roy. Soc.* **152**, 152 (1935) leads to the same value.

<sup>12</sup> W. Heisenberg and P. Jordan, *Zeits. f. Physik* **37**, 263 (1926).

<sup>13</sup> C. G. Darwin, *Proc. Roy. Soc.* **A115**, 1 (1927); **A116**, 227 (1927).

<sup>14</sup> W. Pauli, *Zeits. f. Physik* **43**, 601 (1927).

tivity we cannot consider them as ultimately satisfactory from the point of view of general theory, and must apply them with caution when discussing problems involving high speed particles. However, as will be shown in a later section of this report, the Pauli theory is a valuable first approach to the more complex theory based on the Dirac equation. We shall present this theory in a form which is actually a compromise between the treatment of Pauli and Darwin, with a view to paving the way for the discussion of the Dirac theory. This may serve as our excuse for devoting more attention to it than would otherwise be necessary, in view of the many discussions available in the literature.

#### §4. THE PAULI SPIN OPERATORS

The first necessary point is to find suitable quantities in terms of which a mathematical discussion of the properties of the electron spin may be given. If one follows the general procedure of the Schrödinger method, it is natural to consider that the components of the electron spin,  $s_x$ ,  $s_y$ ,  $s_z$  should be represented by means of linear operators which operate on the wave functions for the system. As no attempt is made to present a theory of the origin of the spin itself, the search for suitable operators can be made only by analogy with other known operators already available in the Schrödinger theory. Since the spin is to have the physical characteristics of an angular momentum, we start with the consideration of the operators used for the representation of the orbital angular momentum. These are:

$$\begin{aligned} L_x &= -i\hbar(y\partial/\partial z - z\partial/\partial y), \\ L_y &= -i\hbar(z\partial/\partial x - x\partial/\partial z), \\ L_z &= -i\hbar(x\partial/\partial y - y\partial/\partial x). \end{aligned} \quad (2)$$

In these explicit definitions, the expressions on the right-hand sides refer directly to the space coordinates of the particles. Since we do not have any idea of what internal coordinates of the electron might be supposed to be related to the spin angular momentum in the same way that the space coordinates are related to the orbital angular momentum, it would be difficult to generalize these expressions directly to the spin operators. But it follows at once from these equations that the following operator relations are satisfied identically:

$$\begin{aligned} L_x L_y - L_y L_x &= i\hbar L_z, \\ L_y L_z - L_z L_y &= i\hbar L_x, \\ L_z L_x - L_x L_z &= i\hbar L_y. \end{aligned} \quad (3)$$

These equations may be symbolized by the single vector operator equation:

$$\mathbf{L} \times \mathbf{L} = i\hbar \mathbf{L}.$$

Since this last set of equations contains explicitly only the operators  $L_x$ ,  $L_y$ , and  $L_z$  themselves, they are more suited to formal generalization than are Eqs. (2).

By analogy let us assume that the spin angular momentum can be characterized by three spin operators  $s_x$ ,  $s_y$ , and  $s_z$ , corresponding, respectively, to the components of the spin, and satisfying the same formal equations as do  $L_x$ ,  $L_y$ , and  $L_z$ : i.e.

$$\begin{aligned} s_x s_y - s_y s_x &= i\hbar s_z, \\ s_y s_z - s_z s_y &= i\hbar s_x, \\ s_z s_x - s_x s_z &= i\hbar s_y, \end{aligned} \quad (4)$$

or vectorially:

$$\mathbf{s} \times \mathbf{s} = i\hbar \mathbf{s}.$$

In addition to these relations, we assume that the following equations are also satisfied

$$(s_x)^2 = (s_y)^2 = (s_z)^2 = (\frac{1}{2}\hbar)^2. \quad (5)$$

The orbital angular momentum operators do not satisfy this latter set of relations. It will be shown that they are valid also in the Dirac theory (§16). They embody the fact that the square of the magnitude of the spin is given by

$$s^2 = s_x^2 + s_y^2 + s_z^2 = \frac{1}{2}(\frac{1}{2} + 1)\hbar^2 = \frac{3}{4}\hbar^2 \quad (6)$$

in agreement with the hypothesis of Uhlenbeck and Goudsmit. From Eqs. (4) and (5) the following operator relations can be readily derived

$$\begin{aligned} s_x s_y &= -s_y s_x = i\frac{1}{2}\hbar s_z, \\ s_y s_z &= -s_z s_y = i\frac{1}{2}\hbar s_x, \\ s_z s_x &= -s_x s_z = i\frac{1}{2}\hbar s_y. \end{aligned} \quad (7)$$

The spin operators thus *anticommute* with each other.

#### §5. THE PAULI WAVE FUNCTION WITH SPIN

In the Schrödinger theory, as exemplified in the problem of the hydrogen atom, it is shown that if the orbital angular momentum  $\mathbf{L}$  is visualized as a vector, and if a given direction in space is chosen as reference, then the component

of  $\mathbf{L}$  along this direction can assume only a discrete set of values. These values are all integral multiples of  $\hbar$ , and may be expressed in the form:

$$m_l \hbar, \quad m_l = -l, -l+1, \dots, +l$$

where  $l$  is the *azimuthal* or *orbital angular momentum quantum number* which determines the magnitude of the orbital angular momentum by the equation:

$$|\mathbf{L}|^2 = l(l+1)\hbar^2.$$

$m_l$  is called the *axial* or *magnetic quantum number*: For the various states of the hydrogen atom,  $l$  assumes the values 0, 1, 2,  $\dots$ .

In physical parlance we say that the component of angular momentum along the field is *quantized*, and has the *quantized values*  $m_l \hbar$ .

If we apply this idea to the spin, we observe that from Eq. (6) the *spin quantum number* is:

$$s = \frac{1}{2}.$$

In contrast with the orbital angular momentum, the spin quantum number assumes but the one value  $+\frac{1}{2}$  for all states.

It will be convenient to choose one of the axes of the coordinate system used for the space variables, say the  $z$  axis, as the axis of quantization of the spin. The  $z$  component of the spin then assumes only the quantized values  $\pm \frac{1}{2}\hbar$ .<sup>14a</sup> This interpretation has been foreshadowed in Eqs. (5) which show that the square of any component of the spin must have the value  $(\frac{1}{2}\hbar)^2$ .

It should perhaps be emphasized that one of the implications contained in this argument is that the behavior of the spin can be completely described in terms of its two orientations with respect to any particular axis which we may choose. If, after having chosen one axis we desire to change to another axis of quantization for the spin, we can do it in a perfectly definite way which will be discussed in §8. The important point is that after the change has been made, the quantized values of the spin, along the new axis, will also be  $\pm \frac{1}{2}\hbar$ . This preserves the physical meaning of spin quantization for an arbitrary choice of the axis of quantization. More par-

<sup>14a</sup> Experimental evidence for the truth of this theory is supplied by the observations on the Stern-Gerlach effect in which a beam of hydrogen or other atoms with one valence electron which is in an  $s$  state is passed through an inhomogeneous magnetic field. The orbital angular momentum of these atoms is zero, so that only the spin is effective. One obtains a splitting into the two allowed components.

ticularly, it assures us that if it were possible to send a beam of electrons through one Stern-Gerlach apparatus,<sup>14b</sup> and then to take one of the separated beams of electrons, say that in which the electrons had their spins oriented in the direction of the field, and analyze these electrons in a second Stern-Gerlach apparatus with its field in a different direction from the first, we should expect to find a resolution into two further beams, corresponding, respectively, to electrons with their spins oriented parallel and anti-parallel to the direction of the field in the second apparatus.

These considerations show us that *there are only two independent quantized states for the spin*. We introduce two spin symbols<sup>15</sup> ("spin functions")  $\mathbf{a}_1$ , and  $\mathbf{a}_2$  to represent, respectively, the states in which  $s_z$  has the values  $+\frac{1}{2}\hbar$  and  $-\frac{1}{2}\hbar$ .

The complete wave function, inclusive of both orbital and spin variables, will be written in the form:

$$\psi = \chi_1(xyzt)\mathbf{a}_1 + \chi_2(xyzt)\mathbf{a}_2. \quad (8)$$

In order that we may keep as close contact as possible with the methods commonly used in wave mechanical theory, we introduce the conjugate<sup>16</sup> spin symbols  $\bar{\mathbf{a}}_1$  and  $\bar{\mathbf{a}}_2$ , such that the complex conjugate wave function is written as:

$$\psi^* = \chi_1^* \bar{\mathbf{a}}_1 + \chi_2^* \bar{\mathbf{a}}_2, \quad (9)$$

where  $\chi_1^*$  and  $\chi_2^*$  are the ordinary complex conjugate functions to  $\chi_1$  and  $\chi_2$ .

The spin symbols will be assumed to have the properties:

$$\bar{\mathbf{a}}_1 \mathbf{a}_1 = 1, \quad \bar{\mathbf{a}}_2 \mathbf{a}_2 = 1, \quad \bar{\mathbf{a}}_1 \mathbf{a}_2 = \bar{\mathbf{a}}_2 \mathbf{a}_1 = 0. \quad (10)$$

It follows from these definitions that  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are linearly independent; i.e.

$$c_1 \mathbf{a}_1 + c_2 \mathbf{a}_2 = 0$$

<sup>14b</sup> We ignore here the obvious practical experimental difficulties in trying to perform a Stern-Gerlach experiment on free electrons. As a matter of fact, according to the Dirac theory, the electron spin in principle cannot be determined in a Stern-Gerlach experiment. (§21.) Cf. also N. F. Mott, Proc. Roy. Soc. **A124**, 425 (1929); C. G. Darwin, Proc. Roy. Soc. **A130**, 632 (1930); W. Pauli, *Handbuch der Physik*, second edition, Vol. 24, p. 241; W. Pauli, Solvay Congress report in *Le Magnetisme* (Gauthier-Villars, 1932) p. 220.

<sup>15</sup> For lack of a better notation we use bold-face type both for space vectors (e.g.  $\mathbf{L}$  and  $\mathbf{S}$ ), and for the spin symbols.

<sup>16</sup> We distinguish between the terms "conjugate" and "complex conjugate." The distinction is discussed at greater length in §18.

if, and only if,  $c_1 = c_2 = 0$ . This is seen at once by multiplying this equation by  $\bar{\mathbf{a}}_1$  and  $\bar{\mathbf{a}}_2$ , respectively, and by using Eqs. (10).

A word on the interpretation of the spin symbols  $\mathbf{a}_1, \mathbf{a}_2, \bar{\mathbf{a}}_1, \bar{\mathbf{a}}_2$  may be appreciated by those unaccustomed to the symbolic methods so useful in general discussions of quantum-mechanical theory. It might seem more natural to introduce a variable  $\sigma$  representing the numerical magnitude of the  $z$  component of the electron spin, and to treat  $a_1$  and  $a_2$  as ordinary (complex) functions of  $\sigma$ , and to put  $\bar{a}_1 = a_1^*, \bar{a}_2 = a_2^*$ . Using the same formal interpretation as for ordinary wave functions in the Schrödinger theory, one might assume that:  $|a_1(\sigma)|^2 d\sigma$  and  $|a_2(\sigma)|^2 d\sigma$  are the probabilities that  $\sigma$  lies between  $\sigma$  and  $\sigma + d\sigma$  in the states represented by  $a_1(\sigma)$  and  $a_2(\sigma)$ ; i.e., in the states in which the  $z$  component of the spin is known to have the values  $+\frac{1}{2}\hbar$  and  $-\frac{1}{2}\hbar$ , respectively. These functions would then be considered to be normalized and orthogonal in the sense

$$\int_{-\infty}^{+\infty} |a_1(\sigma)|^2 d\sigma = \int_{-\infty}^{+\infty} |a_2(\sigma)|^2 d\sigma = 1,$$

$$\int_{-\infty}^{+\infty} a_1^*(\sigma) a_2(\sigma) d\sigma = 0$$

if we let  $\sigma$  range formally from  $-\infty$  to  $+\infty$ .

Such an interpretation would require that

$$a_1(\sigma) = 0 \quad \text{if} \quad \sigma \neq +\frac{1}{2}\hbar,$$

$$a_2(\sigma) = 0 \quad \text{if} \quad \sigma \neq -\frac{1}{2}\hbar.$$

It is clear that there exist no ordinary continuous functions, integrable in the Riemannian sense, which satisfy all of these conditions. Consequently, this treatment of the spin functions could have only a formal significance.

A more correct, and indeed quite satisfactory, method would be to treat  $\sigma$  as a discontinuous variable which assumes only the two values  $\pm\frac{1}{2}\hbar$ , and to assign to  $a_1(\sigma)$  and  $a_2(\sigma)$  the properties

$$|a_1(+\frac{1}{2}\hbar)| = 1, \quad |a_1(-\frac{1}{2}\hbar)| = 0,$$

$$|a_2(+\frac{1}{2}\hbar)| = 0, \quad |a_2(-\frac{1}{2}\hbar)| = 1.$$

This procedure seems quite natural in the Pauli theory, where the variable  $\sigma$  has a simple physical interpretation, but its extension to the Dirac theory where *four* instead of only *two*  $\mathbf{a}$  functions must be used, seems more artificial, since the physical interpretation of the four "states" represented by the  $\mathbf{a}$ 's is not at once so obvious.

For this reason we have preferred to retain a certain measure of symbolic treatment for the spin functions even in the Pauli theory.

The physical interpretation of the wave function  $\psi$  is based on the following hypothesis, which is an immediate generalization of the corresponding statement in the Schrödinger theory:

$$\psi^* \psi \Delta x \Delta y \Delta z$$

is the (relative) probability that, at the time  $t$ , the electron is in the volume element  $\Delta x \Delta y \Delta z$  at the point  $(x, y, z)$ .

From Eqs. (8), (9) and (10) we find:

$$\psi^* \psi = |\psi|^2 = |\chi_1|^2 + |\chi_2|^2. \quad (11)$$

In case  $|\psi|^2$  is an integrable function of  $x, y, z$  over the allowed range for these coordinates we can multiply  $\psi$  by an appropriate constant such that

$$\iiint |\psi|^2 dx dy dz = 1,$$

in which case  $|\psi|^2$  may be considered as an absolute, rather than merely as a relative probability density.

It would be possible, in fact, to go even further by interpreting  $|\chi_1|^2 \Delta x \Delta y \Delta z$  as the (relative) probability that, at the time  $t$ , the electron is in the volume element  $\Delta x \Delta y \Delta z$  at  $(x, y, z)$  with its  $z$  component of spin equal to  $+\frac{1}{2}\hbar$ , with a similar interpretation of  $|\chi_2|^2$  when the  $z$  component of spin is  $-\frac{1}{2}\hbar$ . Such an interpretation is often convenient in problems in which no spin terms are introduced in the energy operator. In case the hamiltonian (energy) operator does not commute with the spin operators, as in the Dirac theory, such an interpretation loses much of its value, but may still be useful on occasion.

## §6. THE PAULI SPIN MATRICES

We must now consider the manner in which the spin operators  $s_x, s_y, s_z$  are to be defined in terms of their operations on the spin functions  $\mathbf{a}_1$  and  $\mathbf{a}_2$ . Our first assumption will be that the results of the operation of any one of them (or of any spin operator) on either spin function can be written as a linear sum in  $\mathbf{a}_1$  and  $\mathbf{a}_2$  i.e.,

$$s_k \mathbf{a}_1 = \mathbf{a}_1 \cdot (1 |s_k | 1) + \mathbf{a}_2 \cdot (2 |s_k | 1),$$

$$s_k \mathbf{a}_2 = \mathbf{a}_1 \cdot (1 |s_k | 2) + \mathbf{a}_2 \cdot (2 |s_k | 2), \quad (12)$$

where the expressions  $(1 |s_k | 1)$ , etc., are merely complex numbers. These equations can be symbolized more succinctly by arranging the coefficients in the form of a *matrix*,

$$s_k \sim \begin{vmatrix} (1 |s_k | 1) & (1 |s_k | 2) \\ (2 |s_k | 1) & (2 |s_k | 2) \end{vmatrix}.$$

The coefficients are called the *matrix elements* of  $s_k$ .

According to our considerations, the spin functions  $\mathbf{a}_1$  and  $\mathbf{a}_2$  by definition represent the states in which  $s_z$  is quantized, and has the

quantized values  $\pm\frac{1}{2}\hbar$ . The appropriate mathematical expression of this is that

$$s_x \mathbf{a}_1 = +\frac{1}{2}\hbar \mathbf{a}_1, \quad s_x \mathbf{a}_2 = -\frac{1}{2}\hbar \mathbf{a}_2. \quad (13)$$

For the *modus operandi* of  $s_x$  and  $s_y$  on  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , we can now appeal to Eqs. (7). It will be found that these equations do not completely determine the matrix elements of  $s_x$  and  $s_y$ ; minor adjustments of phases are possible. For our future work, we adopt the following solutions as most suitable:

$$\begin{aligned} s_x \mathbf{a}_1 &= \frac{1}{2}\hbar \mathbf{a}_2, & s_x \mathbf{a}_2 &= \frac{1}{2}\hbar \mathbf{a}_1, \\ s_y \mathbf{a}_1 &= i\frac{1}{2}\hbar \mathbf{a}_2, & s_y \mathbf{a}_2 &= -i\frac{1}{2}\hbar \mathbf{a}_1. \end{aligned} \quad (14)$$

The matrices for  $s_x$ ,  $s_y$ ,  $s_z$  are now:

$$\begin{aligned} s_x &\sim \begin{vmatrix} 0 & \frac{1}{2}\hbar \\ \frac{1}{2}\hbar & 0 \end{vmatrix}, & s_y &\sim \begin{vmatrix} 0 & -i\frac{1}{2}\hbar \\ i\frac{1}{2}\hbar & 0 \end{vmatrix}, \\ s_z &\sim \begin{vmatrix} \frac{1}{2}\hbar & 0 \\ 0 & -\frac{1}{2}\hbar \end{vmatrix}. \end{aligned} \quad (15)$$

The quantization of  $s_z$  is expressed by the diagonality of its matrix.

It will be convenient in later work to introduce three operators defined by

$$\sigma_1 = 2s_x/\hbar, \quad \sigma_2 = 2s_y/\hbar, \quad \sigma_3 = 2s_z/\hbar \quad (16)$$

having the matrices

$$\sigma_1 \sim \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \quad \sigma_2 \sim \begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix}, \quad \sigma_3 \sim \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}. \quad (17)$$

These are known as the *Pauli operators* (or matrices). They satisfy the relations

$$\sigma_1 \sigma_2 = -\sigma_2 \sigma_1 = i\sigma_3, \text{ etc.} \quad (18)$$

The operator representing "unity" (i.e. the unit transformation on  $\mathbf{a}_1$  and  $\mathbf{a}_2$ ) is

$$\sigma_4 \sim \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}. \quad (19)$$

It is easily seen that the four matrices for  $\sigma_1, \dots, \sigma_4$  form a complete set, in the sense that any two-dimensional matrix can be written as a linear sum in terms of them. Thus if

$$\begin{aligned} \Gamma &\sim \begin{vmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{vmatrix}, \\ \Gamma &= \frac{1}{2}(\gamma_{12} + \gamma_{21})\sigma_1 + i\frac{1}{2}(\gamma_{12} - \gamma_{21})\sigma_2 \\ &\quad + \frac{1}{2}(\gamma_{11} - \gamma_{22})\sigma_3 + \frac{1}{2}(\gamma_{11} + \gamma_{22})\sigma_4. \end{aligned} \quad (20)$$

We interpret this in terms of *operators* by saying that the four operators  $\sigma_1, \dots, \sigma_4$  form a complete set such that any other operator depending on spin quantities only can be expressed as a linear sum in terms of them. This will be of use to us in §8.

From the definition of  $\sigma_4$  we find from Eq. (19) that

$$\sigma_4 \psi = \psi,$$

from which  $\psi^* \sigma_4 \psi = |\psi|^2$ .

By virtue of this equation we shall refer to  $\sigma_4$  as the *probability density operator*.

## §7. THE TOTAL ANGULAR MOMENTUM AND ITS QUANTIZATION IN THE PAULI THEORY

As a simple example of the application of the Pauli theory we shall study the quantization of the total angular momentum, for a single particle. This is of importance in many problems, particularly those dealing with motion in a central field. This calculation, including spin, is a generalization of the corresponding analysis in the Schrödinger theory in which one orders the states (and wave functions) of the electron as  $s, p, d, f, \dots$  by a classification of the wave functions in terms of the orbital angular momentum.

The operators for the components of the total angular momentum vector  $\mathbf{J}$  are assumed to be simple sums of those for the components of  $\mathbf{L}$  and  $\mathbf{s}$ .

$$J_x = L_x + s_x, \quad J_y = L_y + s_y, \quad J_z = L_z + s_z. \quad (21)$$

They satisfy the relations  $\mathbf{J} \times \mathbf{J} = i\hbar \mathbf{J}$ , etc. The operator for the square of the total angular momentum is

$$\begin{aligned} \mathbf{J}^2 &= J_x^2 + J_y^2 + J_z^2 \\ &= \mathbf{L}^2 + \mathbf{s}^2 + 2(L_x s_x + L_y s_y + L_z s_z) \\ &= \mathbf{L}^2 + \mathbf{s}^2 + (L_+ s_- + L_- s_+ + 2L_z s_z) \end{aligned} \quad (22)$$

$$\text{with } L_{\pm} = L_x \pm iL_y, \quad s_{\pm} = s_x \pm is_y. \quad (23)$$

In the discussion of central field problems, it is usually preferable to introduce spherical polar coordinates by

$$x = r \sin \theta \cos \varphi, \quad y = r \sin \theta \sin \varphi, \quad z = r \cos \theta.$$

The orbital angular momentum operators in polar form are tabulated in Appendix A.

Our problem now is to find the particular

functions for  $\chi_1(r, \theta, \varphi)$  and  $\chi_2(r, \theta, \varphi)$  which must be put in Eq. (8) in order that  $\psi$  may represent a state in which the square of the total angular momentum  $\mathbf{J}^2$  and one of the components, say  $J_z$ , are quantized, i.e.,  $\psi$  must satisfy the differential equations

$$J_z \psi = A \psi; \quad \mathbf{J}^2 \psi = B \psi, \quad (24)$$

where  $A$  and  $B$  are constants.

Now

$$\begin{aligned} (J_z - A)\psi &= (-i\hbar \partial / \partial \varphi + s_z - A)(\chi_1 \mathbf{a}_1 + \chi_2 \mathbf{a}_2) \\ &= (-i\hbar \partial / \partial \varphi + \frac{1}{2}\hbar - A)\chi_1 \mathbf{a}_1 \\ &\quad + (-i\hbar \partial / \partial \varphi - \frac{1}{2}\hbar - A)\chi_2 \mathbf{a}_2. \end{aligned}$$

Since this expression must vanish identically, the coefficient of each spin function must be zero. ( $\mathbf{a}_1$  and  $\mathbf{a}_2$  are linearly independent!)

This yields the two equations:

$$\begin{aligned} (-i\hbar \partial / \partial \varphi + \frac{1}{2}\hbar - A)\chi_1 &= 0, \\ (-i\hbar \partial / \partial \varphi - \frac{1}{2}\hbar - A)\chi_2 &= 0. \end{aligned} \quad (25)$$

In a similar manner, the second equation of (24) yields the two differential equations:

$$\begin{aligned} (\mathbf{L}^2 + \frac{3}{4}\hbar^2 + \hbar L_z - B)\chi_1 + \hbar L_- \chi_2 &= 0, \\ \hbar L_+ \chi_1 + (\mathbf{L}^2 + \frac{3}{4}\hbar^2 - \hbar L_z - B)\chi_2 &= 0. \end{aligned} \quad (26)$$

We shall not carry out all of the steps in the solution of these equations, which can be done by an analysis very similar to that used in the solution of the corresponding differential equation for the angular function in the Schrödinger equation for the hydrogen atom. The appropriate values for the constants  $A$  and  $B$  are found to be

$$\begin{aligned} A &= M\hbar, & M &= \pm \frac{1}{2}, \pm \frac{3}{2}, \dots, \\ B &= J(J+1)\hbar^2, & J &= \frac{1}{2}, \frac{3}{2}, \dots, \quad J \geq |M|. \end{aligned}$$

The quantized values of  $J_z$  and  $\mathbf{J}^2$  are thus  $M\hbar$  and  $J(J+1)\hbar^2$ , respectively. The solutions for given choices of  $M$  and  $J$  are

$$\begin{aligned} \chi_1(r, \theta, \varphi) &= f(r) \left( \frac{J+1-M}{2(J+1)} \right)^{\frac{1}{2}} Y_{J+\frac{1}{2}, M-\frac{1}{2}}(\theta, \varphi) \\ &\quad + g(r) \left( \frac{J+M}{2J} \right)^{\frac{1}{2}} Y_{J-\frac{1}{2}, M-\frac{1}{2}}(\theta, \varphi), \\ \chi_2(r, \theta, \varphi) &= -f(r) \left( \frac{J+1+M}{2(J+1)} \right)^{\frac{1}{2}} Y_{J+\frac{1}{2}, M+\frac{1}{2}}(\theta, \varphi) \\ &\quad + g(r) \left( \frac{J-M}{2J} \right)^{\frac{1}{2}} Y_{J-\frac{1}{2}, M+\frac{1}{2}}(\theta, \varphi). \end{aligned} \quad (27)$$

The functions  $f(r)$  and  $g(r)$  are not determined by the differential equations (24).

The functions  $Y_{J+\frac{1}{2}, M-\frac{1}{2}} \dots$  are just the angular functions encountered in the solution of the Schrödinger equation for the hydrogen atom. Their definitions and principal properties are tabulated in Appendix B. In the Schrödinger theory these functions appear in the wave functions representing states in which the orbital angular momentum is quantized.

The reader may note that if we set  $g(r)=0$  we get a solution representing quantization of  $\mathbf{L}^2$ , with the orbital quantum number  $l=J+\frac{1}{2}$ , while if we set  $f(r)=0$  we get a solution corresponding to  $l=J-\frac{1}{2}$ . The possibility of doing this is a consequence of the commutation of  $\mathbf{L}^2$  with the operators  $J_x, J_y, J_z$  and  $\mathbf{J}^2$ . But since  $L_z$  does not commute with  $\mathbf{J}^2$  we cannot avoid using functions with  $m=M \pm \frac{1}{2}$  simultaneously. This is clear, of course, from the vector coupling model also.

## §8. BEHAVIOR OF THE PAULI SPIN OPERATORS AND WAVE FUNCTIONS UNDER ROTATIONS OF THE COORDINATE AXES

One of the most important considerations arising in connection with quantum-mechanical problems concerns the behavior of the wave functions under a rotation of the coordinate axes.<sup>17</sup> Suppose that in studying a given system, we choose a particular set of coordinate axes in terms of which to describe the space and spin coordinates and for which we find the solutions of the wave equation. It is apparent that in the absence of any external fields, or of any considerations which single out one particular set of coordinate axes as fundamental, the choice of axes which we happen to have made will not be in any way unique, and we might as well have chosen some other set oriented in an arbitrary way with respect to the first set.<sup>18</sup> Mathematically, this means that the energy operator and the wave equation should have exactly the same form in the two sets of axes.

<sup>17</sup> W. Pauli, *Zeits. f. Physik* **43**, 601 (1927). Cf. also, B. L. van der Waerden, *Die Gruppentheoretische Methode in der Quantenmechanik* (Springer, 1932). E. Wigner, *Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren* (Vieweg and Sohn, 1931).

<sup>18</sup> This is true also with respect to translations of the axes, but in Euclidean space pure translations without rotation introduce no new features.



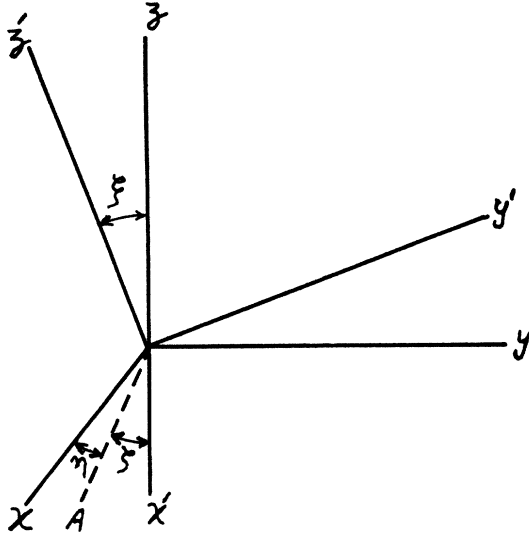


FIG. 1. Rotation of coordinate axes.

If then we consider the solutions of the wave equations obtained separately for two sets of axes, the problem arises of relating these two sets of solutions in a one-to-one manner which will maintain the characteristics from which we draw the physical interpretation of the problem, e.g. the interpretation of  $|\psi|^2$  as a probability density.

Let us consider the two sets of coordinate axes  $(x, y, z)$  and  $(x', y', z')$  related as shown in Fig. 1.<sup>19</sup>

According to our previous analysis, these functions are to be expressed in the forms

$$\begin{aligned}\psi &= \chi_1(xyz) \mathbf{a}_1 + \chi_2(xyz) \mathbf{a}_2, \\ \psi' &= \chi_1'(x'y'z') \mathbf{a}_1' + \chi_2'(x'y'z') \mathbf{a}_2',\end{aligned}\quad (28)$$

where  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are the spin functions appropriate to quantization of the spin components along the  $z$  axis, while  $\mathbf{a}_1'$  and  $\mathbf{a}_2'$  are the spin functions appropriate to quantization of the spin component along the  $z'$  axis. Since the "state" of the spin is supposed to be determinable in terms of its quantization along *any* axis, we assume that these two pairs of spin functions are expressible in terms of each other by a linear relation of the form

<sup>19</sup> In Fig. 1 the line  $A$  is the intersection of the  $(x, y)$  and  $(x', y')$  planes. The transformation from  $(x, y, z)$  to  $(x', y', z')$  can be carried out by (1) a rotation about  $z$  through an angle  $\eta$ , (2) a rotation about  $A$  through an angle  $\xi$ , (3) a rotation about  $z'$  through an angle  $\zeta$ .

$$\begin{aligned}\mathbf{a}_1' &= \mathbf{a}_1 \cdot (1|U|1) + \mathbf{a}_2 \cdot (2|U|1), \\ \mathbf{a}_2' &= \mathbf{a}_1 \cdot (1|U|2) + \mathbf{a}_2 \cdot (2|U|2),\end{aligned}\quad (29)$$

where  $(1|U|1) \dots$  are ordinary complex functions, depending on the relative orientations of the two sets of axes.

It will be convenient to look upon this transformation as induced by an operator  $U$ , having the property that

$$\mathbf{a}_1' = U\mathbf{a}_1, \quad \mathbf{a}_2' = U\mathbf{a}_2. \quad (30)$$

The matrix of  $U$  (as expressed in terms of its operation on the symbols  $\mathbf{a}_1$  and  $\mathbf{a}_2$ ) is

$$U \sim \begin{vmatrix} (1|U|1) & (1|U|2) \\ (2|U|1) & (2|U|2) \end{vmatrix}.$$

As these equations must be reversible, we can write

$$\mathbf{a}_1 = U^{-1}\mathbf{a}_1', \quad \mathbf{a}_2 = U^{-1}\mathbf{a}_2'. \quad (31)$$

$U^{-1}$  may also be expressed by a matrix

$$U^{-1} \sim \begin{vmatrix} (1|U^{-1}|1) & (1|U^{-1}|2) \\ (2|U^{-1}|1) & (2|U^{-1}|2) \end{vmatrix}$$

such that

$$\begin{aligned}\mathbf{a}_1 &= \mathbf{a}_1' \cdot (1|U^{-1}|1) + \mathbf{a}_2' \cdot (2|U^{-1}|1), \\ \mathbf{a}_2 &= \mathbf{a}_1' \cdot (1|U^{-1}|2) + \mathbf{a}_2' \cdot (2|U^{-1}|2).\end{aligned}\quad (32)$$

By elimination we find

$$\begin{aligned}\sum_{l=1}^2 (k|U|l)(l|U^{-1}|m) \\ = \sum_{l=1}^2 (k|U^{-1}|l)(l|U|m) = \delta_{km}\end{aligned}\quad (33)$$

or  $UU^{-1} = U^{-1}U = \sigma_4$  (unit operator!).

The conjugate spin symbols for the two sets of axes must be assumed to be related by the equations<sup>20</sup>

$$\begin{aligned}\bar{\mathbf{a}}_1' &= (1|U^{-1}|1) \cdot \bar{\mathbf{a}}_1 + (1|U^{-1}|2) \cdot \bar{\mathbf{a}}_2, \\ \bar{\mathbf{a}}_2' &= (2|U^{-1}|1) \cdot \bar{\mathbf{a}}_1 + (2|U^{-1}|2) \cdot \bar{\mathbf{a}}_2, \\ \bar{\mathbf{a}}_1 &= (1|U|1) \cdot \bar{\mathbf{a}}_1' + (1|U|2) \cdot \bar{\mathbf{a}}_2', \\ \bar{\mathbf{a}}_2 &= (2|U|1) \cdot \bar{\mathbf{a}}_1' + (2|U|2) \cdot \bar{\mathbf{a}}_2',\end{aligned}\quad (34)$$

in order that relations of the form (10) may be preserved for the spin functions in both sets of axes.

<sup>20</sup> We have written these relations out in detail for the reader who is not too conversant with matrix notations.

TABLE I. Transformation coefficients.

	$x$	$y$	$z$
$x'$	$\cos \zeta \cos \eta$ $-\sin \zeta \cos \xi \sin \eta$	$\cos \zeta \sin \eta$ $+\sin \zeta \cos \xi \cos \eta$	$\sin \eta \sin \xi$
$y'$	$-\sin \zeta \cos \eta$ $-\cos \zeta \cos \xi \sin \eta$	$-\sin \zeta \sin \eta$ $+\cos \zeta \cos \xi \cos \eta$	$\cos \eta \sin \xi$
$z'$	$\sin \xi \sin \eta$	$-\sin \xi \cos \eta$	$\cos \xi$

For the analysis of this section, we assume further that

$$(k|U^{-1}|l) = (l|U|k)^*. \quad (35)$$

The operator  $U$  is then said to be *unitary*.

The transformation coefficients between the two sets of axes are as given in Table I. If we set  $x_1 = x$ ,  $x_2 = y$ ,  $x_3 = z$  this may be written as:

$$x_k' = \sum_{l=1}^3 \omega_{kl} x_l, \quad x_k = \sum_{l=1}^3 \omega_{lk} x_l', \quad (37)$$

where the  $\omega_{lk}$  are the coefficients in Table I.

We shall base our explicit computation of the transformation operator  $U$  on the supposition that the operators representing the components of the spin transform like the components of a vector under a rotation of axes, i.e., like  $x$ ,  $y$ ,  $z$ . If  $s_x', s_y', s_z'$  are the operators for the components of the spin in the primed axes, we write from the table of transformation coefficients (36)

$$\begin{aligned} s_x' &= (\cos \zeta \cos \eta - \sin \zeta \cos \xi \sin \eta) s_x \\ &\quad + (\cos \zeta \sin \eta + \sin \zeta \cos \xi \cos \eta) s_y \\ &\quad + (\sin \eta \sin \xi) s_z, \quad \text{etc.} \end{aligned}$$

$$\text{or} \quad s_k' = \sum_{l=1}^3 \omega_{kl} s_l, \quad s_k = \sum_{l=1}^3 \omega_{lk} s_l'. \quad (37a)$$

Thus (as applied to the spin functions  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , in the sense of Eq. (12)), the matrices of these operators are:

$$\begin{aligned} s_x' &\sim \frac{1}{2}\hbar \begin{vmatrix} \sin \zeta \sin \xi & (\cos \zeta - i \sin \zeta \cos \xi) e^{-i\eta} \\ (\cos \zeta + i \sin \zeta \cos \xi) e^{i\eta} & -\sin \zeta \sin \xi \end{vmatrix}, \\ s_y' &\sim \frac{1}{2}\hbar \begin{vmatrix} \cos \zeta \sin \xi & (-\sin \zeta - i \cos \zeta \cos \xi) e^{-i\eta} \\ (-\sin \zeta + i \cos \zeta \cos \xi) e^{i\eta} & -\cos \zeta \sin \xi \end{vmatrix}, \\ s_z' &\sim \frac{1}{2}\hbar \begin{vmatrix} \cos \xi & i(\sin \xi) e^{-i\eta} \\ -i(\sin \xi) e^{i\eta} & -\cos \xi \end{vmatrix}. \end{aligned} \quad (38)$$

These operators (and their matrices) may be looked upon as more general solutions of Eqs. (4), and (5). They reduce to  $s_x, s_y, s_z$  for  $\xi, \eta, \zeta \rightarrow 0$ .

Now according to our hypothesis that the operators  $s_x', s_y', s_z'$  are related to the spin functions  $\mathbf{a}_1'$  and  $\mathbf{a}_2'$  in exactly the same way that the operators  $s_x, s_y, s_z$  are related to  $\mathbf{a}_1$  and  $\mathbf{a}_2$  we have by comparison with Eqs. (13) and (14)

$$\begin{aligned} s_x' \mathbf{a}_1' &= \frac{1}{2}\hbar \mathbf{a}_2', & s_x' \mathbf{a}_2' &= \frac{1}{2}\hbar \mathbf{a}_1', \\ s_y' \mathbf{a}_1' &= i\frac{1}{2}\hbar \mathbf{a}_2', & s_y' \mathbf{a}_2' &= -i\frac{1}{2}\hbar \mathbf{a}_1', \\ s_z' \mathbf{a}_1' &= \frac{1}{2}\hbar \mathbf{a}_1', & s_z' \mathbf{a}_2' &= -\frac{1}{2}\hbar \mathbf{a}_2'. \end{aligned}$$

Let us introduce the operators  $\sigma_1 \cdots \sigma_4$  from Eq. (16) and their counterparts in the primed set of axes

$$\sigma_k' = \frac{2}{\hbar} s_k', \quad k=1, 2, 3, \quad \sigma_4' = \sigma_4.$$

We see that the matrix elements of the four operators  $\sigma_1' \cdots \sigma_4'$  when operating on the functions  $\mathbf{a}_1', \mathbf{a}_2'$  are exactly the same as those of the operators  $\sigma_1, \cdots, \sigma_4$ , when operating on the functions  $\mathbf{a}_1, \mathbf{a}_2$  so that we can write

$$\sigma_k' \mathbf{a}_r' = \sum_{l=1}^2 \mathbf{a}_l' \cdot (l|\sigma_k|r).$$

Substituting from Eqs. (30) we get

$$\sigma_k' U \mathbf{a}_r = U \sum_{l=1}^2 \mathbf{a}_l \cdot (l|\sigma_k|r) = U \sigma_k \mathbf{a}_r$$

since

$$\sigma_k \mathbf{a}_r = \sum_{l=1}^2 \mathbf{a}_l \cdot (l|\sigma_k|r).$$

From this result we see that the relation between the operators  $\sigma'$  and  $\sigma$  is

$$\sigma_k' U = U \sigma_k, \quad k=1, 2, 3, 4. \quad (39)$$

These equations, taken with Eqs. (33, 35) furnish the basis for the determination of the operator  $U$ , and its dependence on the parameters specifying the rotation of the axes, e.g., the Eulerian angles.

In §6 we showed that any two-dimensional matrix, representing an operator on the spin functions, could be written as a linear sum of the

operators  $\sigma_1, \dots, \sigma_4$ . This leads us to write, as in Eq. (20),

$$U = u_1\sigma_1 + u_2\sigma_2 + u_3\sigma_3 + u_4\sigma_4 \quad (40)$$

with

$$\begin{aligned} u_1 &= \frac{1}{2}[(1|U|2) + (2|U|1)], \\ u_2 &= i\frac{1}{2}[(1|U|2) - (2|U|1)], \\ u_3 &= \frac{1}{2}[(1|U|1) - (2|U|2)], \\ u_4 &= \frac{1}{2}[(1|U|1) + (2|U|2)]. \end{aligned}$$

On the other hand, we know the transformation formulas of the  $s$  operators from Eq. (37a) for a given rotation of the system of axes, and if we let

$$\omega_{41} = \omega_{42} = \omega_{43} = \omega_{34} = \omega_{24} = \omega_{14} = 0, \quad \omega_{44} = 1,$$

we can write the transformation of the *four*  $\sigma$  operators as

$$\sigma_k' = \sum_{l=1}^4 \omega_{kl} \sigma_l, \quad \sigma_k = \sum_{l=1}^4 \omega_{lk} \sigma_l'. \quad (41)$$

These operator equations can be used for the explicit determination of the coefficients  $u_1, u_2, u_3, u_4$ . Using Eqs. (41) we get

$$\sigma_k' U = \left( \sum_{l=1}^4 \omega_{kl} \sigma_l \right) \left( \sum_{m=1}^4 u_m \sigma_m \right), \quad U \sigma_k = \sum_{n=1}^4 u_n \sigma_n \sigma_k,$$

so that finally

$$\sum_{l=1}^4 \sum_{m=1}^4 u_m \omega_{kl} \sigma_l \sigma_m = \sum_{n=1}^4 u_n \sigma_n \sigma_k. \quad (42)$$

If we work out both sides explicitly we find that they each consist of a sum of terms in  $\sigma_1, \dots, \sigma_4$ . Equating coefficients of corresponding  $\sigma$  operators on each side we get a family of linear equations satisfied by the  $u$ 's. The details of the computation are given in Appendix C. They lead to the following results, which may be verified directly by the reader,

$$\begin{aligned} u_1 &= -i \sin \frac{1}{2} \xi \cdot \cos \frac{1}{2} (\eta - \zeta), \\ u_2 &= -i \sin \frac{1}{2} \xi \cdot \sin \frac{1}{2} (\eta - \zeta), \\ u_3 &= -i \cos \frac{1}{2} \xi \cdot \sin \frac{1}{2} (\eta + \zeta), \\ u_4 &= \cos \frac{1}{2} \xi \cdot \cos \frac{1}{2} (\eta + \zeta). \end{aligned} \quad (43)$$

It should be noted that these quantities are not single-valued functions of the relative orientations of the two systems. If we change any one of the angles by  $2\pi$  we find that

$$(u_1, u_2, u_3, u_4) \rightarrow -(u_1, u_2, u_3, u_4).$$

The operator  $U$  is a multiple-valued function of  $\xi, \eta, \zeta$ .

For the matrix of  $U$  we find<sup>20a</sup>

$$U(\{\xi, \eta, \zeta\}) \sim \begin{vmatrix} \cos \frac{1}{2} \xi \cdot e^{-i\frac{1}{2}(\eta+\zeta)} & -i \sin \frac{1}{2} \xi \cdot e^{-i\frac{1}{2}(\eta-\zeta)} \\ -i \sin \frac{1}{2} \xi \cdot e^{i\frac{1}{2}(\eta-\zeta)} & \cos \frac{1}{2} \xi \cdot e^{i\frac{1}{2}(\eta+\zeta)} \end{vmatrix}. \quad (44)$$

In order to determine the transformations of the functions  $\chi_1$  and  $\chi_2$  we proceed as follows: Suppose that  $\psi$  and  $\psi'$  are the solutions of the wave equations carried out independently in the two sets of axes, *but both representing the same physical state of the system under consideration*. In order to preserve the invariance of the probability density we shall assume that<sup>21</sup>

$$\psi = \psi'$$

or

$$\begin{aligned} \chi_1'(x'y'z't)\mathbf{a}_1' + \chi_2'(x'y'z't)\mathbf{a}_2' \\ = \chi_1(xyzt)\mathbf{a}_1 + \chi_2(xyzt)\mathbf{a}_2. \end{aligned} \quad (45)$$

On substitution from Eqs. (29) or Eqs. (31) we find

$$\chi_1' = \chi_1 \cdot (1|U|1)^* + \chi_2 \cdot (2|U|1)^*, \quad (46)$$

$$\chi_2' = \chi_1 \cdot (1|U|2)^* + \chi_2 \cdot (2|U|2)^*,$$

and

$$\chi_1 = (1|U|1) \cdot \chi_1' + (1|U|2) \cdot \chi_2', \quad (47)$$

$$\chi_2 = (2|U|1) \cdot \chi_1' + (2|U|2) \cdot \chi_2'.$$

With the matrix (44), Eqs. (46) become

$$\begin{aligned} \chi_1' &= \chi_1 \cdot \cos \frac{1}{2} \xi \cdot e^{i\frac{1}{2}(\eta+\zeta)} + \chi_2 \cdot i \sin \frac{1}{2} \xi \cdot e^{-i\frac{1}{2}(\eta-\zeta)}, \\ \chi_2' &= \chi_1 \cdot i \sin \frac{1}{2} \xi \cdot e^{i\frac{1}{2}(\eta-\zeta)} + \chi_2 \cdot \cos \frac{1}{2} \xi \cdot e^{-i\frac{1}{2}(\eta+\zeta)}. \end{aligned} \quad (48)$$

It is evident that the pair of quantities  $\chi_1$  and  $\chi_2$  do not transform under a rotation of axes like

<sup>20a</sup> The convenient notation  $U(\{\xi, \eta, \zeta\})$  for the operator  $U$  as a function of the rotation parameters is adopted from Wigner, *Gruppentheorie*, reference 17.

<sup>21</sup> More generally one could assume  $\psi = e^{i\theta} \psi'$  where  $\theta$  is any real number. This generalization is unnecessary, however, since the factor  $e^{i\theta}$  can be absorbed in the transformation operator  $U$ . The reader may note at this point that the operator  $U$  is not uniquely determined by the conditions (39) and (35). Cf. Appendix C.

the components of a vector or tensor of higher rank. They are called the components of a *spinor* (of rank 1).

The significance of the spin components as rotation operators can be exhibited very nicely from this analysis. If  $\eta = \zeta = 0$  and  $\xi (= \Delta\xi)$  be infinitesimal, an infinitesimal rotation about the  $x$  axis through the angle  $\Delta\xi$  is induced, with the transformation operator <sup>21a</sup>

$$U(\{\Delta\xi, 0, 0\}) = -i\frac{1}{2}\Delta\xi \cdot \sigma_1 + \sigma_4 = \sigma_4 + \Delta\xi(-iS_x/\hbar),$$

from which

$$(\partial U/\partial \xi)_{(\xi, \eta, \zeta)=0} = -iS_x/\hbar.$$

$U$  can be expressed as

$$U(\{\xi, 0, 0\}) = e^{-i\xi S_x/\hbar} = e^{-i\frac{1}{2}\xi \sigma_1}$$

if the exponential function is defined formally by

$$\begin{aligned} e^{-i\frac{1}{2}\xi \sigma_1} &= 1 + (-i\frac{1}{2}\xi \sigma_1) + (1/2!)(-i\frac{1}{2}\xi \sigma_1)^2 + \dots \\ &= (\cos \frac{1}{2}\xi)\sigma_4 - i(\sin \frac{1}{2}\xi)\sigma_1. \end{aligned}$$

In view of the noncommutativity of these operators, the exponential form loses the happy faculty of addition of the exponents in the composition of two rotations. Extensive use has been made of this representation by Eddington in his recent book.<sup>22</sup>

#### §9. BEHAVIOR OF THE PAULI OPERATORS AND SPIN FUNCTIONS UNDER REFLECTIONS

In addition to rotations of the coordinate axes, it is sometimes necessary to consider the characteristics of the wave functions with respect to various reflections. Problems of this kind arise in the study of systems in which the energy operator has certain symmetry properties with respect to operations of this type, e.g., spherical or axial symmetry.

We confine our attention to two operators of this kind, (a) the operation  $R_y$  which reflects the system in the  $(x, z)$  plane, and (b) the operation  $R_0$  which reflects the system in the origin of the

<sup>21a</sup> The minus sign appears in these expressions because  $U$  is the operator which rotates the coordinate axes in "spin space"; i.e.,  $\mathbf{a}_1$  and  $\mathbf{a}_2$ . More customarily one deals with the operator  $U^{-1}$  which transforms the *components*  $x_1$  and  $x_2$ , in which the negative sign does not appear.

<sup>22</sup> A. S. Eddington, *The Relativity Theory of Protons and Electrons* (Cambridge University Press, 1936).

coordinates (inversion). All other reflection operators in ordinary space which leave the origin of coordinates fixed can be made up from these two combined with appropriate operators representing rotations of the axes.

By inspection of the orbital angular momentum operators (2) we see that under these two reflections they undergo the following transformations:<sup>9</sup>

$$R_y: L_x \rightarrow -L_x, \quad L_y \rightarrow +L_y, \quad L_z \rightarrow -L_z,$$

$$R_0: L_x \rightarrow L_x, \quad L_y \rightarrow L_y, \quad L_z \rightarrow L_z.$$

We assume that the spin operators are subject to the same transformations under these reflections. By a reasoning entirely analogous to that of the previous section, we conclude that the corresponding transformation operators, analogous to the  $U$  of Eq. (40) are:

$$\begin{aligned} R_y: U(R_y) &= \pm \sigma_2, \\ R_0: U(R_0) &= \pm \sigma_4. \end{aligned} \quad (49)$$

The double sign for  $U(R_y)$  and  $U(R_0)$  has been introduced here explicitly to show the freedom in the choice of  $U$  (cf. footnote 21). For pure reflections only the choice of  $+$  or  $-$  is allowed, since a further reflection of the same sort returns the system to its original configuration.

#### §10. THE EXTENSION OF THE PAULI THEORY TO MANY ELECTRONS

Although it does not lie within the scope of the present article to discuss the problems of many particles in detail, we may pause to indicate the manner in which the Pauli theory is extended to more than one particle. Since each electron has a spin, we must introduce  $2n$  individual spin functions for  $n$  electrons.

$$\mathbf{a}_1(1), \mathbf{a}_2(1); \quad \mathbf{a}_1(2), \mathbf{a}_2(2); \quad \dots; \quad \mathbf{a}_1(n), \mathbf{a}_2(n).$$

The index in brackets designates the electron, e.g.,  $\mathbf{a}_1(1)$  is associated with a state in which the  $z$ -component of the spin of electron No. 1 is  $+\frac{1}{2}\hbar$ .

A spin wave function representing a particular state for the spins of *all* of the electrons can be made up by taking a product of an arbitrary choice of these functions, one for each electron, e.g.,

$$\mathbf{a}_1(1)\mathbf{a}_1(2)\mathbf{a}_2(3)\dots\mathbf{a}_1(n).$$

In all, we can make up  $2^n$  products of this sort, representing the complete set of spin states of the system.

The complete wave function is then written in the form

$$\psi = \sum_{k, l, \dots=1}^2 \chi_{klm\dots r}(x_1, y_1, z_1; \dots; x_n, y_n, z_n; t) \times \mathbf{a}_k(1)\mathbf{a}_l(2)\dots\mathbf{a}_r(n), \quad (50)$$

where the sum runs over the  $2^n$  spin functions.

In applying this method to electrons we must take cognizance of the Pauli exclusion principle which requires that the function  $\psi$  change sign if we interchange the variables of any two electrons. In such an interchange we consider the index numbers of the electrons appearing in the spin functions as subject to interchange in the same manner as the space variables.

In many practical calculations it is convenient to write the functions  $\chi_{kl\dots}$  as products, or sums of products, of functions each depending on the coordinates of a single electron (i.e. one electron wave functions).<sup>23</sup>

#### §11. THE ESTABLISHMENT OF THE DIRAC WAVE EQUATION

In turning from the Pauli theory to that of Dirac, we enter on a new phase of ideas centering around the problem of developing a theory which will satisfy the requirements of the theory of relativity. As is well known, the special theory of relativity is concerned with the transformation properties of the equations of mathematical physics under the group of Lorentz transformations. These transformations relate the space and time variables used by two "observers" moving with constant velocity with respect to each other. The specific requirement which is ordinarily imposed is that the equations employed in physical theory must have the same form for the two observers, and furthermore, that the solutions obtained by the two observers for the representation of a given physical phenomenon must be related in a one-to-one manner which will preserve the physical significance attached to them. In itself, this requirement is

<sup>23</sup> Cf. Wigner, *Gruppentheorie* (reference 17) or any book on advanced quantum-mechanical theory.

not very restrictive, and leaves considerable freedom in the choice of the actual mathematical form for the equations. The final selection must be made on the basis of arguments concerning the physical phenomena to be described.

Prior to the appearance of Dirac's theory, several authors<sup>23a</sup> had proposed relativistic generalizations of the Schrödinger equation. These had in common the characteristic that they contained *second* partial differential coefficients in the time variable  $t$ , unlike the simple Schrödinger equation which contains only a first partial derivative in  $t$ . The starting point of Dirac's theory was the observation that the success of quantum mechanics in the construction of a comprehensive description of stationary states is due, in large measure, to the appearance of but the first-order time derivative in the wave equation

$$\mathcal{H}\psi = i\hbar\partial\psi/\partial t. \quad (51)$$

The importance of this restriction may be seen from several points of view. The most weighty concerns the definition of a probability density, which from its physical meaning must be positive everywhere. The form of wave equation assumed determines the expression for the probability density in terms of the wave function  $\psi$ . The relativistic equation proposed by Schrödinger leads to a probability density which is not necessarily positive.<sup>24</sup>

From another angle we can see that if the wave equation were to contain a term in  $\partial^2\psi/\partial t^2$ , then in order to specify the behavior of a system for  $t > t_0$ , in terms of its condition at  $t = t_0$ , it would be necessary to specify both  $\psi$  and  $\partial\psi/\partial t$  at  $t = t_0$ . In speaking of an atom such a statement as "at time  $t_0$  the atom is in state  $A$ " would not be adequate, but would need to be amplified to "at time  $t_0$  the atom is in the state  $A$ , and its state is changing in some specified manner." In the absence of any physical evidence that such a drastic extension of our specification of the behavior of systems in terms of their stationary states is required, it seems only reasonable to avoid it if possible.

<sup>23a</sup> E. Schrödinger, *Ann. d. Physik* **81**, 109 (1926). O. Klein, *Zeits. f. Physik* **37**, 895 (1926). V. Fock, *Zeits. f. Physik* **38**, 242 (1926); **39**, 226 (1926). J. Kudar, *Ann. d. Physik* **81**, 632 (1926).

<sup>24</sup> Cf. W. Pauli, *Handbuch der Physik*, second edition, Vol. 24, p. 214.

On the other hand, the symmetrical manner in which the special theory of relativity treats the four variables  $x_1=x$ ,  $x_2=y$ ,  $x_3=z$ ,  $x_4=ict$ , is strong evidence that whatever equation is assumed should contain them symmetrically. The requirements of both quantum-mechanical theory and the relativity theory, when taken together, suggest that the wave equation should be of the form (51), and that the hamiltonian operator  $\mathcal{H}$  should contain only first partial differential coefficients in  $x$ ,  $y$ ,  $z$ .

As the result of his quest for a hamiltonian operator satisfying these requirements, Dirac proposed<sup>25</sup> the following form for the description of the motion of a single particle in an external electromagnetic field.

$$\mathcal{H}_D = -c[\alpha_1\Pi_1 + \alpha_2\Pi_2 + \alpha_3\Pi_3 + \alpha_4m_0c] + \epsilon\phi, \quad (52)$$

where  $\Pi_k = -i\hbar\partial/\partial x_k - \epsilon A_k/c$ ,  $k=1, 2, 3$ .

$A_1=A_x$ ,  $A_2=A_y$ ,  $A_3=A_z$  are the components of the vector potential, and  $\phi$  is the scalar potential, specifying the external field.

$\alpha_1, \alpha_2, \alpha_3, \alpha_4$  are assumed to be operators which do not operate on functions of the space coordinates or time, and which obey the equations

$$\alpha_k\alpha_l + \alpha_l\alpha_k = 2\delta_{kl}, \quad k, l=1, 2, 3, 4. \quad (53)$$

$\delta_{kl}=0$  if  $k \neq l$ ,  $=1$  if  $k=l$ .

As in the nonrelativistic theory the operators for the components of momentum of the particle are retained as

$$p_x \sim -i\hbar\partial/\partial x, \quad p_y \sim -i\hbar\partial/\partial y, \quad p_z \sim -i\hbar\partial/\partial z. \quad (54)$$

A strong argument for the reasonableness of this hamiltonian is the following. Let us consider a free particle for which the hamiltonian is

$$\mathcal{H}_D^0 = -c(\alpha_1p_x + \alpha_2p_y + \alpha_3p_z + \alpha_4m_0c).$$

If we form  $(\mathcal{H}_D^0)^2$  we have by virtue of<sup>26</sup> Eqs. (53)

$$(\mathcal{H}_D^0)^2 = c^2(m_0^2c^2 + p_x^2 + p_y^2 + p_z^2),$$

which is formally just the expression relating the energy and momentum of a free particle used in

<sup>25</sup> P. A. M. Dirac, Proc. Roy. Soc. **A117**, 610 (1928); **A118**, 351 (1928).

<sup>26</sup> This process is permissible since the  $p$  operators commute. The  $\Pi$  operators, with inclusion of external field terms, do not commute and care must be used in arguments involving the iteration of the hamiltonian.

the dynamical equations of the special theory of relativity.

With the hamiltonian (52) we write the *Dirac wave equation*

$$\mathcal{H}_D\psi = [-c(\alpha_1\Pi_1 + \alpha_2\Pi_2 + \alpha_3\Pi_3 + \alpha_4m_0c) + \epsilon\phi]\psi = i\hbar\partial\psi/\partial t, \quad (55)$$

which constitutes the basic starting point of the Dirac theory.<sup>27</sup>

It is sometimes convenient to write the Dirac equation in a more symmetrical form by introducing

$$x_1=x, \quad x_2=y, \quad x_3=z, \quad x_4=ict, \\ A_1=A_x, \quad A_2=A_y, \quad A_3=A_z, \quad A_4=i\phi, \quad (55a)$$

$$\Pi_k = -i\hbar\partial/\partial x_k - \epsilon A_k/c, \quad k=1, 2, 3, 4.$$

The Dirac equation then becomes

$$[-i\Pi_4 + \sum_{k=1}^3 \alpha_k\Pi_k + \alpha_4m_0c]\psi = 0. \quad (56)$$

Another useful form is obtained by multiplying on the left with  $i\alpha_4$  and writing

$$\beta_1 = i\alpha_4\alpha_1, \quad \beta_2 = i\alpha_4\alpha_2, \quad \beta_3 = i\alpha_4\alpha_3, \quad \beta_4 = \alpha_4, \quad (57)$$

which yields the equation

$$\left(\sum_{k=1}^4 \beta_k\Pi_k + im_0c\right)\psi = 0. \quad (58)$$

## §12. THE DIRAC OPERATORS AND SPIN FUNCTIONS

This discussion has thrown no light on the nature of the  $\alpha$  operators, save that we have assumed that they are independent of the space variables, that they do not operate on functions of the space coordinates, and that they commute with all space operators (linear momentum, angular momentum, etc.).

<sup>27</sup> For other reviews of the Dirac theory cf. P. A. M. Dirac, *Quantum Mechanics*, first edition (Oxford University Press, 1930), second edition (1935). H. Weyl, *The Theory of Groups and Quantum Mechanics*, translated from the second German edition by H. P. Robertson (Methuen, 1931). B. L. van der Waerden, *Die Gruppentheoretische Methode in der Quantenmechanik* (Springer, 1932). W. Pauli, *Handbuch der Physik*, second edition, Vol. 24 (1933). L. de Broglie, *L'Electron Magnétique* (Hermann et Cie, 1934). J. Frenkel, *Wave Mechanics: Advanced General Theory* (Oxford University Press, 1934). G. Rumer, *Physik. Zeits.* **32**, 601 (1931). H. A. Kramers, "Theorien des Aufbaues der Materie," in *Hand- und Jahrbuch der Chemischen Physik*, Vol. 1, Nos. 1 and 2 (Akademische Verlagsgesellschaft, 1933-38).

Following the general plan of §5 we introduce "spin symbols" similar to the  $\mathbf{a}_1$  and  $\mathbf{a}_2$  of the Pauli theory. However, it will be necessary to introduce at least four<sup>28</sup> such symbols instead of only two. We call them  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4$ .

For the definition of the mode of operation of the  $\alpha$ 's on  $\mathbf{a}_1, \dots, \mathbf{a}_4$  we proceed by direct analogy with the Pauli theory by assuming that the result of the operation of each of the  $\alpha$ 's on the  $\mathbf{a}$  symbols can be written as a linear sum in the  $\mathbf{a}$ 's; i.e.

$$\alpha_k \mathbf{a}_j = \sum_{l=1}^4 \mathbf{a}_l \cdot (l | \alpha_k | j), \quad k, j = 1, 2, 3, 4. \quad (59)$$

In this way we define matrices representing the  $\alpha$ 's of the form

$$\alpha_k \sim \begin{vmatrix} (1 | \alpha_k | 1) & (1 | \alpha_k | 2) & (1 | \alpha_k | 3) & (1 | \alpha_k | 4) \\ (2 | \alpha_k | 1) & \cdot & \cdot & \cdot \\ (3 | \alpha_k | 1) & \cdot & \cdot & \cdot \\ (4 | \alpha_k | 1) & \cdot & \cdot & (4 | \alpha_k | 4) \end{vmatrix}.$$

As in the Pauli theory, the defining equations (53) for the  $\alpha$ 's do not determine the matrix elements uniquely. For the purposes of this report, we choose the matrices in the form given below

$$\alpha_1 = i\beta_1\beta_4 \sim \begin{vmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{vmatrix};$$

$$\alpha_2 = i\beta_2\beta_4 \sim \begin{vmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{vmatrix};$$

$$\alpha_3 = i\beta_3\beta_4 \sim \begin{vmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{vmatrix};$$

$$\alpha_4 = \beta_4 \sim \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix}.$$

The operator representing "unity" (i.e.  $I_{\mathbf{a}_k} = \mathbf{a}_k$ ) has the matrix

$$I \sim \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix}.$$

In our future work we shall need the matrices representing various other operators which can be made up from the  $\alpha$ 's. For reference we give a list below. These operators are adjusted so that their squares are all +1.

$$i\alpha_2\alpha_3 = i\beta_2\beta_3 \sim \begin{vmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{vmatrix};$$

$$i\alpha_3\alpha_1 = i\beta_3\beta_1 \sim \begin{vmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{vmatrix};$$

$$i\alpha_1\alpha_2 = i\beta_1\beta_2 \sim \begin{vmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix};$$

$$i\alpha_1\alpha_4 = -\beta_1 \sim \begin{vmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{vmatrix};$$

$$i\alpha_2\alpha_4 = -\beta_2 \sim \begin{vmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{vmatrix};$$

<sup>28</sup> The reader can easily verify from the results of §6 that no operator  $\Gamma$  (cf. Eq. (20)) can be found which will anti-commute with  $\sigma_1, \sigma_2, \sigma_3$  but which is not a multiple of one of these. The possibility of using two-dimensional matrices is thus eliminated. For the more general discussion cf. W. Pauli, *Zeeman Verhandelingen* (Nijhoff, 1935), p. 31.

$$\begin{aligned}
i\alpha_3\alpha_4 = -\beta_3 &\sim \begin{vmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{vmatrix}; \\
i\alpha_2\alpha_3\alpha_4 = i\beta_2\beta_3\beta_4 &\sim \begin{vmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{vmatrix}; \\
i\alpha_3\alpha_1\alpha_4 = i\beta_3\beta_1\beta_4 &\sim \begin{vmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{vmatrix}; \\
i\alpha_1\alpha_2\alpha_4 = i\beta_1\beta_2\beta_4 &\sim \begin{vmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix}; \\
i\alpha_1\alpha_2\alpha_3 = \beta_1\beta_2\beta_3\beta_4 &\sim \begin{vmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{vmatrix}; \\
\alpha_1\alpha_2\alpha_3\alpha_4 = i\beta_1\beta_2\beta_3 &\sim \begin{vmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{vmatrix}.
\end{aligned}$$

All of these matrices are hermitian as well as unitary.<sup>29</sup>

It is to be noted that all of the quantities which can be made up by multiplication of any number of  $\alpha$ 's can be reduced to one of these forms, or to one of them multiplied by  $\pm 1$  or  $\pm i$ . This is a direct result of the commutation rules (53). Consequently any general operator function of

<sup>29</sup> A matrix  $\Gamma$  is said to be hermitian if  $\Gamma = \Gamma^\dagger$  where  $\Gamma^\dagger$  is the matrix obtained from  $\Gamma$  by interchanging rows and columns and then changing all elements to their complex conjugates.  $\Gamma$  is said to be *unitary* if  $\Gamma^{-1} = \Gamma^\dagger$  (cf. Eq. (35)).  $\Gamma^\dagger$  is usually called the *adjoint* of  $\Gamma$ . For the purposes of this article we refer to an operator as hermitian or unitary if the matrix used to represent it is hermitian or unitary, as the case may be.

the  $\alpha$ 's can be expressed as a linear sum of these 16 operators, and similarly any 4-rowed square matrix can be written as a linear sum of those 16 matrices. This is a generalization of the similar theorem found in §6 for the Pauli operators.

### §13. THE DIRAC WAVE FUNCTION

Following the same procedure as in §5 we write the complete Dirac wave function in the form

$$\psi = \chi_1 \mathbf{a}_1 + \chi_2 \mathbf{a}_2 + \chi_3 \mathbf{a}_3 + \chi_4 \mathbf{a}_4. \quad (60)$$

We then introduce as in §5 the *conjugate spin symbols*:

$$\bar{\mathbf{a}}_1, \bar{\mathbf{a}}_2, \bar{\mathbf{a}}_3, \bar{\mathbf{a}}_4, \quad (61)$$

which have the property that

$$\bar{\mathbf{a}}_k \mathbf{a}_l = \delta_{kl}. \quad (62)$$

The complex conjugate function to  $\psi$  will be written as

$$\psi^* = \chi_1^* \bar{\mathbf{a}}_1 + \chi_2^* \bar{\mathbf{a}}_2 + \chi_3^* \bar{\mathbf{a}}_3 + \chi_4^* \bar{\mathbf{a}}_4, \quad (63)$$

where  $\chi_1^*, \dots, \chi_4^*$  are the ordinary complex conjugates of the functions  $\chi_1, \dots, \chi_4$ .

In §21 we shall discuss the physical interpretation to be attached to the "internal states" of the electron which are represented by the symbols  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4$ . Anticipating this analysis, we may note that, with our definitions, the matrices of §12 show that these states are such that the operators  $\alpha_4$  and  $i\alpha_1\alpha_2$  are quantized; i.e.

$$\begin{aligned}
\alpha_4 \begin{cases} \mathbf{a}_1 \\ \mathbf{a}_2 \end{cases} &= \begin{cases} \mathbf{a}_1 \\ \mathbf{a}_2 \end{cases}, & \alpha_4 \begin{cases} \mathbf{a}_3 \\ \mathbf{a}_4 \end{cases} &= \begin{cases} -\mathbf{a}_3 \\ -\mathbf{a}_4 \end{cases}, \\
i\alpha_1\alpha_2 \begin{cases} \mathbf{a}_1 \\ \mathbf{a}_3 \end{cases} &= \begin{cases} -\mathbf{a}_1 \\ -\mathbf{a}_3 \end{cases}, & i\alpha_1\alpha_2 \begin{cases} \mathbf{a}_2 \\ \mathbf{a}_4 \end{cases} &= \begin{cases} \mathbf{a}_2 \\ \mathbf{a}_4 \end{cases}.
\end{aligned}$$

We shall find that  $S_z = -\frac{1}{2}\hbar i\alpha_1\alpha_2$  is the operator for the  $z$  component of the electron spin, while  $\Lambda = -m_0\alpha_4$  is interpretable as a kind of "rest mass" operator. We may then characterize  $\mathbf{a}_1$  as representing a state in which  $S_z$  has the value  $+\frac{1}{2}\hbar$  and  $\Lambda$  has the value  $-m_0$ . Similar statements follow for the other states.

In one important respect the Pauli theory permits a type of simplification which is not possible in the Dirac theory. In the former, the energy operator used in most practical problems is of such form that it is possible to employ wave functions which contain but one spin function; i.e., solutions of the form  $\chi_1 \mathbf{a}_1$  or  $\chi_2 \mathbf{a}_2$ . In fact, solutions of this form are commonly used in the literature. In contrast with this, the form of the Dirac hamiltonian is such that, *even for a free particle*, it is not possible to consider the "internal" states as separable. That is, one cannot dispense with the use of all four functions  $\chi_1, \dots, \chi_4$ .



By substitution of  $\psi$  from Eq. (60) in the wave equation (55) we can work out the equations for the functions  $\chi_1, \chi_2, \chi_3, \chi_4$ . The result is

$$\begin{aligned} (i\hbar\partial/\partial t - \epsilon\phi + m_0c^2)\chi_1 + c\Pi_- \chi_4 + c\Pi_3 \chi_3 &= 0, \\ (i\hbar\partial/\partial t - \epsilon\phi + m_0c^2)\chi_2 + c\Pi_+ \chi_3 - c\Pi_3 \chi_4 &= 0, \\ (i\hbar\partial/\partial t - \epsilon\phi - m_0c^2)\chi_3 + c\Pi_- \chi_2 + c\Pi_3 \chi_1 &= 0, \\ (i\hbar\partial/\partial t - \epsilon\phi - m_0c^2)\chi_4 + c\Pi_+ \chi_1 - c\Pi_3 \chi_2 &= 0 \end{aligned} \quad (64)$$

with  $\Pi_{\pm} = \Pi_1 \pm i\Pi_2$ .

#### §14. THE PROBABILITY AND CURRENT DENSITY EXPRESSIONS

The physical interpretation of the Dirac wave function is based on the same fundamental hypothesis as in the Schrödinger and Pauli theories (cf. §5).

The probability density is defined by

$$|\psi|^2 = \psi^* \psi = |\chi_1|^2 + |\chi_2|^2 + |\chi_3|^2 + |\chi_4|^2, \quad (65)$$

which is never negative.

The possibility of endowing this expression with the physical meaning of a probability function depends on the existence of a probability current density  $\mathfrak{J}$  such that

$$\frac{\partial}{\partial t} |\psi|^2 + \text{div } \mathfrak{J} = 0$$

for then only can we be assured that the total probability of finding the electron somewhere will be constant in time; i.e.

$$(\partial/\partial t) \iiint |\psi|^2 dx dy dz = 0.$$

From Eqs. (64) and their complex conjugates we find

$$\begin{aligned} \frac{\partial}{\partial t} |\psi|^2 + c \frac{\partial}{\partial x} (-\chi_1^* \chi_4 - \chi_2^* \chi_3 - \chi_3^* \chi_2 - \chi_4^* \chi_1) \\ + c \frac{\partial}{\partial y} (i\chi_1^* \chi_4 - i\chi_2^* \chi_3 + i\chi_3^* \chi_2 - i\chi_4^* \chi_1) \\ + c \frac{\partial}{\partial z} (-\chi_1^* \chi_3 + \chi_2^* \chi_4 - \chi_3^* \chi_1 + \chi_4^* \chi_2) = 0. \end{aligned} \quad (66)$$

The components of the probability current density can be identified as

$$\begin{aligned} \mathfrak{J}_x &= -c(\chi_1^* \chi_4 + \chi_2^* \chi_3 + \chi_3^* \chi_2 + \chi_4^* \chi_1) \\ &= \psi^* (-c\alpha_1) \psi, \\ \mathfrak{J}_y &= ic(\chi_1^* \chi_4 - \chi_2^* \chi_3 + \chi_3^* \chi_2 - \chi_4^* \chi_1) \\ &= \psi^* (-c\alpha_2) \psi, \\ \mathfrak{J}_z &= -c(\chi_1^* \chi_3 - \chi_2^* \chi_4 + \chi_3^* \chi_1 - \chi_4^* \chi_2) \\ &= \psi^* (-c\alpha_3) \psi. \end{aligned} \quad (67)$$

If we multiply by the charge  $\epsilon$  we get the charge and current density expressions

$$\rho = \epsilon |\psi|^2 = \epsilon \psi^* I \psi; \quad \mathbf{j} = \epsilon \psi^* (-c\boldsymbol{\alpha}) \psi. \quad (68)$$

The second of these equations suggests that the (vector) operator  $-c\boldsymbol{\alpha}$  represents the *velocity* of the electron in the Dirac theory. This interpretation is due to Breit.<sup>30</sup> It is significant that in the Schrödinger theory, there exists no operator for the velocity, but only for the momentum. The further development of this conception is deferred to §21.

#### §15. THE FREE PARTICLE SOLUTIONS

In the absence of an external electromagnetic field

$$A_1 = A_2 = A_3 = A_4 = 0$$

the Dirac equation becomes from Eq. (64) and (55a)

$$\begin{aligned} \left(i\hbar \frac{\partial}{\partial t} + m_0c^2\right)\chi_1 - i\hbar c \left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\chi_4 - i\hbar c \frac{\partial}{\partial z}\chi_3 &= 0, \\ \left(i\hbar \frac{\partial}{\partial t} + m_0c^2\right)\chi_2 - i\hbar c \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\chi_3 + i\hbar c \frac{\partial}{\partial z}\chi_4 &= 0, \\ \left(i\hbar \frac{\partial}{\partial t} - m_0c^2\right)\chi_3 - i\hbar c \left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\chi_2 - i\hbar c \frac{\partial}{\partial z}\chi_1 &= 0, \\ \left(i\hbar \frac{\partial}{\partial t} - m_0c^2\right)\chi_4 - i\hbar c \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\chi_1 + i\hbar c \frac{\partial}{\partial z}\chi_2 &= 0. \end{aligned} \quad (69)$$

We can obtain particular solutions of these equations by assuming that the  $\chi$ 's can be written in the form

$$\chi_\mu = \eta_\mu \cdot \exp(i/\hbar)(p_1x + p_2y + p_3z - Et),$$

$$\mu = 1, 2, 3, 4,$$

<sup>30</sup> G. Breit, Proc. Nat. Acad. Sci. **14**, 553 (1928); **17**, 70 (1931).

where  $\eta_1, \dots, \eta_4; p_1, \dots, p_3, E$  are all constants; the  $\eta$ 's are complex and the others real. By substitution we obtain the following algebraic equations for the  $\eta$ 's:

$$\begin{aligned} (E+m_0c^2)\eta_1+0\cdot\eta_2+c p_3\eta_3+c(p_1-ip_2)\eta_4 &= 0, \\ 0\cdot\eta_1+(E+m_0c^2)\eta_2+c(p_1+ip_2)\eta_3-c p_3\eta_4 &= 0, \\ c p_3\eta_1+c(p_1-ip_2)\eta_2+(E-m_0c^2)\eta_3+0\cdot\eta_4 &= 0, \\ c(p_1+ip_2)\eta_1-c p_3\eta_2+0\cdot\eta_3+(E-m_0c^2)\eta_4 &= 0. \end{aligned}$$

The necessary and sufficient condition for the existence of nonvanishing solutions to these equations is the vanishing of the determinant of the coefficients; i.e.

$$\begin{vmatrix} E+m_0c^2 & 0 & c p_3 & c(p_1-ip_2) \\ 0 & E+m_0c^2 & c(p_1+ip_2) & -c p_3 \\ c p_3 & c(p_1-ip_2) & E-m_0c^2 & 0 \\ c(p_1+ip_2) & -c p_3 & 0 & E-m_0c^2 \end{vmatrix} = 0.$$

On expansion the determinant yields

$$[E^2 - m_0^2c^4 - c^2(p_1^2 + p_2^2 + p_3^2)]^2 = 0,$$

from which we obtain the two (double) roots

$$E_{\pm} = \pm c(m_0^2c^2 + p_1^2 + p_2^2 + p_3^2)^{\frac{1}{2}}. \quad (70)$$

As both roots are double, for each root two of the  $\eta$ 's may be given arbitrary values, while the other two can be obtained from the equations. If we let  $A, B, C, D$  be arbitrary complex constants, we can write the solutions in the form

$$\begin{aligned} E = E_+ \quad \eta_3^+ &= A, \quad \eta_4^+ = B, \\ \eta_1^+ &= -c \frac{p_3A + (p_1 - ip_2)B}{E_+ + m_0c^2}; \\ \eta_2^+ &= -c \frac{(p_1 + ip_2)A - p_3B}{E_+ + m_0c^2}; \\ \psi_+ &= \exp(i/\hbar)(\mathbf{p} \cdot \mathbf{r} - E_+t) \\ &\quad \times (\eta_1^+ \mathbf{a}_1 + \eta_2^+ \mathbf{a}_2 + \eta_3^+ \mathbf{a}_3 + \eta_4^+ \mathbf{a}_4); \quad (71) \\ E = E_- \quad \eta_1^- &= C, \quad \eta_2^- = D, \\ \eta_3^- &= -c \frac{p_3C + (p_1 - ip_2)D}{E_- - m_0c^2}; \end{aligned}$$

$$\eta_4^- = -c \frac{(p_1 + ip_2)C - p_3D}{E_- - m_0c^2};$$

$$\begin{aligned} \psi_- &= \exp(i/\hbar)(\mathbf{p} \cdot \mathbf{r} - E_-t) \\ &\quad \times (\eta_1^- \mathbf{a}_1 + \eta_2^- \mathbf{a}_2 + \eta_3^- \mathbf{a}_3 + \eta_4^- \mathbf{a}_4). \quad (72) \end{aligned}$$

For small values of the  $p$ 's (i.e.  $p_1^2 + p_2^2 + p_3^2 \ll m_0^2c^2$ )

$$E_+ \sim +m_0c^2, \quad E_- \sim -m_0c^2,$$

so that

$$\begin{aligned} |\eta_3^+|, \quad |\eta_4^+| &\gg |\eta_1^+|, \quad |\eta_2^+|, \\ |\eta_1^-|, \quad |\eta_2^-| &\gg |\eta_3^-|, \quad |\eta_4^-|. \end{aligned}$$

The existence of solutions of the Dirac equation for  $E < -m_0c^2$  (negative energy solutions) has been the cause of much doubt and speculation concerning their proper physical interpretation. In a series of very interesting papers, Schrödinger<sup>31</sup> some years ago studied the possibility of eliminating the negative energy solutions by an altered definition of the operators used for the representation of physical quantities.

In fact, however, an exactly similar difficulty is present in classical relativistic mechanics, in which the energy expression for a free particle in terms of its momentum components could be taken as either of the expressions of Eq. (70). But the difficulty can be evaded in this case by requiring that in the motion of a particle its energy, as well as its momentum, can change only continuously. A particle moving with an initially positive energy could never attain a negative energy, since the finite interval  $2m_0c^2$  separating the positive and negative energies could not be negotiated by continuous stages.

But in quantum-mechanical theory the trouble is much more serious and fundamental, since discontinuous transitions between different states are not only permitted, but form a basic element in the applications to actual physical problems. A preliminary investigation of transitions between positive and negative energy states was made by Klein,<sup>32</sup> soon after the publication of Dirac's equation (*Klein paradox*). Klein studied the

<sup>31</sup> E. Schrödinger, Sitzungsber. Preuss. Akad. Wiss. Phys.-Math. Klasse, p. 418 (1930); p. 63 (1931); Annales de l'Institut Henri Poincaré 2, 269 (1932).

<sup>32</sup> O. Klein, Zeits. f. Physik 53, 157 (1929).

reflection of electrons at a "potential barrier" separating two regions in which the potential energy of the particle is  $O$  and  $P$ , respectively. In Fig. 2 is shown a schematic energy diagram for the two regions (treated as one-dimensional) with the energy intervals of width  $2m_0c^2$  in which no solutions exist for the free particle marked by cross hatching. For  $P \geq 2m_0c^2$  it is possible to fit the solutions together at the boundary between the two regions such that a positive energy solution on the left is fitted with a negative energy solution on the right. Under these conditions it would appear that the particle could penetrate the barrier by making a transition from a positive to a negative energy state. Klein computed a coefficient of transmission, which increases from zero for  $P = E + m_0c^2$  to

$$2 \frac{(E^2 - m_0^2c^4)^{\frac{1}{2}}}{E + (E^2 - m_0^2c^4)^{\frac{1}{2}}}$$

for  $P \rightarrow \infty$ .

Bohr made the suggestion that the high coefficient of transmission arose from the discontinuity in the potential, which would be associated with an infinitely great acceleration. The problem was examined more in detail by Sauter,<sup>33</sup> who supposed that the energy changed in a gradual manner from one region to the other. He concluded that the coefficient of transmission for an electron would be small unless the energy gradient exceeded

$$m_0c^2/(\hbar/m_0c) \approx 10^{16} \text{ electron volts/cm.}$$

Although this indicates that transition probabilities between positive and negative energy states are small for the fields ordinarily available in nature, the theoretical difficulty of their existence remains.

Some question might be raised concerning calculations of this type, since in physical problems we must consider the fields not as purely external things, but as having a dynamical origin. However, all attempts to eliminate transitions from the positive to the negative energy states have but established more firmly the conviction that the negative energy solutions of the Dirac equation must be considered on a par with those for positive energies. Further dis-

<sup>33</sup> F. Sauter, *Zeits. f. Physik* **69**, 742 (1931); **73**, 547 (1931).

cussion of this point is given in a later section (§23).

It should be observed that the distinction between "negative energy states" and "positive energy states" can be made exact only in the absence of external fields. In most applications the electron is considered to be *practically* free, but is caused to make transitions between its various states by the external field, which is treated as a perturbing influence. The distinction between positive and negative energy states retains its physical significance.

#### §16. THE SPIN ANGULAR MOMENTUM OPERATORS. QUANTIZATION OF THE TOTAL ANGULAR MOMENTUM

In this section we shall study the operators representing the components of the angular momentum in the Dirac theory, and shall develop the relationship of the four  $\alpha$ -operators to the electron spin.

The operators for the components of the orbital angular momentum are defined by exactly the same equations as in the Schrödinger and Pauli theories (§4).

We can no longer define the spin angular momentum operators in an *a priori* manner as in the Pauli theory, but must appeal directly to the structure of the Dirac equation itself. The criteria which we shall use are that:

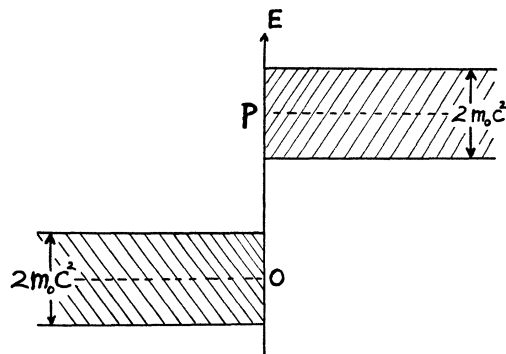


FIG. 2. Schematic one-dimensional energy diagram.

(a) The total angular momentum operator shall be a (vector) sum of the orbital and spin angular momentum operators.

(b) The total angular momentum operator shall commute with the Dirac hamiltonian for the electron in a central field.

The first condition is the natural generalization of the Pauli definitions (21); the second is the necessary and sufficient condition that the total angular momentum may be quantized in the stationary states of the hydrogen atom, just as is the case for the orbital angular momentum in the Schrödinger theory.

The operators for the components of the spin angular momentum must be chosen to satisfy the equations

$$(\mathcal{H}_D^c)\mathbf{J} - \mathbf{J}(\mathcal{H}_D^c) = 0, \quad (73)$$

where  $(\mathcal{H}_D^c)$  is the special form assumed by the Dirac hamiltonian for the electron in a central field

$$\mathcal{H}_D^c = -c(\alpha_1 p_x + \alpha_2 p_y + \alpha_3 p_z + \alpha_4 m_0 c) + \epsilon\phi(r).$$

The operators  $p$  are defined by (54).

On writing out the equations (73) in detail (for each component), the reader will easily find that the following operators satisfy these conditions,

$$\begin{aligned} J_x &= L_x - \frac{1}{2}\hbar i\alpha_2\alpha_3, \\ J_y &= L_y - \frac{1}{2}\hbar i\alpha_3\alpha_1, \\ J_z &= L_z - \frac{1}{2}\hbar i\alpha_1\alpha_2. \end{aligned} \quad (74)$$

The operators for the spin angular momentum are seen to be

$$\begin{aligned} S_x &= -\frac{1}{2}\hbar i\alpha_2\alpha_3, \\ S_y &= -\frac{1}{2}\hbar i\alpha_3\alpha_1, \\ S_z &= -\frac{1}{2}\hbar i\alpha_1\alpha_2. \end{aligned} \quad (75)$$

It follows immediately by use of Eqs. (53) that these operators satisfy exactly the formal equations of the Pauli theory.

$$\begin{aligned} S_x S_y &= -S_y S_x = i\hbar S_z/2, \quad \text{etc.}, \\ S_x^2 &= S_y^2 = S_z^2 = (\frac{1}{2}\hbar)^2. \end{aligned}$$

*The square of the magnitude of the spin angular momentum has exactly the value  $\frac{3}{4}\hbar^2$  required in the hypothesis of Uhlenbeck and Goudsmit.*

The automatic appearance of appropriate spin operators constitutes one of the principal triumphs of the Dirac theory, and has had much to do with its adoption as the most fundamental starting point at present available for the discussion of problems involving high energy electrons.

We can now carry through a calculation of the quantization of the total angular momentum analogous to that of §7. We seek a wave function  $\psi$  satisfying the two equations

$$J_z \psi = A \psi; \quad \mathbf{J}^2 \psi = B \psi, \quad (76)$$

where  $A$  and  $B$  are constants.

We substitute  $\psi = \chi_1 \mathbf{a}_1 + \chi_2 \mathbf{a}_2 + \chi_3 \mathbf{a}_3 + \chi_4 \mathbf{a}_4$  in these equations and work out the solutions for  $\chi_1, \dots, \chi_4$ . We find

$$(L_z + \frac{1}{2}\hbar - A) \begin{cases} \chi_1 \\ \chi_3 \end{cases} = 0, \quad (L_z - \frac{1}{2}\hbar - A) \begin{cases} \chi_2 \\ \chi_4 \end{cases} = 0,$$

$$(\mathbf{L}^2 + \frac{3}{4}\hbar^2 + \hbar L_z - B) \begin{cases} \chi_1 \\ \chi_3 \end{cases} + \hbar L_- \begin{cases} \chi_2 \\ \chi_4 \end{cases} = 0,$$

$$(\mathbf{L}^2 + \frac{3}{4}\hbar^2 - \hbar L_z - B) \begin{cases} \chi_2 \\ \chi_4 \end{cases} + \hbar L_+ \begin{cases} \chi_1 \\ \chi_3 \end{cases} = 0.$$

Inspection shows these equations fall into two sets, one containing only  $\chi_1$  and  $\chi_2$ , and the other only  $\chi_3$  and  $\chi_4$ . Furthermore we see that each pair is identical in form with Eqs. (25) and (26) of §7. The results of that section can be taken over *in toto*, so that we may write the solutions in the form

$$\begin{aligned} \chi_1(r, \theta, \varphi) &= f(r) \left( \frac{J+1-M}{2(J+1)} \right)^{\frac{1}{2}} Y_{J+\frac{1}{2}, M-\frac{1}{2}}(\theta, \varphi) + g(r) \left( \frac{J+M}{2J} \right)^{\frac{1}{2}} Y_{J-\frac{1}{2}, M-\frac{1}{2}}(\theta, \varphi), \\ \chi_2(r, \theta, \varphi) &= -f(r) \left( \frac{J+1+M}{2(J+1)} \right)^{\frac{1}{2}} Y_{J+\frac{1}{2}, M+\frac{1}{2}}(\theta, \varphi) + g(r) \left( \frac{J-M}{2J} \right)^{\frac{1}{2}} Y_{J-\frac{1}{2}, M+\frac{1}{2}}(\theta, \varphi), \end{aligned} \quad (77)$$

$$\begin{aligned}\chi_3(r, \theta, \varphi) &= F(r) \left( \frac{J+1-M}{2(J+1)} \right)^{\frac{1}{2}} Y_{J+1, M-1}(\theta, \varphi) + G(r) \left( \frac{J+M}{2J} \right)^{\frac{1}{2}} Y_{J-1, M-1}(\theta, \varphi), \\ \chi_4(r, \theta, \varphi) &= -F(r) \left( \frac{J+1+M}{2(J+1)} \right)^{\frac{1}{2}} Y_{J+1, M+1}(\theta, \varphi) + G(r) \left( \frac{J-M}{2J} \right)^{\frac{1}{2}} Y_{J-1, M+1}(\theta, \varphi)\end{aligned}$$

where the radial functions  $f, g, F, G$  are not determined by Eqs. (76).

The quantized values of  $J_z$  and  $\mathbf{J}^2$  are again

$$A = M\hbar, \quad B = J(J+1)\hbar^2,$$

where

$$J = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots, \quad M = -J, -J+1, \dots, +J.$$

### §17. THE HYDROGENIC ATOM. FINE STRUCTURE FORMULA

Apart from the solution of the problem of electron spin, the most signal success afforded by the Dirac theory has been the derivation of the Sommerfeld fine structure formula for the energy levels of an electron in the field of a single nucleus. This formula was originally derived from an extension of the Bohr theory to include the variation of mass of the electron with velocity, long before the discovery of quantum mechanics. After the discovery of the electron spin and the development of quantum mechanics, the problem had a checkered career involving much uncertainty over the significance of the electron spin and mass variation effects. The derivation of the identical Sommerfeld formula<sup>34</sup> in 1928 from Dirac's equation, restored the problem to the realm of exact theory, and created a strong argument in favor of the validity of the new wave equation.

We shall confine ourselves to a discussion of the derivation of the fine structure formula and of the wave functions for the energy levels. For the discussion of the empirical data on the spectra of the alkali atoms, and to the x-ray levels of heavy atoms, the reader may refer to various accounts in the literature.<sup>34, 35</sup>

The Coulomb field of the nucleus is defined by

$$A_1 = A_2 = A_3 = 0, \quad A_4 = i\phi = i(Ze/r) \quad (\epsilon = -e = -4.80 \times 10^{-10} \text{ e.s.u.}).$$

Equations (64) now reduce to

$$\begin{aligned}\left( i\hbar \frac{\partial}{\partial t} + \frac{Ze^2}{r} + m_0c^2 \right) \chi_1 - i\hbar c \left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \chi_4 - i\hbar c \frac{\partial}{\partial z} \chi_3 &= 0, \\ \left( i\hbar \frac{\partial}{\partial t} + \frac{Ze^2}{r} + m_0c^2 \right) \chi_2 - i\hbar c \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \chi_3 + i\hbar c \frac{\partial}{\partial z} \chi_4 &= 0, \\ \left( i\hbar c \frac{\partial}{\partial t} + \frac{Ze^2}{r} - m_0c^2 \right) \chi_3 - i\hbar c \left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \chi_2 - i\hbar c \frac{\partial}{\partial z} \chi_1 &= 0, \\ \left( i\hbar c \frac{\partial}{\partial t} + \frac{Ze^2}{r} - m_0c^2 \right) \chi_4 - i\hbar c \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \chi_1 + i\hbar c \frac{\partial}{\partial z} \chi_2 &= 0.\end{aligned}\tag{78}$$

We set

$$\chi_k = \chi_k^0(r, \theta, \varphi) e^{-(i/\hbar)Et}\tag{79}$$

and introduce for  $\chi_1^0, \dots, \chi_4^0$  the functions of Eq. (77). It follows from the commutation of the hamiltonian operator with the components of  $\mathbf{J}$ , discussed in the last section, that the wave functions for the stationary states are of the form of Eqs. (77).

<sup>34</sup> C. G. Darwin, Proc. Roy. Soc. **A118**, 654 (1928).

<sup>35</sup> H. Bethe, *Handbuch der Physik*, second edition, Vol. 24, p. 316.

The differential equations (78) could be transformed to polar coordinates, but by use of the formulas given in Appendix B this is not necessary. The expressions (77) may be substituted directly and the terms containing the individual spherical harmonics collected together. By virtue of the linear independence of the spherical harmonics the coefficients of each separate harmonic must vanish. This straightforward, but somewhat laborious, calculation may be left to the reader. As the end result, we find the following differential equations for  $f$ ,  $g$ ,  $F$ ,  $G$ .

$$df/dr + (J + \frac{3}{2})(f/r) + (i/\hbar c)[E + (Ze^2/r) - m_0c^2]G = 0, \quad (80)$$

$$dG/dr - (J - \frac{1}{2})(G/r) + (i/\hbar c)[E + (Ze^2/r) + m_0c^2]f = 0,$$

$$dF/dr + (J + \frac{3}{2})(F/r) + (i/\hbar c)[E + (Ze^2/r) + m_0c^2]g = 0, \quad (81)$$

$$dg/dr - (J - \frac{1}{2})(g/r) + (i/\hbar c)[E + (Ze^2/r) - m_0c^2]F = 0.$$

The separation of these equations into two groups, each containing but one pair of functions, shows that we can find two independent solutions for  $\psi$  for each allowed value of  $E$ , by letting either of the pairs of functions ( $f$ ,  $G$ ) or ( $F$ ,  $g$ ) vanish.

We shall carry out the solution of Eqs. (80) in detail. The work for Eqs. (81) proceeds along the same lines.

Let us set<sup>35a</sup>

$$\alpha = e^2/\hbar c, \quad \lambda = (m_0c/\hbar)(1 - \epsilon^2)^{\frac{1}{2}}, \quad \epsilon = E/m_0c^2, \quad \rho = 2\lambda r, \quad (82)$$

$$f(r) = N_1 i (1 - \epsilon)^{\frac{1}{2}} (e^{-\lambda r}/r) (\varphi_1 - \varphi_2), \quad G(r) = N_1 (1 + \epsilon)^{\frac{1}{2}} (e^{-\lambda r}/r) (\varphi_1 + \varphi_2), \quad (83)$$

where  $N_1$  is a normalizing factor to be determined later.

By substitution in Eqs. (80) we find that  $\varphi_1$  and  $\varphi_2$  satisfy the differential equations

$$\frac{d\varphi_1}{d\rho} = \left(1 - \frac{Z\alpha}{\rho} \frac{\epsilon}{(1 - \epsilon^2)^{\frac{1}{2}}}\right) \varphi_1 + \left(\frac{J + \frac{1}{2}}{\rho} - \frac{Z\alpha}{\rho(1 - \epsilon^2)^{\frac{1}{2}}}\right) \varphi_2, \quad (84)$$

$$\frac{d\varphi_2}{d\rho} = \left(\frac{J + \frac{1}{2}}{\rho} + \frac{Z\alpha}{\rho(1 - \epsilon^2)^{\frac{1}{2}}}\right) \varphi_1 + \left(\frac{Z\alpha}{\rho} \frac{\epsilon}{(1 - \epsilon^2)^{\frac{1}{2}}}\right) \varphi_2.$$

We reduce these equations one step further by writing

$$\varphi_1 = \rho^\gamma \Lambda_1, \quad \varphi_2 = \rho^\gamma \Lambda_2, \quad (85)$$

where  $\Lambda_1$  and  $\Lambda_2$  satisfy the equations

$$\begin{aligned} \frac{d\Lambda_1}{d\rho} &= \left[1 - \frac{\gamma}{\rho} - \frac{Z\alpha\epsilon}{\rho(1 - \epsilon^2)^{\frac{1}{2}}}\right] \Lambda_1 + \left[\frac{J + \frac{1}{2}}{\rho} - \frac{Z\alpha}{\rho(1 - \epsilon^2)^{\frac{1}{2}}}\right] \Lambda_2, \\ \frac{d\Lambda_2}{d\rho} &= \left[\frac{J + \frac{1}{2}}{\rho} + \frac{Z\alpha}{\rho(1 - \epsilon^2)^{\frac{1}{2}}}\right] \Lambda_1 + \left[-\frac{\gamma}{\rho} + \frac{Z\alpha\epsilon}{\rho(1 - \epsilon^2)^{\frac{1}{2}}}\right] \Lambda_2. \end{aligned} \quad (86)$$

The solutions of these equations may be found in the form of series

$$\Lambda_1 = 1 + c_1\rho + c_2\rho^2 + \dots, \quad \Lambda_2 = d_0 + d_1\rho + d_2\rho^2 + \dots. \quad (87)$$

By substitution we obtain the recursion formulas

$$c_k \left[ \gamma + k + \frac{Z\alpha\epsilon}{(1 - \epsilon^2)^{\frac{1}{2}}} \right] - d_k \left[ J + \frac{1}{2} - \frac{Z\alpha}{(1 - \epsilon^2)^{\frac{1}{2}}} \right] = c_{k-1}, \quad c_k \left[ J + \frac{1}{2} + \frac{Z\alpha}{(1 - \epsilon^2)^{\frac{1}{2}}} \right] - d_k \left[ \gamma + k - \frac{Z\alpha\epsilon}{(1 - \epsilon^2)^{\frac{1}{2}}} \right] = 0. \quad (88)$$

<sup>35a</sup> In the remainder of this section, and in Appendix D, the electronic charge is designated by  $e$ , and the energy in units of  $m_0c^2$  by  $\epsilon$ .

For the lowest term  $k=0$  ( $c_{-1}=0$ ) we get two homogeneous equations for  $c_0$  and  $d_0$  which admit nonvanishing solutions if, and only if, the determinantal equation

$$\begin{vmatrix} \left( \gamma + \frac{Z\alpha\epsilon}{(1-\epsilon^2)^{\frac{1}{2}}} \right) & - \left( J + \frac{1}{2} - \frac{Z\alpha}{(1-\epsilon^2)^{\frac{1}{2}}} \right) \\ \left( J + \frac{1}{2} + \frac{Z\alpha}{(1-\epsilon^2)^{\frac{1}{2}}} \right) & - \left( \gamma - \frac{Z\alpha\epsilon}{(1-\epsilon^2)^{\frac{1}{2}}} \right) \end{vmatrix} = 0$$

is satisfied. One of the solutions of this equation is

$$\gamma = +[(J + \frac{1}{2})^2 - Z^2\alpha^2]^{\frac{1}{2}}. \quad (89)$$

The other is the negative of this expression, which must be discarded since from Eqs. (83) and (85) the behavior of the wave function in the neighborhood of  $r=0$  would then be like

$$1/r^{1+[(J+\frac{1}{2})^2-Z^2\alpha^2]^{\frac{1}{2}}}.$$

This choice would lead to a nonintegrable value of  $|\psi|^2$ , which would not be suitable for the representation of a real stationary state. With the choice (89) the behavior of  $|\psi|^2$  for small values of  $r$  is as

$$1/r^{1-[(J+\frac{1}{2})^2-Z^2\alpha^2]^{\frac{1}{2}}}.$$

It is worthy of note that  $\alpha \sim 1/137$  (Eddington's value), so that for all known atoms

$$Z\alpha < 1.$$

As the minimum value of  $J$  is  $+\frac{1}{2}$ , it follows that  $\gamma$  is always real. From Eqs. (88) our recursion formulas now become:

$$c_k = \frac{(\gamma + k)(1 - \epsilon^2)^{\frac{1}{2}} - Z\alpha\epsilon}{k(2\gamma + k)(1 - \epsilon^2)^{\frac{1}{2}}} c_{k-1}, \quad d_k = \frac{(J + \frac{1}{2})(1 - \epsilon^2)^{\frac{1}{2}} + Z\alpha}{(\gamma + k)(1 - \epsilon^2)^{\frac{1}{2}} - Z\alpha\epsilon} c_k. \quad (90)$$

In order that the solutions may be of the form of polynomials let the highest nonvanishing coefficient in the series for  $c_k$  be

$$c_{n'-1} \neq 0, \quad c_{n'} = c_{n'+1} = \dots = 0.$$

Then

$$\gamma + n' - Z\alpha\epsilon / (1 - \epsilon^2)^{\frac{1}{2}} = 0, \quad (91)$$

from which

$$E = \epsilon m_0 c^2 = m_0 c^2 [1 + Z^2 \alpha^2 / (n' + \gamma)^2]^{-\frac{1}{2}}. \quad (92)$$

The principal quantum number is defined by

$$n = n' + J + \frac{1}{2}. \quad (93)$$

Introducing this into Eq. (92) we get the energy expression for a hydrogenic atom

$$E_{n,J} = m_0 c^2 \epsilon_{n,J} = m_0 c^2 [1 + Z^2 \alpha^2 / (n - J - \frac{1}{2} + \{(J + \frac{1}{2})^2 - Z^2 \alpha^2\}^{\frac{1}{2}})^2]^{-\frac{1}{2}}. \quad (94)$$

If the rest energy  $m_0 c^2$  of the electron is subtracted out, the residual is

$$W_{n,J} = E_{n,J} - m_0 c^2, \quad (94a)$$

which is the Sommerfeld fine structure formula.

For the explicit determination of the wave functions we let<sup>36</sup>

<sup>36</sup> These functions are related to the confluent hypergeometric function. Cf. Whittaker and Watson, *Modern Analysis*, fourth edition (Cambridge University Press), chapter 16. W. Gordon, *Zeits. f. Physik* **48**, 11 (1928). H. A. Kramers, reference 27, p. 302 *et seq.* H. A. Bethe, reference 35, p. 311.

$$\mathfrak{F}(\xi, \eta; x) = 1 + \frac{\xi}{1! \eta} x + \frac{\xi(\xi+1)}{2! \eta(\eta+1)} x^2 + \dots \quad (95)$$

From the recursion formulas (90) (with  $c_0 = 1$ ) it is easily computed that for  $E = E_{n, J}$

$$\begin{aligned} \varphi_1 &= [\rho^\gamma \cdot \mathfrak{F}(-n'+1, 2\gamma+1; \rho)]_{\epsilon = \epsilon_n, J}, \\ \varphi_2 &= - \left[ \frac{[\gamma + n' + (J + \frac{1}{2})\epsilon]}{n'\epsilon} \rho^\gamma \cdot \mathfrak{F}(-n', 2\gamma+1; \rho) \right]_{\epsilon = \epsilon_n, J}. \end{aligned} \quad (96)$$

A similar analysis can be carried out for Eqs. (81) by writing

$$F = N_2 i(1 + \epsilon)^{\frac{1}{2}} (e^{-\lambda r/r})(\theta_1 - \theta_2), \quad g = N_2 (1 - \epsilon)^{\frac{1}{2}} (e^{-\lambda r/r})(\theta_1 + \theta_2). \quad (97)$$

We find

$$\begin{aligned} \theta_1 &= \left[ \frac{[\gamma + n' - (J + \frac{1}{2})\epsilon]}{n'\epsilon} \rho^\gamma \cdot \mathfrak{F}(-n', 2\gamma+1; \rho) \right]_{\epsilon = \epsilon_n, J} \\ \theta_2 &= [\rho^\gamma \cdot \mathfrak{F}(-n'+1, 2\gamma+1; \rho)]_{\epsilon = \epsilon_n, J}. \end{aligned} \quad (98)$$

The normalization factors  $N_1$  and  $N_2$  can be computed by the method given in Appendix D and are found to be

$$\begin{aligned} N_1 &= \left\{ \frac{\lambda}{\Gamma(2\gamma+1)} \left[ \frac{\hbar}{2Z\alpha m_0 c} \frac{n'\epsilon}{\gamma + n' + (J + \frac{1}{2})\epsilon} \frac{\Gamma(2\gamma+1+n')}{(n'-1)!} \right]^{\frac{1}{2}} \right\}_{\epsilon = \epsilon_n, J}, \\ N_2 &= \left\{ \frac{\lambda}{\Gamma(2\gamma+1)} \left[ \frac{\hbar}{2Z\alpha m_0 c} \frac{n'\epsilon}{\gamma + n' - (J + \frac{1}{2})\epsilon} \frac{\Gamma(2\gamma+1+n')}{(n'-1)!} \right]^{\frac{1}{2}} \right\}_{\epsilon = \epsilon_n, J}, \end{aligned} \quad (99)$$

where  $\Gamma$  refers to the gamma-function.

It can be verified from the explicit formulas or can be seen from the differential equations (80, 81) that

$$|G| \gg |f|, \quad |F| \gg |g|.$$

For each of the two solutions for the energy state  $E_{n, J}$  one of the components of the wave function is much larger than the other. If we designate the two independent solutions as

$$\text{I. } F = g = 0, \quad \text{II. } f = G = 0,$$

we see that for (I) the big components have the angular factors

$$Y_{J-\frac{1}{2}, M \pm \frac{1}{2}},$$

indicating that the orbital angular quantum number is  $l = J - \frac{1}{2}$ , while for (II) the big components have the angular factor  $Y_{J+\frac{1}{2}, M \pm \frac{1}{2}}$  for which  $l = J + \frac{1}{2}$ . In a rough way we get the vector coupling scheme of the Pauli theory. But the existence of the small components with the angular factors in the reverse order shows that the vector coupling model is only approximate at best.<sup>37</sup>

## §18. THE RELATIVISTIC PROPERTIES OF THE DIRAC EQUATION

We turn now to the discussion of the relativistic invariance of the Dirac equation. This involves

<sup>37</sup> Interesting pictorial representations of the probability density  $\psi^* \psi$  for the hydrogenic atom are given by H. E. White, *Phys. Rev.* **38**, 513 (1931), with a comparison with the classical orbit model with vector coupling of **L** and **S**.

specifically the study of its behavior under the group of Lorentz transformations.<sup>38</sup>

<sup>38</sup> J. von Neumann, *Zeits. f. Physik* **48**, 868 (1928). F. Möglich, *Zeits. f. Physik* **48**, 852 (1928). C. G. Darwin, *Proc. Roy. Soc.* **A118**, 654 (1928). W. Pauli, *Handbuch der Physik*, Vol. 24, p. 222 gives an interesting discussion based on the infinitesimal elements of the Lorentz group. For a different approach cf. A. S. Eddington, *Relativity Theory of Protons and Electrons* (Cambridge, 1936).



In the special theory of relativity,<sup>39</sup> one considers two observers, moving with constant velocity with respect to each other, each describing his observations on the physical world by the use of his appropriate set of space and time variables. If we designate the coordinates of the two observers by

$$\begin{aligned} x_1 = x, \quad x_2 = y, \quad x_3 = z, \quad x_4 = ict, \\ x_1' = x', \quad x_2' = y', \quad x_3' = z', \quad x_4' = ict', \end{aligned}$$

respectively, then, according to the relativity theory these sets of variables will be related by equations of the form

$$x_k' = \sum_{l=1}^4 \omega_{kl} x_l, \quad k = 1, 2, 3, 4, \quad (100)$$

where the  $\omega_{kl}$  are constants.

By reason of the physical interpretation of the transformations ( $x_4$  pure imaginary!!) the following restrictions are imposed on the coefficients  $\omega_{kl}$ :

$$\sum_{l=1}^4 \omega_{lk} \omega_{lj} = \sum_{l=1}^4 \omega_{kl} \omega_{jl} = \delta_{kj}, \quad (A)$$

$$\omega_{jk} \begin{cases} \text{is real if neither } j \text{ nor } k \text{ is equal to } 4, \\ \text{is pure imaginary if } j=4, k=1, 2, 3 \text{ or} \\ \text{if } k=4, j=1, 2, 3, \end{cases} \quad (B)$$

$$\omega_{j4} = \omega_{4j}^*, \quad j = 1, 2, 3, \quad (C)$$

$$\omega_{44} \text{ is real and } > 0. \quad (D)$$

By making use of Eqs. (A) the inverse transformation is found to be

$$x_k = \sum_{l=1}^4 \omega_{lk} x_l'.$$

For the purposes of this section Eq. (58) gives the most useful form of the Dirac equation

$$\left( \sum_{k=1}^4 \beta_k \Pi_k + im_0 c \right) \psi = 0. \quad (101)$$

In analyzing the behavior of this equation and its solutions under the Lorentz transformations (100) we shall follow closely the general line of

<sup>39</sup> R. C. Tolman, *Relativity, Thermodynamics, and Cosmology* (Oxford University Press, 1934). R. Becker, *Theorie der Elektrizität, Band II: Elektronentheorie* (Teubner, 1933). A. S. Eddington, *The Mathematical Theory of Relativity*, second edition (Cambridge, 1924).

reasoning used in §8 for the Pauli theory. Consider an electron moving in an electromagnetic field, its condition being "observed" by two observers moving with constant velocity with respect to each other, and whose coordinates are related by a particular transformation included under (100).

We shall assume that the behavior of the electron will be describable by each of the observers in terms of wave functions which are solutions of the form (60) for each of the observers. If  $\psi$  and  $\psi'$  are these solutions,  $\psi$  satisfies the differential equation (101) while  $\psi'$  satisfies the equation

$$\left( \sum_{k=1}^4 \beta_k' \Pi_k' + im_0 c \right) \psi' = 0, \quad (102)$$

respectively. Here

$$\Pi_k' = -i\hbar(\partial/\partial x_k') - (\epsilon/c)A_k'.$$

In relating the operators  $\Pi_k'$  and  $\Pi_l$  we have

$$\begin{aligned} -i\hbar \frac{\partial}{\partial x_l'} &= -i\hbar \left( \frac{\partial x_1}{\partial x_l'} \frac{\partial}{\partial x_1} + \frac{\partial x_2}{\partial x_l'} \frac{\partial}{\partial x_2} \right. \\ &\quad \left. + \frac{\partial x_3}{\partial x_l'} \frac{\partial}{\partial x_3} + \frac{\partial x_4}{\partial x_l'} \frac{\partial}{\partial x_4} \right) \\ &= -i\hbar \sum_{k=1}^4 \omega_{lk} \frac{\partial}{\partial x_k}. \end{aligned}$$

The vector potential transforms like a 4-vector in the same manner, so that finally

$$\Pi_l' = \sum_{k=1}^4 \omega_{lk} \Pi_k. \quad (103)$$

An inspection of the operators in Eqs. (101) and (102) shows that these conditions are compatible, and that the Dirac equations for the two observers will have the same formal construction if we set

$$\beta_l' = \sum_{m=1}^4 \omega_{lm} \beta_m, \quad (104)$$

$$\psi' = \psi. \quad (105)$$

These two relations will be adopted as the basis of our calculations. The first requires that the four operators  $\beta_1', \dots, \beta_4'$  in the primed

axes be related to their analogs  $\beta_1, \dots, \beta_4$  in the unprimed axes like the components of a 4 vector. Eqs. (104), (105) are directly analogous to our considerations of §8 on the transformation of the Pauli spin operators under a rotation of the ordinary 3-dimensional coordinate axes.

For the Dirac wave functions in the two sets of axes we write

$$\begin{aligned}\psi &= \chi_1 \mathbf{a}_1 + \chi_2 \mathbf{a}_2 + \chi_3 \mathbf{a}_3 + \chi_4 \mathbf{a}_4, \\ \psi' &= \chi_1' \mathbf{a}_1' + \chi_2' \mathbf{a}_2' + \chi_3' \mathbf{a}_3' + \chi_4' \mathbf{a}_4'.\end{aligned}\quad (106)$$

The analysis of §8 can now be carried over directly. We seek an operator  $U$  such that

$$\mathbf{a}_k' = U \mathbf{a}_k, \quad k = 1, 2, 3, 4.$$

We suppose that  $\beta_1', \dots, \beta_4'$  are to have exactly the same properties as operators on  $\mathbf{a}_1', \dots, \mathbf{a}_4'$  that  $\beta_1, \dots, \beta_4$  have as operators on  $\mathbf{a}_1, \dots, \mathbf{a}_4$  so that

$$\beta_k' \mathbf{a}_l' = \sum_{m=1}^4 \mathbf{a}_m' (m | \beta_k | l)$$

or

$$\beta_k' U \mathbf{a}_l = U \sum_{m=1}^4 \mathbf{a}_m (m | \beta_k | l) = U \beta_k \mathbf{a}_l,$$

from which follows the operator relation

$$\beta_k' U = U \beta_k, \quad (107)$$

where  $\beta_k'$  is given by Eq. (104).

For the explicit determination of  $U$  we can generalize the method of §8. The 16 matrices of §12 have the property that an arbitrary matrix of four rows and four columns can be written as a linear sum in terms of them. This leads to the general expression<sup>40</sup>

$$\begin{aligned}U &= u_1 \beta_1 + u_2 \beta_2 + u_3 \beta_3 + u_4 \beta_4 + u_5 i \beta_1 \beta_4 \\ &+ u_6 i \beta_2 \beta_4 + u_7 i \beta_3 \beta_4 + u_8 i \beta_2 \beta_3 + u_9 i \beta_3 \beta_1 \\ &+ u_{10} i \beta_1 \beta_2 + u_{11} i \beta_1 \beta_2 \beta_3 + u_{12} i \beta_2 \beta_3 \beta_4 \\ &+ u_{13} i \beta_3 \beta_1 \beta_4 + u_{14} i \beta_1 \beta_2 \beta_4 \\ &+ u_{15} \beta_1 \beta_2 \beta_3 \beta_4 + u_{16} I, \quad (108)\end{aligned}$$

where  $u_1, \dots, u_{16}$  are ordinary complex quantities. If desired, this expression can be worked out in terms of the  $\alpha$ 's from Eqs. (57).

<sup>40</sup> Cf. especially W. Pauli, *Zeeman Verhandelingen* (Nijhoff, 1935), p. 31. Eddington, reference 38, Chaps. 2 and 3.

The problem now reduces to the determination of the coefficients  $u_1, \dots, u_{16}$  from Eqs. (107). The analysis can be carried out in a manner exactly analogous to that of the determination of the transformation function of the Pauli theory.

One point of considerable importance must be noted here. In the discussion of the Pauli theory (§8) it was assumed that the operator  $U$  was unitary, i.e.<sup>29</sup>

$$U^\dagger = U^{-1}.$$

This condition can be preserved in the relativistic theory only for the sub-group of rotations in ordinary space. The Lorentz transformations involving transformations between systems in relative motion lead to nonunitary values for  $U$  (cf. below for a special Lorentz transformation). This has as a consequence the circumstance that the *complex conjugate* wave function

$$\psi^* = \chi_1^* \bar{\mathbf{a}}_1 + \chi_2^* \bar{\mathbf{a}}_2 + \chi_3^* \bar{\mathbf{a}}_3 + \chi_4^* \bar{\mathbf{a}}_4$$

has rather awkward transformation properties. This is implied in the notation that  $\bar{\mathbf{a}}_k$  is *not* to be treated as the complex conjugate of  $\mathbf{a}_k$ . This is possible in general only when  $U$  is unitary, as it is for space relations. In order to develop the symbolic theory in a simple fashion, it would be necessary to introduce another type of wave function

$$\Phi = \nu_1 \bar{\mathbf{a}}_1 + \nu_2 \bar{\mathbf{a}}_2 + \nu_3 \bar{\mathbf{a}}_3 + \nu_4 \bar{\mathbf{a}}_4,$$

where the functions  $\nu_1, \dots, \nu_4$  are not simply the complex conjugates of  $\chi_1, \dots, \chi_4$ . The transformation of  $\chi_1^*, \dots, \chi_4^*$  is found below to be

$$\chi_k'^* = \sum_{l=1}^4 (k | U^{-1} | l)^* \chi_l^*,$$

whereas the  $\nu$ 's would be required to transform like

$$\nu_k' = \sum_{l=1}^4 \nu_l (l | U | k).$$

These expressions agree if  $U$  is unitary.

Even if  $U$  is not unitary, it will be found that

$$\Phi' = \Phi \quad \text{and} \quad \psi' = \psi,$$

while

$$\psi'^* \neq \psi^*.$$

Because of the special characteristics of the operator  $U$  for the Lorentz transformation group, it is possible to take for the conjugate function

$$\Phi = i \beta_4 \psi^*,$$

from which

$$\nu_1 = i \chi_1^*, \quad \nu_2 = i \chi_2^*, \quad \nu_3 = -i \chi_3^*, \quad \nu_4 = -i \chi_4^*.$$

The detailed proof can be given most readily by the spinor formulation of the theory. In a more formal way it can be seen from the fact that

$$\Phi \psi = i (|\chi_1|^2 + |\chi_2|^2 - |\chi_3|^2 - |\chi_4|^2)$$

is invariant under Lorentz transformations. (Table I.)<sup>40a</sup>

<sup>40a</sup> Cf. Pauli, *Handbuch der Physik*, Vol. 24, p. 220 *et seq.* A. S. Eddington, *Relativity Theory of Protons and Electrons* (Cambridge, 1936), Chap. 6.

The transformation equations for the  $\chi$ 's can be determined from Eqs. (105) and (106). We have

$$\begin{aligned} \mathbf{a}_k' &= U\mathbf{a}_k = \sum_{l=1}^4 \mathbf{a}_l(l|U|k); \\ \therefore \Psi' &= \sum_{k=1}^4 \chi_k' \mathbf{a}_k' = \sum_{k=1}^4 \sum_{l=1}^4 \chi_k' \mathbf{a}_l(l|U|k), \\ \Psi &= \sum_{l=1}^4 \chi_l \mathbf{a}_l. \end{aligned}$$

By comparison of coefficients

$$\chi_l = \sum_{k=1}^4 (l|U|k) \chi_k'. \quad (109)$$

Since  $U$  now is not unitary in general, we must use its reciprocal explicitly in the inversion of these relations. The result is:

$$\chi_k' = \sum_{l=1}^4 (k|U^{-1}|l) \chi_l. \quad (110)$$

These equations are the direct analogs of Eqs. (46) and (47) of §8.

The determination of the form of  $U$  for the most general Lorentz transformation is a matter of some complexity. We tabulate the results below for the general space rotation, and for the customary special Lorentz transformations (cf. Appendix E). For further discussion see Appendix H.

#### General rotation in space (cf. §8)

$$\begin{aligned} U(\{\xi, \eta, \zeta\}) &= (i \sin \frac{1}{2} \xi \cos \frac{1}{2}(\eta - \zeta)) i \beta_2 \beta_3 \\ &+ (i \sin \frac{1}{2} \xi \sin \frac{1}{2}(\eta - \zeta)) i \beta_3 \beta_1 \\ &+ (i \cos \frac{1}{2} \xi \sin \frac{1}{2}(\eta + \zeta)) i \beta_1 \beta_2 \\ &+ (\cos \frac{1}{2} \xi \cos \frac{1}{2}(\eta + \zeta)) I. \quad (111) \end{aligned}$$

The relationship of this transformation function to the transformation function of the Pauli theory is at once obvious. The reader will find it instructive to write out the matrix of this function and compare it with (44).

This operator is unitary, so that

$$U = U^\dagger.$$

The transformation of the  $\chi$ 's is

$$\begin{aligned} \chi_1' &= \cos \frac{1}{2} \xi \cdot e^{i\frac{1}{2}(\eta+\zeta)} \cdot \chi_1 + i \sin \frac{1}{2} \xi \cdot e^{-i\frac{1}{2}(\eta-\zeta)} \cdot \chi_2, \\ \chi_2' &= i \sin \frac{1}{2} \xi \cdot e^{i\frac{1}{2}(\eta-\zeta)} \cdot \chi_1 + \cos \frac{1}{2} \xi \cdot e^{-i\frac{1}{2}(\eta+\zeta)} \cdot \chi_2, \\ \chi_3' &= \cos \frac{1}{2} \xi \cdot e^{i\frac{1}{2}(\eta+\zeta)} \cdot \chi_3 + i \sin \frac{1}{2} \xi \cdot e^{-i\frac{1}{2}(\eta-\zeta)} \cdot \chi_4, \\ \chi_4' &= i \sin \frac{1}{2} \xi \cdot e^{i\frac{1}{2}(\eta-\zeta)} \cdot \chi_3 + \cos \frac{1}{2} \xi \cdot e^{-i\frac{1}{2}(\eta+\zeta)} \cdot \chi_4. \end{aligned} \quad (112)$$

#### Special Lorentz transformation

We consider only the special transformation

$$\begin{aligned} x' &= \frac{x - \beta ct}{(1 - \beta^2)^{\frac{1}{2}}}, \quad y' = y, \quad z' = z, \quad t' = \frac{t - \beta x/c}{(1 - \beta^2)^{\frac{1}{2}}}, \\ \beta &= v/c. \end{aligned}$$

Let

$$\cosh \vartheta = (1 - \beta^2)^{-\frac{1}{2}}, \quad \sinh \vartheta = \beta(1 - \beta^2)^{-\frac{1}{2}}.$$

The transformation function is (Appendix E)

$$U = (-\sinh \frac{1}{2} \vartheta) i \beta_1 \beta_4 + (\cosh \frac{1}{2} \vartheta) I \quad (113)$$

with the reciprocal.

$$U^{-1} = (\sinh \frac{1}{2} \vartheta) i \beta_1 \beta_4 + (\cosh \frac{1}{2} \vartheta) I. \quad (114)$$

From Eq. (110)

$$\begin{aligned} \chi_1' &= \cosh \frac{1}{2} \vartheta \cdot \chi_1 + \sinh \frac{1}{2} \vartheta \cdot \chi_4, \\ \chi_2' &= \cosh \frac{1}{2} \vartheta \cdot \chi_2 + \sinh \frac{1}{2} \vartheta \cdot \chi_3, \\ \chi_3' &= \cosh \frac{1}{2} \vartheta \cdot \chi_3 + \sinh \frac{1}{2} \vartheta \cdot \chi_2, \\ \chi_4' &= \cosh \frac{1}{2} \vartheta \cdot \chi_4 + \sinh \frac{1}{2} \vartheta \cdot \chi_1. \end{aligned} \quad (115)$$

The reader may be interested to note the characteristics of the function  $U$  with respect to inverse transformations. For example the transformation operator for a rotation about the  $x$  axis through an angle  $\xi$  in the positive sense is

$$(i \sin \frac{1}{2} \xi) i \beta_2 \beta_3 + (\cos \frac{1}{2} \xi) I.$$

The inverse transformation is that which *returns* the axes to their original position, by a rotation through the angle  $-\xi$ . It should then be

$$(-i \sin \frac{1}{2} \xi) i \beta_2' \beta_3' + (\cos \frac{1}{2} \xi) I,$$

where  $\beta_2'$  and  $\beta_3'$  are the appropriate operators *in the rotated system*. But from the equations

$$\beta_2' = \beta_2 \cos \xi + \beta_3 \sin \xi, \quad \beta_3' = -\beta_2 \sin \xi + \beta_3 \cos \xi,$$

it is found at once that

$$i \beta_2' \beta_3' = i \beta_2 \beta_3.$$

A similar analysis for the special Lorentz transformation given above shows that

$$i\beta_1'\beta_4' = i\beta_1\beta_4,$$

so that the transformation operator satisfies the rule that it is changed into its reciprocal by replacing  $v/c$  by  $-v/c$ .

#### §19. THE BEHAVIOR OF THE DIRAC WAVE FUNCTIONS UNDER GAUGE TRANSFORMATIONS

It has been emphasized by Weyl<sup>41</sup> that there is a type of invariance of the equations of electrodynamics which is of importance for theoretical considerations. The equations connecting the field vectors and the scalar and vector potentials in an electromagnetic field are

$$\mathbf{H} = \text{curl } \mathbf{A}, \quad \mathbf{E} = -\text{grad } \phi - (1/c)(\partial\mathbf{A}/\partial t) \quad (116)$$

with a connecting equation between  $\mathbf{A}$  and  $\phi$

$$\text{div } \mathbf{A} + (1/c)(\partial\phi/\partial t) = 0. \quad (117)$$

The substitution

$$\mathbf{A} = \mathbf{A} + \text{grad } \omega, \quad \phi = \phi - (1/c)(\partial\omega/\partial t), \quad (118)$$

where  $\omega$  is any function for which

$$[\nabla^2 - (1/c^2)(\partial^2/\partial t^2)]\omega = 0 \quad (119)$$

will lead to the same field strengths. This is called a gauge transformation.

We consider the fields, and not the potentials, as the quantities of physical importance, so that we are led to examine the characteristics of the Dirac equation under this transformation.

In 4-vector notation

$$\mathbf{A}_1 = \mathbf{A}_1 + (\partial\omega/\partial x_1), \quad \dots, \quad \mathbf{A}_4 = i\phi = \mathbf{A}_4 + (\partial\omega/\partial x_4).$$

The wave equation in the form (58) becomes

$$\left[ \sum_{k=1}^4 \beta_k \left( -i\hbar \frac{\partial}{\partial x_k} - \frac{\epsilon}{c} A_k \right) + im_0c - \sum_{k=1}^4 \beta_k \frac{\partial \omega}{\partial x_k} \right] \psi = 0.$$

The transformation

$$\psi' = e^{(i/\hbar)(\epsilon/c)\omega} \cdot \psi \quad (120)$$

is easily seen to restore the equation to its original form.

<sup>41</sup> H. Weyl, *The Theory of Groups and Quantum Mechanics*, chap. IV, §6; Proc. Nat. Acad. Sci. 15, 323 (1929). V. Fock, Zeits. f. Physik 57, 261 (1929).

#### §20. THE BEHAVIOR OF THE DIRAC OPERATORS AND WAVE FUNCTIONS UNDER REFLECTIONS

It is interesting, and for some purposes important, to examine the properties of the Dirac equation with respect to various reflections.<sup>42</sup> We shall consider the inversion (§9)

$$R_0: x \rightarrow -x, \quad y \rightarrow -y, \quad z \rightarrow -z, \quad t \rightarrow t \quad (121)$$

and the "time reversal"

$$R_t: x \rightarrow x, \quad y \rightarrow y, \quad z \rightarrow z, \quad t \rightarrow -t. \quad (122)$$

The Maxwell field equations for the scalar and vector potentials are

$$\text{div } \mathbf{A} + (1/c)(\partial\phi/\partial t) = 0;$$

$$[\nabla^2 - (1/c^2)(\partial^2/\partial t^2)]\mathbf{A} = -4\pi\mathbf{j}/c;$$

$$[\nabla^2 - (1/c^2)(\partial^2/\partial t^2)]\phi = -4\pi\rho,$$

where  $\rho$  and  $\mathbf{j}$  are the ordinary charge and current densities of electrodynamics. In view of their physical interpretation  $\rho$  and  $\mathbf{j}$  undergo the transformation<sup>43</sup>

$$\rho \rightarrow \rho, \quad \mathbf{j} \rightarrow -\mathbf{j}$$

under either of the reflections  $R_0, R_t$ , so that the potentials undergo the transformation

$$\phi \rightarrow +\phi, \quad \mathbf{A} \rightarrow -\mathbf{A}. \quad (123)$$

Under the space inversion  $R_0: \Pi_k \rightarrow -\Pi_k, k=1, 2, 3$ . An inspection shows that Eqs. (64) will be invariant in form under  $R_0$  if the  $\chi$ 's undergo the transformation:

$$R_0: \chi_1 \rightarrow \chi_1, \quad \chi_2 \rightarrow \chi_2, \quad \chi_3 \rightarrow -\chi_3, \quad \chi_4 \rightarrow -\chi_4. \quad (124)$$

This is just the transformation which would be induced by the operator

$$U(R_0) = \beta_4.$$

A consideration of the equation

$$\beta_k' U = U \beta_k$$

shows that the same result could have been obtained by postulating that the  $\beta$ 's transforms under  $R_0$  like the four quantities  $(x, y, z, ict)$ .

<sup>42</sup> Weyl, reference 41.

<sup>43</sup> It must be recalled that  $\rho$  and  $\mathbf{j}$  are *density* expressions, so that  $\rho|\Delta x \Delta y \Delta z|$  measures the amount of charge in  $\Delta x \Delta y \Delta z$ . In classical electromagnetic theory  $\mathbf{j}$  is expressible as  $\rho \mathbf{v}$  where  $\mathbf{v}$  is the velocity of the charge at the point considered. For more general considerations cf. Eddington, *The Mathematical Theory of Relativity*, second edition, §49.

In working out the transformation properties under the "time reversal"  $R_t$  we must proceed a little more cautiously. It is observed first that:

$$\begin{aligned}\Pi_k &= (-i\hbar\partial/\partial x_k - \epsilon A_k/c) \\ \rightarrow (-i\hbar\partial/\partial x_k + \epsilon A_k/c) &= -\Pi_k^*, \quad k=1, 2, 3, \quad (125) \\ \Pi_+ \rightarrow -(\Pi_1^* + i\Pi_2^*) &= -\Pi_-^*, \\ \Pi_- \rightarrow -(\Pi_1^* - i\Pi_2^*) &= -\Pi_+^*.\end{aligned}$$

On substituting these expressions in Eqs. (64) and at the same time replacing  $t$  by  $-t$ , we see that the equations will be changed into their complex conjugates if we make the substitution

$$R_t: \quad \chi_1 \rightarrow \chi_2^*, \quad \chi_2 \rightarrow -\chi_1^*, \\ \chi_3 \rightarrow \chi_4^*, \quad \chi_4 \rightarrow -\chi_3^*. \quad (126)$$

These results may be exhibited on the wave functions for the free particle (§15). A simple inspection shows that the transformations (124, 126) both change the wave functions representing a particle with linear momentum  $\mathbf{p}$  into functions representing the particle with momentum  $-\mathbf{p}$ .

Dirac<sup>44</sup> has pointed out another type of transformation which emphasizes strikingly the importance of the negative energy solutions. This "Dirac transformation" is

$$R_D: \quad \epsilon \rightarrow -\epsilon.$$

The electromagnetic potentials and the coordinates  $(x, y, z, t)$  are left unchanged. The operators  $\Pi_k$  again transform by Eqs. (125), and we find that the Dirac equations (64) transform into their complex conjugates with the substitution

$$R_D: \quad \chi_1 \rightarrow \chi_4^*, \quad \chi_2 \rightarrow -\chi_3^*, \\ \chi_3 \rightarrow -\chi_2^*, \quad \chi_4 \rightarrow \chi_1^*. \quad (127)$$

But this transformation interchanges the roles of the "small" and "big" components of  $\psi$ , and in fact, changes a negative energy solution into a positive energy solution. A negative energy solution for a particle of charge  $\epsilon$  in a given external electromagnetic field is equivalent to a positive energy solution of a particle of charge  $-\epsilon$  moving in the same external field. This observation leads directly to Dirac's theory of the positron (§23).

<sup>44</sup> P. A. M. Dirac, *Quantum Mechanics*, second edition, p. 270.

## §21. THE PHYSICAL INTERPRETATION OF THE DIRAC THEORY

The physical interpretation of the Dirac theory is based primarily on the characteristics of various expressions which are made up by suitable combinations of the four functions  $\chi_1, \chi_2, \chi_3, \chi_4$  and their complex conjugates. In working out the properties of these expressions we must lean heavily on the study of their mathematical transformation properties under Lorentz transformations.

In §14 we saw that the charge and current density expressions for the Dirac equation are

$$\rho = \psi^*(\epsilon I)\psi, \quad \mathbf{j} = \psi^*(-\epsilon c\boldsymbol{\alpha})\psi.$$

We have already remarked on the interpretation suggested by Breit, that the operators

$$-c\alpha_1, \quad -c\alpha_2, \quad -c\alpha_3$$

represent the components of *velocity* of the electron.

The requirement of invariance of the equation of continuity

$$\partial\rho/\partial t + \text{div } \mathbf{j} = 0$$

under Lorentz transformations implies that the four quantities

$$j_1 = j_x, \quad j_2 = j_y, \quad j_3 = j_z, \quad j_4 = ic\rho$$

transform as the components of a 4 vector; i.e. by the same expression (100) as the coordinates

$$j_k' = \sum_{l=1}^4 \omega_{kl} j_l, \quad k=1, 2, 3, 4.$$

The direct verification of this formula for the special transformations given in the preceding section may be left to the reader.

In developing this idea further, it will be instructive to study specifically the free particle, for which the wave functions are given in §15. Let us consider first the derivation of the Einstein mass-energy relation.

We adopt Breit's interpretation and compute the average values of the velocity components by the relation

$$\mathbf{v}_A = \psi^*(-c\boldsymbol{\alpha})\psi/\psi^*\psi.$$

From Eqs. (71, 72) we find for

$$E = E_+$$

$$(\mathbf{v}^+)_A = \mathbf{p} \cdot (c^2/E_+);$$

$$E = E_-$$

$$(\mathbf{v}^-)_A = \mathbf{p} \cdot (c^2/E_-).$$

(128)

The (average) velocity and the momentum vectors are oppositely directed to each other in the negative energy states.

These relations can be summarized in the equations

$$(v_k^\pm)_{Av} = (\partial E_\pm / \partial p_k).$$

If we define

$$(\beta_{Av})^2 = (v^\pm)_{Av}^2 / c^2$$

we get the relations<sup>45</sup>

$$E_\pm = \pm m_0 c^2 (1 - \beta_{Av}^2)^{-1/2}, \quad (129)$$

which is the formulation of the Einstein mass-energy relation in the present theory. This gives us

$$\mathbf{p} = \pm m_0 (1 - \beta_{Av}^2)^{-1/2} (\mathbf{v}^\pm)_{Av} \quad (130)$$

as the exact relation between the momentum and the velocity.

Since the characteristic values of the velocity operators  $-\alpha_1, -\alpha_2, -\alpha_3$  are all  $\pm c$ , one must consider that a single "instantaneous" measurement of any component of velocity of the electron would yield either  $+c$  or  $-c$ . This would seem to be in paradoxical contradiction to the consideration of relativity theory that for a particle having a finite rest mass, the proper mass should become indefinitely large as the speed of the particle approaches  $c$ . The arguments given above show that the solution of the paradox lies in the fact that it is only the *average* speed (an average between  $+c$  and  $-c$ !) which appears in the Einstein mass-velocity formula.

It is interesting to resolve the paradox in another way. Suppose we consider a set of axes ( $I$ ) in which the *momentum* of the electron vanishes. By Eqs. (128) its average velocity will also vanish in this set of axes. But there are still two types of motion of the electron, represented by the wave functions

$$\begin{aligned} (\psi_+)_{II} &= (A\mathbf{a}_3 + B\mathbf{a}_4) e^{-(i/\hbar)m_0 c^2 t}, \\ (\psi_-)_{II} &= (C\mathbf{a}_1 + D\mathbf{a}_2) e^{(i/\hbar)m_0 c^2 t}, \end{aligned}$$

where  $A, B, C, D$  are constants (cf. Eqs. (71, 72)).

We can now introduce a set of axes ( $II$ ) associated with an "observer" moving with a speed  $-v$  along the  $x$  direction, for whom the original reference system is moving along the  $x$  direction with speed  $+v$ . The wave functions for the electron can now be found from the transformation equations of Eq. (115), by using  $\beta = -v/c$ . A simple calculation leads to the result<sup>46</sup>

$$\begin{aligned} (\psi_+)_{II} &= [(c/E_+ + m_0 c^2)(-p_1' B' \mathbf{a}_1' - p_1' A' \mathbf{a}_2') \\ &\quad + A' \mathbf{a}_3' + B' \mathbf{a}_4'] e^{(i/\hbar)(p_1' x' - E_+ t')}, \\ (\psi_-)_{II} &= [C' \mathbf{a}_1' + D' \mathbf{a}_2' + (c/E_- - m_0 c^2) \\ &\quad \times (p_1' C' \mathbf{a}_3' + p_1' D' \mathbf{a}_4')] e^{(i/\hbar)(-p_1' x' - E_- t')}, \end{aligned}$$

where

$$p_1' = m_0 c \beta (1 - \beta^2)^{-1/2}; \quad E_\pm = \pm m_0 c^2 (1 - \beta^2)^{-1/2}.$$

On referring to Eqs. (71, 72) of §15 we see that  $(\psi_+)_{II}$  represents the particle having momentum  $p_1'$  in the  $x'$

direction and energy  $E_+ > m_0 c^2$ ; while  $(\psi_-)_{II}$  represents it having momentum  $-p_1'$  in the  $x'$  direction and energy  $E_- < -m_0 c^2$ .

The "velocity"  $v$  enters here as a kinematical, rather than as a dynamical quantity, since it involves only the relative speed of two "observers." This shows in detail how the Einstein mass-energy relation is preserved, and how the reversed relation between momentum and velocity for the "negative energy" states arises automatically in the application of a Lorentz transformation.

The expression for the current density can be thrown into a form which will bring out more clearly its connection with the Schrödinger theory.<sup>47</sup>

From Eq. (58) we can write the Dirac equation as

$$\begin{aligned} \psi &= \frac{i}{m_0 c} \sum_{l=1}^4 \beta_l \Pi_l \psi, \\ \psi^* &= -\frac{i}{m_0 c} \sum_{l=1}^4 \beta_l^* \Pi_l^* \psi^*. \end{aligned}$$

The components of the current density can now be put in the form

$$\begin{aligned} j_k &= i e c \psi^* \beta_4 \beta_k \psi \\ &= \frac{e}{2m_0} \sum_{l=1}^4 [(\beta_l^* \Pi_l^* \psi^*)(\beta_4 \beta_k \psi) - \psi^* (\beta_4 \beta_k \beta_l \Pi_l \psi)]. \end{aligned}$$

By a little manipulation<sup>48</sup> this can be written as

$$j_k = \frac{e}{2m_0} \sum_{l=1}^4 [(\Pi_l^* \psi^*)(\beta_l \beta_4 \beta_k \psi) - \psi^* (\Pi_l \beta_4 \beta_k \beta_l \psi)]. \quad (131)$$

Let us separate out the term for which  $l=k$ , by writing

$$j_k = j_k^{(0)} + j_k^{(1)}$$

with

$$j_k^{(0)} = -\frac{e}{2m_0} [\psi^* (\Pi_k \beta_4 \psi) + (\Pi_l^* \psi^*)(\beta_4 \psi)], \quad (132)$$

$$\begin{aligned} j_k^{(1)} &= -\frac{e}{2m_0} \sum_{l \neq k} [\psi^* (\Pi_l \beta_4 \beta_k \beta_l \psi) \\ &\quad - (\Pi_l^* \psi^*)(\beta_l \beta_4 \beta_k \psi)]. \quad (133) \end{aligned}$$

<sup>45</sup> This is obtained by substituting for  $p^2$  in Eq. (70) from Eqs. (128).

<sup>46</sup> These equations have been reduced to the standard form of §15 by writing

$$A' = A \cosh \vartheta, \quad B' = B \cosh \vartheta.$$

<sup>47</sup> W. Gordon, Zeits. f. Physik 50, 630 (1927). W. Pauli, *Handbuch der Physik*, second edition, Vol. 24, p. 238.

<sup>48</sup> Note that here the  $\beta$ 's are allowed to operate on the  $\mathbf{a}$ 's by the same formal rules as on the  $\mathbf{a}$ 's. It follows that  $(\beta^* \mathbf{a}_k) \mathbf{a}_n = \mathbf{a}_k \beta \mathbf{a}_n = (k|\beta|n)$ .

On writing out  $j_k^{(0)}$  we find

$$\begin{aligned} \mathbf{j}^{(0)} = & -\frac{i\epsilon\hbar}{2m_0}[-\chi_1^*\nabla\chi_1 - \chi_2^*\nabla\chi_2 + \chi_3^*\nabla\chi_3 \\ & + \chi_4^*\nabla\chi_4 + \chi_1\nabla\chi_1^* + \chi_2\nabla\chi_2^* - \chi_3\nabla\chi_3^* - \chi_4\nabla\chi_4^*] \\ & + \frac{\epsilon^2}{m_0c}\mathbf{A}[|\chi_1|^2 + |\chi_2|^2 - |\chi_3|^2 - |\chi_4|^2]. \quad (134) \end{aligned}$$

The terms in the "large" components  $\chi_3$  and  $\chi_4$  give just the usual form for the current vector in the Schrödinger theory. The remaining terms in the "small" components  $\chi_1$  and  $\chi_2$  are of the same form, but have reversed signs. This reversal of sign is due to the presence of the operator  $\beta_4$  in (131).

If the expression for  $\mathbf{j}^{(1)}$  is written out in detail for each component, it will be found to give the following contributions to the charge density, and the three-dimensional current density:

$$\begin{aligned} \rho^{(1)} &= -\text{div}(\psi^*\mathbf{P}\psi), \\ \mathbf{j}^{(1)} &= c \text{curl}(\psi^*\mathbf{M}\psi) + (\partial/\partial t)(\psi^*\mathbf{P}\psi), \quad (135) \end{aligned}$$

where the vector operators  $\mathbf{P}$  and  $\mathbf{M}$  are defined by their components

$$\begin{aligned} P_x &= \frac{\epsilon\hbar}{2m_0c} \cdot i\alpha_1\alpha_4, & P_y &= \frac{\epsilon\hbar}{2m_0c} i\alpha_2\alpha_4, & P_z &= \frac{\epsilon\hbar}{2m_0c} i\alpha_3\alpha_4, \\ M_x &= \frac{\epsilon\hbar}{2m_0c} i\alpha_2\alpha_3\alpha_4, & M_y &= \frac{\epsilon\hbar}{2m_0c} i\alpha_3\alpha_1\alpha_4, & M_z &= \frac{\epsilon\hbar}{2m_0c} i\alpha_1\alpha_2\alpha_4. \end{aligned}$$

These equations are exactly of the type ordinarily introduced in macroscopic electromagnetic theory<sup>49</sup> for the study of the "effective" charge and current densities due to an electrical polarization (electrical moment per unit volume)  $\mathbf{P}$ , and a magnetic polarization  $\mathbf{M}$ . Having this analogy in mind, one is led to interpret  $\mathbf{P}$  and  $\mathbf{M}$  as the operators representing the electric and the magnetic polarizations.

Although the basis of these expressions in classical electromagnetic theory is entirely differ-

ent from their interpretation in the present theory, the mathematical analogy is still sufficiently close to bring out the interpretation of the polarization vectors as arising from these added terms in the Dirac current density expressions.<sup>50</sup> The procedure is actually just the reverse of the classical theory, in which the polarizations  $\mathbf{P}$  and  $\mathbf{M}$  are introduced *a priori*, and are then replaced by effective charges and currents.

The relativistic transformation properties of the density expressions for the electric and the magnetic moment require also that the operators be of the above form, and give definite indication that the magnetic moment operators are not numerical multiples of the spin operators. Instead

$$\mathbf{M}_x = -(\epsilon/m_0c)\mathbf{S}_x\alpha_4.$$

It will be seen in the next section that this association is intimately related to the existence of the negative energy solutions of the Dirac equation.

We give in Table II a tabulation of the 16 operators of §12 with their transformation properties. This table is based on one given by de Broglie,<sup>51</sup> which we have amplified by giving the transformation properties of the various density expressions under the "reflection" operations  $R_0, R_i, R_D$ . A - or + indicates that the expression does, or does not, change its sign under the reflection.

The spin 4 vector  $(S_x, S_y, S_z, S_4)$  and the operator  $\alpha_1\alpha_2\alpha_3\alpha_4$  are sometimes referred to as a *pseudo-vector* and a *pseudo-scalar*, respectively, because of their behavior under the space inversion  $R_0$ .

By inspection of this table (or of the matrices (§12)) it is seen that the "internal" states represented by the separate functions  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4$  are arranged to represent quantized (i.e., characteristic) states for the operators

$$\begin{aligned} \rho &= \epsilon I, & \Lambda &= -m_0\alpha_4, & S_z &= -\frac{1}{2}\hbar \cdot i\alpha_1\alpha_2, \\ & & & & M_z &= (\epsilon\hbar/2m_0c) \cdot i\alpha_1\alpha_2\alpha_4. \end{aligned}$$

We tabulate the characteristic values of these operators in Table III.

<sup>49</sup> Frenkel, *Lehrbuch der Elektrodynamik*, Vol. 2, p. 12. R. Becker, *Theorie der Elektrizität*, Vol. 2, p. 124.

<sup>50</sup> Eqs. (135) may be used to explain the behavior of  $\mathbf{M}$  and  $\mathbf{P}$  under the reflections  $R_0$  and  $R_i$ . Since  $\rho^{(1)}$  and  $\mathbf{j}^{(1)}$  transform as shown in Table I, these equations show the transformations of  $\mathbf{M}$  and  $\mathbf{P}$  to be as given.

<sup>51</sup> L. de Broglie, *L'Électron Magnétique*, p. 225.

TABLE II. Transformation properties of Dirac operators.

NAME	OPERATOR	DENSITY EXPRESSION	R <sub>0</sub> R <sub>t</sub> R <sub>D</sub>	LORENTZ TRANSFORMATIONS
"Rest Mass Operator" (?)	$\Lambda = -m_0\alpha_4$	$-m_0( \chi_1 ^2 +  \chi_2 ^2 -  \chi_3 ^2 -  \chi_4 ^2)$	+ + -	Invariant (Scalar)
Current Density	$j_x = -e c \alpha_1$ $j_y = -e c \alpha_2$ $j_z = -e c \alpha_3$	$-e c (\chi_1^* \chi_4 + \chi_2^* \chi_3 + \chi_3^* \chi_2 + \chi_4^* \chi_1)$ $-e c (-i \chi_1^* \chi_4 + i \chi_2^* \chi_3 - i \chi_3^* \chi_2 + i \chi_4^* \chi_1)$ $-e c (\chi_1^* \chi_3 - \chi_2^* \chi_4 + \chi_3^* \chi_1 - \chi_4^* \chi_2)$	- - -	4-vector $j_1 = j_x, j_2 = j_y, j_3 = j_z, j_4 = i c \rho$
Charge Density	$\rho = e I$	$e ( \chi_1 ^2 +  \chi_2 ^2 +  \chi_3 ^2 +  \chi_4 ^2)$	+ + -	
Spin Angular Momentum	$S_x = -\frac{1}{2} \hbar \cdot i \alpha_2 \alpha_3$ $S_y = -\frac{1}{2} \hbar \cdot i \alpha_3 \alpha_1$ $S_z = -\frac{1}{2} \hbar \cdot i \alpha_1 \alpha_2$ ?	$\frac{1}{2} \hbar (\chi_1^* \chi_2 + \chi_2^* \chi_1 + \chi_3^* \chi_4 + \chi_4^* \chi_3)$ $\frac{1}{2} \hbar (-i \chi_1^* \chi_2 + i \chi_2^* \chi_1 - i \chi_3^* \chi_4 + i \chi_4^* \chi_3)$ $\frac{1}{2} \hbar ( \chi_1 ^2 -  \chi_2 ^2 +  \chi_3 ^2 -  \chi_4 ^2)$ $\frac{1}{2} \hbar (-i \chi_1^* \chi_3 - i \chi_2^* \chi_4 - i \chi_3^* \chi_1 - i \chi_4^* \chi_2)$	+ - -	Completely antisymmetrical tensor of rank 3 = 4-vector (pseudo-vector) $\mathcal{E}_{231} = S_x, \mathcal{E}_{311} = S_y, \mathcal{E}_{124} = S_z, \mathcal{E}_{321} = S_4$
Magnetic Polarization	$M_x = \frac{e \hbar}{2 m_0 c} \cdot i \alpha_2 \alpha_3 \alpha_4$ $M_y = \frac{e \hbar}{2 m_0 c} \cdot i \alpha_3 \alpha_1 \alpha_4$ $M_z = \frac{e \hbar}{2 m_0 c} \cdot i \alpha_1 \alpha_2 \alpha_4$	$\frac{e \hbar}{2 m_0 c} (-\chi_1^* \chi_2 - \chi_2^* \chi_1 + \chi_3^* \chi_4 + \chi_4^* \chi_3)$ $\frac{e \hbar}{2 m_0 c} (i \chi_1^* \chi_2 - i \chi_2^* \chi_1 - i \chi_3^* \chi_4 + i \chi_4^* \chi_3)$ $\frac{e \hbar}{2 m_0 c} (- \chi_1 ^2 +  \chi_2 ^2 +  \chi_3 ^2 -  \chi_4 ^2)$	+ - -	Antisymmetrical tensor of rank 2 = 6-vector $\mu_{23} = M_x, \mu_{31} = M_y, \mu_{12} = M_z$ $\mu_{14} = i P_x, \mu_{24} = i P_y, \mu_{34} = i P_z$
Electric Polarization	$P_x = \frac{e \hbar}{2 m_0 c} \cdot i \alpha_1 \alpha_4$ $P_y = \frac{e \hbar}{2 m_0 c} \cdot i \alpha_2 \alpha_4$ $P_z = \frac{e \hbar}{2 m_0 c} \cdot i \alpha_3 \alpha_4$	$\frac{e \hbar}{2 m_0 c} (-i \chi_1^* \chi_4 - i \chi_2^* \chi_3 + i \chi_3^* \chi_2 + i \chi_4^* \chi_1)$ $\frac{e \hbar}{2 m_0 c} (-\chi_1^* \chi_4 + \chi_2^* \chi_3 + \chi_3^* \chi_2 - \chi_4^* \chi_1)$ $\frac{e \hbar}{2 m_0 c} (-i \chi_1^* \chi_3 + i \chi_2^* \chi_4 + i \chi_3^* \chi_1 - i \chi_4^* \chi_2)$	- + -	
?	$\Omega = \alpha_1 \alpha_2 \alpha_3 \alpha_4$	$(-i \chi_1^* \chi_3 - i \chi_2^* \chi_4 + i \chi_3^* \chi_1 + i \chi_4^* \chi_2)$	- - -	Invariant (pseudo-scalar).

TABLE III. Characteristic values of operators.

	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>
$\rho$	+e	+e	+e	+e
$\Lambda$	-m <sub>0</sub>	-m <sub>0</sub>	+m <sub>0</sub>	+m <sub>0</sub>
$S_x$	+ $\frac{1}{2} \hbar$	- $\frac{1}{2} \hbar$	+ $\frac{1}{2} \hbar$	- $\frac{1}{2} \hbar$
$M_x$	-e $\hbar/2m_0c$	+e $\hbar/2m_0c$	+e $\hbar/2m_0c$	-e $\hbar/2m_0c$

Since the actual wave function  $\psi$  is a linear superposition of the symbols **a**<sub>1</sub>, **a**<sub>2</sub>, **a**<sub>3</sub>, **a**<sub>4</sub> it represents a state in which the values to be assigned to these physical quantities are weighted averages of their characteristic values.

The designation of the operator  $\Lambda = -m_0\alpha_4$  as a "rest mass" operator which is due to de Broglie,<sup>52</sup> is suggested by the way in which it enters into the density expressions for **M** and **P**. We can compute the average value of the operator  $\Lambda$  from the equation,

$$(\Lambda)_{Av} = \frac{-|\chi_1|^2 - |\chi_2|^2 + |\chi_3|^2 + |\chi_4|^2}{|\chi_1|^2 + |\chi_2|^2 + |\chi_3|^2 + |\chi_4|^2}$$

<sup>52</sup> L. de Broglie, reference 51, p. 223.

With the wave function of the free particle this reduces to

$$(\Lambda^\pm)_{Av} = m_0 \cdot (m_0 c^2 / E_\pm) = m_0 [\pm (1 - \beta_{Av}^2)^{\frac{1}{2}}]$$

as  $|\mathbf{p}| \rightarrow 0 \quad (\Lambda^\pm)_{Av} \rightarrow \pm m_0$ ,

$$|\mathbf{p}| \rightarrow \infty \quad (\beta_{Av} \rightarrow 1) \quad (\Lambda^\pm)_{Av} \rightarrow 0.$$

The relation of the operator  $\Lambda$  to the nonquantum mechanical theory may be noted by introducing the "proper time"  $\tau$  (the time variable in the system of coordinates in which the electron is at "rest"). According to the arguments of the special theory of relativity

$$dt = d\tau / (1 - \beta^2)^{\frac{1}{2}},$$

from which we see that

$$|\Lambda_{Av} dt| = m_0 d\tau,$$

which is invariant under Lorentz transformations. The integral

$$\int m_0 c^2 d\tau$$

is the action integral of relativity theory.



## §22. THE REDUCTION OF THE DIRAC THEORY TO THE PAULI THEORY

In §15 it was pointed out that for

$$|p| \ll m_0c$$

two of the four Dirac  $\chi$ 's are much larger than the other two. For positive energy states  $|\chi_3^+|$ ,  $|\chi_4^+| \gg |\chi_1^+|$ ,  $|\chi_2^+|$  and for negative energy states  $|\chi_1^-|$ ,  $|\chi_2^-| \gg |\chi_3^-|$ ,  $|\chi_4^-|$ . This disparity between the pairs of functions permits the development of an approximate wave equation involving explicitly only the two large components, which can be compared directly with the Pauli theory. In order that the differing roles of the positive and negative energy states may be made more apparent, we state them separately.

### Positive energy states

Let

$$\begin{aligned}\phi_0 &= e^{(i/\hbar)m_0c^2t}(\chi_1\mathbf{a}_1 + \chi_2\mathbf{a}_2), \\ \psi_0 &= e^{(i/\hbar)m_0c^2t}(\chi_3\mathbf{a}_1 + \chi_4\mathbf{a}_2).\end{aligned}\quad (136)$$

By means of the operator  $\Omega_0 = i\alpha_1\alpha_2\alpha_3 = \beta_1\beta_2\beta_3\beta_4$  we can write the Dirac wave function as

$$\psi = e^{-(i/\hbar)m_0c^2t}(\phi_0 - \Omega_0\psi_0) \quad (137)$$

since

$$\Omega_0\mathbf{a}_1 = -\mathbf{a}_3, \quad \Omega_0\mathbf{a}_2 = -\mathbf{a}_4.$$

Further

$$\begin{aligned}i\hbar\partial\psi/\partial t &= [m_0c^2(\phi_0 - \Omega_0\psi_0) \\ &+ i\hbar(\partial\phi_0/\partial t - \Omega_0\partial\psi_0/\partial t)]e^{-(i/\hbar)m_0c^2t}.\end{aligned}$$

Substituting in the Dirac wave equation (55) we obtain

$$\begin{aligned}[-c\sum_{k=1}^3\alpha_k\Pi_k - \alpha_4m_0c^2 + \epsilon\phi](\phi_0 - \Omega_0\psi_0) \\ = m_0c^2(\phi_0 - \Omega_0\psi_0) \\ + i\hbar((\partial\phi_0/\partial t) - \Omega_0(\partial\psi_0/\partial t)).\end{aligned}\quad (138)$$

It will be convenient to introduce the operators  $\sigma_1$ ,  $\sigma_2$ ,  $\sigma_3$ , of the Pauli theory, and let them operate on  $\mathbf{a}_1$  and  $\mathbf{a}_2$  by the rules of §6. Then we have

$$\begin{aligned}\alpha_k\phi_0 &= -\Omega_0\sigma_k\phi_0, & \alpha_k\Omega_0\psi_0 &= -\sigma_k\psi_0, & k &= 1, 2, 3, \\ \alpha_4\phi_0 &= \phi_0, & \alpha_4\Omega_0\psi_0 &= -\Omega_0\psi_0.\end{aligned}\quad (139)$$

By means of these expressions we can separate the wave equation (138) into two equations

$$\begin{aligned}(2m_0c^2 + i\hbar(\partial/\partial t) - \epsilon\phi)\phi_0 + c(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})\psi_0 &= 0, \\ (i\hbar(\partial/\partial t) - \epsilon\phi)\psi_0 + c(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})\phi_0 &= 0,\end{aligned}\quad (140)$$

where we have introduced the abbreviated vector notation

$$\boldsymbol{\sigma}\cdot\boldsymbol{\Pi} = \sigma_1\Pi_1 + \sigma_2\Pi_2 + \sigma_3\Pi_3.$$

Since  $\phi_0$  is a small term we can eliminate it by successive approximations based on the first of these equations, by the expansion

$$\phi_0 = \phi_0^{(1)} + \phi_0^{(2)} + \dots,$$

where

$$\begin{aligned}\phi_0^{(1)} &= -\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\Pi}}{2m_0c}\psi_0, \\ \phi_0^{(2)} &= (1/4m_0^2c^3)(i\hbar\partial/\partial t - \epsilon\phi)(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})\psi_0, \dots\end{aligned}\quad (141)$$

We shall retain only terms as far as the second approximation.

If we substitute this expression for  $\phi_0$  in the second of Eqs. (140) we find the approximate equation for  $\psi_0$ :

$$\begin{aligned}(i\hbar\partial/\partial t - \epsilon\phi)\psi_0 &= -c(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})[-(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})/2m_0c \\ &+ (1/4m_0^2c^3)(i\hbar(\partial/\partial t) - \epsilon\phi)(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})]\psi_0.\end{aligned}\quad (142)$$

This can be reduced by writing out the operators, and introducing the expressions for the field strengths

$$\mathbf{E} = -(1/c)(\partial\mathbf{A}/\partial t) - \text{grad } \phi, \quad \mathbf{H} = \text{curl } \mathbf{A}.$$

The operators in the last term of (142) can be interchanged by use of the relation

$$\begin{aligned}(i\hbar\partial/\partial t - \epsilon\phi)(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi}) \\ = (\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})[i\hbar\partial/\partial t - \epsilon\phi] + i\epsilon\hbar(\boldsymbol{\sigma}\cdot\mathbf{E}).\end{aligned}$$

We can now rearrange the equation (142) to give

$$\begin{aligned}(i\hbar\partial/\partial t - \epsilon\phi)\psi_0 &= \\ &= -c(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})\{-\boldsymbol{\sigma}\cdot\boldsymbol{\Pi}/2m_0c \\ &+ (\boldsymbol{\sigma}\cdot\boldsymbol{\Pi}/4m_0^2c^3)[i\hbar\partial/\partial t - \epsilon\phi] \\ &+ (i\epsilon\hbar/4m_0^2c^3)(\boldsymbol{\sigma}\cdot\mathbf{E})\}\psi_0.\end{aligned}\quad (143)$$

To our degree of approximation we can replace the term  $(i\hbar\partial/\partial t - \epsilon\phi)\psi_0$  on the right-hand side by  $[(\boldsymbol{\sigma} \cdot \boldsymbol{\Pi})^2/2m_0]\psi_0$ . Further

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \boldsymbol{\Pi})^2 &= (\Pi_1^2 + \Pi_2^2 + \Pi_3^2) - (\epsilon\hbar/c)(\boldsymbol{\sigma} \cdot \mathbf{H}) \\ &= \sum_{k=1}^3 (-i\hbar\partial/\partial x_k - \epsilon A_k/c)^2 - (\epsilon\hbar/c)(\boldsymbol{\sigma} \cdot \mathbf{H}), \end{aligned} \quad (144)$$

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \boldsymbol{\Pi})(\boldsymbol{\sigma} \cdot \mathbf{E}) &= (\sigma_1\Pi_1 + \sigma_2\Pi_2 + \sigma_3\Pi_3)(\sigma_1E_x + \sigma_2E_y + \sigma_3E_z) \\ &= (\Pi_1E_x + \Pi_2E_y + \Pi_3E_z) + \sigma_1\sigma_2(\Pi_1E_y - \Pi_2E_x) + \dots \\ &= (E_x\Pi_1 - i\hbar\partial E_x/\partial x + \dots) + i\sigma_3(E_y\Pi_1 - i\hbar\partial E_y/\partial x - E_x\Pi_2 + i\hbar\partial E_x/\partial y) + \dots \\ &= (\mathbf{E} \cdot \boldsymbol{\Pi}) - i\hbar \operatorname{div} \mathbf{E} - i(\boldsymbol{\sigma} \cdot [\mathbf{E} \times \boldsymbol{\Pi}]) + \hbar(\boldsymbol{\sigma} \cdot \operatorname{curl} \mathbf{E}). \end{aligned} \quad (145)$$

From the Maxwell field equations in free space we have

$$\operatorname{div} \mathbf{E} = 0, \quad \operatorname{curl} \mathbf{E} = -(1/c)(\partial \mathbf{H}/\partial t).$$

Substituting these expressions back in Eq. (143), we arrive at our final form of the reduced wave equation

$$\begin{aligned} i\hbar\partial\psi_0/\partial t &= \left\{ \sum_{k=1}^3 (1/2m_0)(-i\hbar\partial/\partial x_k - \epsilon A_k/c)^2 \right. \\ &+ \epsilon\phi - (\boldsymbol{\sigma} \cdot \boldsymbol{\Pi})^4/8m_0^3c^2 - (\epsilon/m_0c)(\mathbf{S} \cdot \mathbf{H}) \\ &- \frac{1}{2}(\epsilon/m_0^2c^3)(\mathbf{S} \cdot [\mathbf{E} \times \boldsymbol{\Pi}]) \left. \right\} \psi_0 - (i\epsilon\hbar/4m_0^2c^2) \\ &\quad \times \{ (\mathbf{E} \cdot \boldsymbol{\Pi}) - (2/c)(\mathbf{S} \cdot \partial \mathbf{H}/\partial t) \} \psi_0. \end{aligned} \quad (146)$$

The first two terms on the right-hand side constitute just the hamiltonian operator  $\mathcal{H}_S$  of the Schrödinger equation.

If we drop the external field in the third term it becomes<sup>53</sup>

$$-\mathbf{p}^4/8m_0^3c^2 = -(\mathcal{H}_S - \epsilon\phi)^2/2m_0c^2,$$

which is the correction term ordinarily added to the Schrödinger equation to account for the variation of mass with velocity.

The fourth term is the energy term for the spin in an external magnetic field, with the correct gyromagnetic ratio  $+\epsilon/m_0c$  ( $\epsilon = -e$  for the electron!).

The fifth term is the so-called Thomas term, to which the "spin-orbit" coupling is attributed. Again replacing  $\boldsymbol{\Pi}$  by  $\mathbf{p}$ , this term becomes

$$-\frac{1}{2}(\epsilon/m_0^2c^2)(\mathbf{S} \cdot [\mathbf{E} \times \mathbf{p}]). \quad (147)$$

<sup>53</sup> Cf. E. C. Kemble, *The Fundamental Principles of Quantum Mechanics* for the discussion of these terms by perturbation methods in the Schrödinger wave equation.

For an electron in the Coulomb field of a nucleus of charge  $Ze$

$$\mathbf{E} = (Ze/r^3)\mathbf{r}$$

which reduces the expression for a hydrogenic atom to

$$+\frac{1}{2}(Ze^2/m_0^2c^2r^3)(\mathbf{S} \cdot \mathbf{L})$$

with  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$  and gives the correct perturbation term inclusive of the Thomas correction factor.

By rearranging the factors in Eq. (147) we can write it as

$$\frac{1}{2}(\epsilon/m_0^2c^2)(\mathbf{E} \cdot [\mathbf{S} \times \mathbf{p}]),$$

from which we can interpret it as the energy term arising from the existence of an electrical moment associated with the operator

$$-(\epsilon/m_0^2c^2)\mathbf{S} \times \mathbf{p}.$$

The last two small terms in Eq. (146) are not ordinarily considered in the Schrödinger theory.

For an illuminating discussion of the interpretation of these interaction terms in the non-relativistic approximation, the reader is referred to two recent papers by Breit.<sup>54</sup>

### Negative energy states

The same formal process as that just given may be employed in the derivation of an approximate "Schrödinger equation" for energies in the neighborhood of  $-m_0c^2$ . The appropriate substitution is now

$$\hat{\phi}^0 = e^{-(i/\hbar)m_0c^2t}(\chi_1\mathbf{a}_1 + \chi_2\mathbf{a}_2),$$

$$\psi^0 = e^{-(i/\hbar)m_0c^2t}(\chi_3\mathbf{a}_1 + \chi_4\mathbf{a}_2),$$

$$\psi = e^{(i/\hbar)m_0c^2t}(\hat{\phi}^0 - \Omega_0\psi^0).$$

<sup>54</sup> G. Breit, *Phys. Rev.* **51**, 248 (1937); **53**, 153 (1938). Cf. also D. R. Inglis, *Phys. Rev.* **50**, 783 (1936); W. H. Furry, *Phys. Rev.* **50**, 784 (1936).

The equations for  $\phi^0$  and  $\psi^0$  become

$$\begin{aligned} (i\hbar\partial/\partial t - \epsilon\phi)\phi^0 + c(\boldsymbol{\sigma}\cdot\mathbf{\Pi})\psi^0 &= 0, \\ (-2m_0c^2 + i\hbar\partial/\partial t - \epsilon\phi)\psi^0 + c(\boldsymbol{\sigma}\cdot\mathbf{\Pi})\phi^0 &= 0. \end{aligned}$$

$\phi^0$  is now the large, and  $\psi^0$  the small, component. Comparison with Eqs. (140) shows that the only formal difference is the interchange in the roles of  $\psi^0$  and  $\phi^0$  and the change in the sign of the mass term. The final result will be an equation similar to Eq. (146) with  $\phi^0$  replacing  $\psi^0$ , and with the sign of the rest mass changed throughout. In particular, we see that the sign of the  $(\mathbf{S}\cdot\mathbf{H})$  term will be changed, indicating the change in sign of the gyromagnetic ratio which was mentioned in the previous section. This exhibits explicitly the necessity for the assignment of the magnetic moment operators by

$$M_x = (\epsilon\hbar/2m_0c)i\alpha_2\alpha_3\alpha_4,$$

rather than by  $(\epsilon\hbar/2m_0c)i\alpha_2\alpha_3$ , as was originally done by Dirac on the basis of an argument depending on the iteration of the hamiltonian. The Thomas term, containing  $m_0^2$ , is not altered in sign.

### §23. THE DIRAC POSITRON THEORY (THEORY OF HOLES)

In previous sections (§15, §20,) we have encountered the problem of the existence of solutions of the Dirac equation associated with energies of the electron for which  $E < -m_0c^2$  (negative energy solutions), and have seen some of their curious dynamical properties.

In 1930, before the experimental discovery of the positron, Dirac<sup>55</sup> advanced a suggestion concerning the negative energy solutions which has since been developed into a fairly comprehensive theory, in spite of many difficulties which it presents. Dirac supposed that in the normal condition of the universe all of the possible states of negative energy might be considered to be already occupied by electrons, and that the Pauli exclusion principle could be invoked to prevent more than one electron from occupying each given state. So long as no hypothesis of "finiteness" of space is made, the number of negative

energy levels available for occupancy would be a high order infinity, so that in fact one needs to suppose an infinite density of "negative energy electrons" to be present. These electrons should produce an infinitely large negative potential, but because of the very uniformity of the distribution, it might be assumed that no observable fields would be produced.

But if an electron were caused to make a transition to a positive energy state, it would leave a void in the distribution of electrons in the negative energy states (i.e., a *hole*) which might be expected to behave, in some respects at least, like a positive particle. Its properties would be such that they could just be compensated by having an electron return to the negative energy state from the positive energy state. In particular, this particle, or "hole" should appear to have a spin angular momentum, just like the electron. With the experimental discovery of the positron in 1932, it was but natural to identify the "hole" of Dirac's theory with the positron as found in the laboratory.

A process in which an electron makes a transition out of a negative energy into a positive energy state is called *pair creation* on this theory, since it would produce an ordinary (i.e. positive energy) electron and a positron. Pair creation requires a supply of energy from the perturbing influence causing it of at least  $2m_0c^2$  ( $\sim 10^6$  ev). The reverse process in which an electron in a positive energy state makes a transition into an unoccupied negative energy level, thereby causing the "disappearance" of an electron and a positron, is called *pair annihilation*. It is associated with the emission of an amount of energy equal to at least  $2m_0c^2$ .

All of these considerations have the very best support from the experimental evidence on the appearance and disappearance of positrons.<sup>55a</sup>

This interpretation has also the advantage from the physical point of view of giving a reason for the fact that the ordinary electron is the normal inhabitant of our world as we find it, while positrons can be observed only under specially designed conditions. For whenever free

<sup>55</sup> P. A. M. Dirac, Proc. Roy. Soc. **A126**, 360 (1930).

<sup>55a</sup> O. Klemperer, Proc. Camb. Phil. Soc. **30**, 347 (1934).  
H. R. Crane and C. C. Lauritsen, Phys. Rev. **45**, 430 (1934).

positrons ("holes") occur, electrons are very soon induced to combine with them with the emission of the *annihilation radiation*.<sup>56</sup>

On the other hand, this theory is attended by several very serious difficulties. In the first place, the infinite density of electrons in negative energy states which is postulated to be present, presents many problems. Although a uniform distribution of charge might set up no observable field under normal conditions, yet there seems to be no reason why it could not be affected by fields due to other charge and current distributions. The properties of a "vacuum" or "free space" now become very complex, and the appearance of infinities in the answers to all of its physical characteristics such as its "index of refraction" for example, can be avoided only by the use of special conventions in the mathematical developments. The field equations are no longer linear, so that electromagnetic fields are no longer strictly superposable; two light beams interact with each other, and so on.

While these troublesome points remain, the theory can hardly be said to have developed much beyond a formative stage. But even so, in the rapidly developing field of nuclear processes during the last few years, it has played an important role in the tentative discussion of the properties of high energy electrons and  $\gamma$ -rays.<sup>56</sup>

#### §24. THE EXTENSION OF THE DIRAC EQUATION TO TWO PARTICLES

With the exception of the discussion of the last section, the whole of our treatment has been limited to the motion of a single particle in an external field. Even in the positron theory in its present form no effective attempt is made to treat the interactions of two or more particles except as a problem in small perturbations, i.e., the influence of one particle on another is supposed to be so slight that it can be handled by approximation methods.

<sup>56</sup> Cf. W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, 1936), for a comprehensive discussion.

In his general theory of the relationship between quantum mechanics and relativity, Eddington<sup>57</sup> has made some very interesting suggestions on the problem of two particles, and has given a discussion of the energy of interaction between two protons. Unfortunately, the authors do not feel it possible to give a discussion of Eddington's theory at the present time, and must refer the reader to the original sources.

It was shown some years ago by Breit,<sup>58</sup> and later by Møller<sup>59</sup> and Bethe and Fermi,<sup>60</sup> that an approximate formula could be obtained for the perturbative energy of interaction between two electrons of the form

$$\mathcal{H}_{12} = (e^2/r_{12}) \left[ 1 - \frac{1}{2}(\boldsymbol{\alpha}^I \cdot \boldsymbol{\alpha}^{II}) - (\boldsymbol{\alpha}^I \cdot \mathbf{r}_{12})(\boldsymbol{\alpha}^{II} \cdot \mathbf{r}_{12})/2r_{12}^2 \right].$$

Each electron is treated as in the Dirac theory, with  $-c\boldsymbol{\alpha}^I$  and  $-c\boldsymbol{\alpha}^{II}$  as the (vector) velocity operators of the two electrons. The hamiltonian operator for the two electrons is written as

$$\mathcal{H} = \mathcal{H}_D(1) + \mathcal{H}_D(2) + \mathcal{H}_{12},$$

where  $\mathcal{H}_D(1)$  is the Dirac hamiltonian for electron 1, etc. The complete wave function now has 16 components, and can be put in the form

$$\psi = \sum_{k, l=1}^4 \chi_{kl} \mathbf{a}_k^I \mathbf{a}_l^{II}.$$

Following a method similar to that of §22 Breit arrived at a system of equations which involve four "big" components, and include approximate perturbative terms between the electrons. He has made extensive applications of his results to the study of hyperfine structure separations.<sup>61</sup>

<sup>57</sup> A. S. Eddington, *The Relativity Theory of Protons and Electrons* (Cambridge University Press, 1936); Proc. Roy. Soc. **A162**, 155 (1937).

<sup>58</sup> G. Breit, Phys. Rev. **34**, 553 (1929); **36**, 383 (1930); **39**, 616 (1932). Cf. also Breit, reference 54.

<sup>59</sup> C. Møller, Zeits. f. Physik **70**, 786 (1931).

<sup>60</sup> H. Bethe and E. Fermi, Zeits. f. Physik **77**, 296 (1932).

<sup>61</sup> Cf. the discussion by Bethe, *Handbuch der Physik*, second edition, Vol. 24, p. 375 *et seq.*

## APPENDIX A. LINEAR AND ORBITAL ANGULAR MOMENTUM OPERATORS IN POLAR COORDINATES

$$\begin{aligned}
x &= r \sin \theta \cos \varphi, & y &= r \sin \theta \sin \varphi, & z &= r \cos \theta, \\
p_x &= -i\hbar \partial / \partial x = -i\hbar [\sin \theta \cos \varphi \partial / \partial r + (\cos \theta \cos \varphi / r) \partial / \partial \theta - (\sin \varphi / r \sin \theta) \partial / \partial \varphi], \\
p_y &= -i\hbar \partial / \partial y = -i\hbar [\sin \theta \sin \varphi \partial / \partial r + (\cos \theta \sin \varphi / r) \partial / \partial \theta + (\cos \varphi / r \sin \theta) \partial / \partial \varphi], \\
p_z &= -i\hbar \partial / \partial z = -i\hbar [\cos \theta \partial / \partial r - (\sin \theta / r) \partial / \partial \theta], \\
L_x &= -i\hbar (y \partial / \partial z - z \partial / \partial y) = -i\hbar (-\sin \varphi \partial / \partial \theta - \cot \theta \cos \varphi \partial / \partial \varphi), \\
L_y &= -i\hbar (z \partial / \partial x - x \partial / \partial z) = -i\hbar (\cos \varphi \partial / \partial \theta - \cot \theta \sin \varphi \partial / \partial \varphi), \\
L_z &= -i\hbar (x \partial / \partial y - y \partial / \partial x) = -i\hbar \partial / \partial \varphi, \\
L_{\pm} &= L_x \pm iL_y = i\hbar e^{\pm i\varphi} (\mp i \partial / \partial \theta + \cot \theta \partial / \partial \varphi), \\
L^2 &= L_x^2 + L_y^2 + L_z^2 = \frac{1}{2}(L_+ L_- + L_- L_+) + L_z^2, \\
&= -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right].
\end{aligned}$$

## APPENDIX B. THE SPHERICAL HARMONICS

In the following definitions  $m$  and  $l$  are integers,  $|m| \leq l$ ,

$$\begin{aligned}
\mu &= \cos \theta, \\
\Theta_{l, m}(\theta) &= (-)^m \left[ \frac{2l+1}{2} \frac{(l-m)!}{(l+m)!} \right]^{\frac{1}{2}} \frac{(1-\mu^2)^{m/2}}{2^l \cdot l!} \frac{d^{l+m}}{d\mu^{l+m}} (\mu^2 - 1)^l, \tag{B1}
\end{aligned}$$

$$Y_{l, m}(\theta, \varphi) = \Theta_{l, m}(\theta) \cdot \frac{e^{im\varphi}}{(2\pi)^{\frac{1}{2}}}. \tag{B2}$$

It follows from (B1) that

$$\Theta_{l, -m}(\theta) = (-)^m \Theta_{l, m}(\theta).$$

The functions  $Y_{l, m}(\theta, \varphi)$  form an orthonormal set on the surface of the unit sphere; i.e.

$$\int_{\theta=0}^{\pi} \int_{\varphi=0}^{2\pi} (Y_{l, m})^* Y_{l', m'} \sin \theta \, d\theta \, d\varphi = \delta_{m, m'} \cdot \delta_{l, l'}.$$

We tabulate below some useful formulas involving these functions. These expressions are not all independent, but the complete table assists materially in reducing the labor of computations. For notation let

$$[a; b] = \left( \frac{a+1-b}{2a+1} \right)^{\frac{1}{2}},$$

$$\begin{aligned}
(\partial / \partial \theta) Y_{l, m} &= -\frac{1}{2}((l+m)(l-m+1))^{\frac{1}{2}} Y_{l, m-1} e^{i\varphi} + \frac{1}{2}((l-m)(l+m+1))^{\frac{1}{2}} Y_{l, m+1} e^{-i\varphi}, \\
m \cot \theta \cdot Y_{l, m} &= -\frac{1}{2}((l+m)(l-m+1))^{\frac{1}{2}} Y_{l, m-1} e^{i\varphi} - \frac{1}{2}((l-m)(l+m+1))^{\frac{1}{2}} Y_{l, m+1} e^{-i\varphi}, \\
\sin \theta (\partial / \partial \theta) Y_{l, m} &= l[l; m][l+1; -m+1] Y_{l+1, m} - (l+1)[l-1; m][l; -m+1] Y_{l-1, m}, \\
L_+ Y_{l, m} &= \hbar((l-m)(l+m+1))^{\frac{1}{2}} Y_{l, m+1}, \\
L_- Y_{l, m} &= \hbar((l+m)(l-m+1))^{\frac{1}{2}} Y_{l, m-1}, \\
L_z Y_{l, m} &= m\hbar Y_{l, m}, \\
L^2 Y_{l, m} &= l(l+1)\hbar^2 Y_{l, m}.
\end{aligned}$$

If  $f(r)$  is a function of  $r$  only

$$\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)fY_{l,m} = -\left(\frac{df}{dr} - \frac{l}{r}f\right)[l; -m][l+1; -m]Y_{l+1,m+1} \\ + \left(\frac{df}{dr} + \frac{l+1}{r}f\right)[l; m+1][l-1; m+1]Y_{l-1,m+1},$$

$$\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)fY_{l,m} = \left(\frac{df}{dr} - \frac{l}{r}f\right)[l; m][l+1; m]Y_{l+1,m-1} \\ - \left(\frac{df}{dr} + \frac{l+1}{r}f\right)[l; -m+1][l-1; -m+1]Y_{l-1,m-1},$$

$$\frac{\partial}{\partial z}fY_{l,m} = \left(\frac{df}{dr} - \frac{l}{r}f\right)[l; m][l+1; -m+1]Y_{l+1,m} + \left(\frac{df}{dr} + \frac{l+1}{r}f\right)[l; -m+1][l-1; m]Y_{l-1,m},$$

$$[l; -m] \cos \theta \cdot Y_{l,m} - [l+1; m+1]Y_{l+1,m} + [l; m+1] \sin \theta \cdot Y_{l,m+1}e^{-i\varphi} = 0,$$

$$\cos \theta \cdot Y_{l,m} - [l; -m][l+1; m+1]Y_{l+1,m} - [l-1; m][l; -m+1]Y_{l-1,m} = 0,$$

$$[l; m] \cos \theta \cdot Y_{l,m} - [l+1; -m+1]Y_{l+1,m} - [l; -m+1] \sin \theta \cdot Y_{l,m-1}e^{i\varphi} = 0,$$

$$[l; -m+1] \cos \theta \cdot Y_{l,m} - [l-1; m]Y_{l-1,m} + [l; m] \sin \theta \cdot Y_{l,m-1}e^{i\varphi} = 0,$$

$$(2m/2l+1) \cos \theta \cdot Y_{l,m} + [l; m+1][l; -m] \sin \theta \cdot Y_{l,m+1}e^{-i\varphi} + [l; m][l; -m+1] \sin \theta \cdot Y_{l,m-1}e^{i\varphi} = 0,$$

$$(2m/2l-1)Y_{l-1,m} + [l; -m][l-1; -m] \sin \theta \cdot Y_{l,m+1}e^{-i\varphi} + [l; m][l-1; m] \sin \theta \cdot Y_{l,m-1}e^{i\varphi} = 0,$$

$$(2m/2l+3)Y_{l+1,m} + [l+1; m+1][l; m+1] \sin \theta \cdot Y_{l,m+1}e^{-i\varphi}$$

$$+ [l+1; -m+1][l; -m+1] \sin \theta \cdot Y_{l,m-1}e^{i\varphi} = 0,$$

$$[l+1; -m+1][l; -m+1]Y_{l+1,m} - [l-1; m][l; m]Y_{l-1,m} + \sin \theta \cdot Y_{l,m-1}e^{i\varphi} = 0,$$

$$[l; m+1] \cos \theta \cdot Y_{l,m} - [l-1; -m]Y_{l-1,m} - [l; -m] \sin \theta \cdot Y_{l,m+1}e^{-i\varphi} = 0,$$

$$\sin \theta \cdot Y_{l,m+1} - [l+1; m+1][l; m+1]Y_{l+1,m}e^{i\varphi} + [l; -m][l-1; -m]Y_{l-1,m}e^{i\varphi} = 0.$$

## References:

Condon and Shortley, *The Theory of Atomic Spectra*, (Cambridge University Press, 1935), p. 52 *et seq.* We have followed these authors in introducing the factor  $(-)^m$  in the definition (B1). It has the advantage of making the phases of the orbital angular momentum and spin matrices the same.

H. Bateman, *Partial Differential Equations* (Cambridge University Press, 1932), Chap. 6.

Whittaker and Watson, *Modern Analysis*, (Cambridge University Press, 1927), Chap. 15.

G. Prevost, *Procès-Verbaux des Séances de la Société des Sciences Physiques et Naturelles de Bordeaux*, 1935-36, p. 23. The formulas given in this reference contain some typographical errors.

## APPENDIX C. THE PAULI TRANSFORMATION FUNCTION (§ 8)

We compute first the special transformation functions corresponding to rotations about the coordinate axes.

### Rotation about the x axis

For such a rotation  $\eta = \zeta = 0$ ,

$$\sigma_1' = \sigma_1, \quad \sigma_4' = \sigma_4,$$

$$\sigma_2' = \sigma_2 \cos \xi + \sigma_3 \sin \xi,$$

$$\sigma_3' = -\sigma_2 \sin \xi + \sigma_3 \cos \xi.$$

It is evident at once that since  $U$  must commute

with  $\sigma_1$ , it has the special form

$$U(\{\xi, 0, 0\}) = u_1\sigma_1 + u_4\sigma_4.$$

Operating on the left with  $\sigma_2'$  and reducing by the use of Eqs. (18) of the text we find

$$\sigma_2' \cdot U(\{\xi, 0, 0\}) = \sigma_2(iu_1 \sin \xi + u_4 \cos \xi) + \sigma_3(-iu_1 \cos \xi + u_4 \sin \xi),$$

$$U(\{\xi, 0, 0\}) \cdot \sigma_2 = u_4\sigma_2 + iu_1\sigma_3.$$

Equating corresponding coefficients of these expressions gives

$$\begin{aligned} -iu_1 \sin \xi + u_4(1 - \cos \xi) &= 0, \\ iu_1(1 + \cos \xi) - u_4 \sin \xi &= 0. \end{aligned}$$

The same equations are obtained from

$$\sigma_3' U(\{\xi, 0, 0\}) = U(\{\xi, 0, 0\}) \sigma_3.$$

The solution for which

$$U(\{\xi, 0, 0\}) \rightarrow 1 \quad \text{as} \quad \xi \rightarrow 0$$

$$\text{is} \quad u_1 = -i \sin \frac{1}{2}\xi, \quad u_4 = \cos \frac{1}{2}\xi,$$

giving

$$U(\{\xi, 0, 0\}) = -i \sin \frac{1}{2}\xi \cdot \sigma_1 + \cos \frac{1}{2}\xi \cdot \sigma_4. \quad (\text{C1})$$

#### Rotation about the z axis

$$\xi = \zeta = 0,$$

$$\sigma_1' = \sigma_1 \cos \eta + \sigma_2 \sin \eta,$$

$$\sigma_2' = -\sigma_1 \sin \eta + \sigma_2 \cos \eta,$$

$$\sigma_3' = \sigma_3, \quad \sigma_4' = \sigma_4.$$

An exactly similar calculation shows that

$$U(\{0, \eta, 0\}) = -i \sin \frac{1}{2}\eta \cdot \sigma_3 + \cos \frac{1}{2}\eta \cdot \sigma_4. \quad (\text{C2})$$

We can now build up the general transformation function by observing that the transformation (36) can be generated by the successive rotations (cf. Fig. 1 of the text).

- (1) A rotation through the angle  $\eta$  about the z axis, followed by
- (2) A rotation through the angle  $\xi$  about the line A, followed by
- (3) A rotation through the angle  $\zeta$  about the z' axis.

The calculation of the operator  $U(\{\xi, \eta, \zeta\})$  for the general rotation may be materially sim-

plified by the following observation. The equation from which  $U$  is to be found is

$$\sigma_k' U = U \sigma_k. \quad (\text{C3})$$

Suppose that we consider a second transformation

$$\sigma_k' \rightarrow \sigma_k''$$

with

$$\sigma_k'' V = V \sigma_k'. \quad (\text{C4})$$

Here  $V$  is to be considered as expressed directly in terms of the operators  $\sigma_1', \dots, \sigma_4'$ .

The resultant operator for  $\sigma_k \rightarrow \sigma_k''$  is found from

$$\sigma_k'' = V \sigma_k' V^{-1} = V U \sigma_k U^{-1} V^{-1} \quad (\text{C5})$$

or

$$\sigma_k'' V U = V U \sigma_k,$$

i.e., the resultant operator is  $VU$ , where  $U$  is expressed directly in terms of the  $\sigma$ 's, and  $V$  of the  $\sigma'$ 's.

But we can proceed in a different manner. If we write Eq. (C3) as

$$\sum_{l=1}^4 \omega_{kl} \sigma_l U = U \sigma_k$$

we can say that to every set of transformation coefficients ( $\omega_{kl}$ ) we associate an operator  $U_\sigma$ , to be found in terms of the  $\sigma$ 's from the above equation.

In carrying out two successive transformations we have

$$\sigma_k' = \sum_{l=1}^4 \omega_{kl} \sigma_l = U_\sigma \sigma_k U_\sigma^{-1},$$

$$\sigma_m'' = \sum_{k=1}^4 \Omega_{mk} \sigma_k' = U_\sigma \left( \sum_{k=1}^4 \Omega_{mk} \sigma_k \right) U_\sigma^{-1}$$

$$= U_\sigma V_\sigma \sigma_m V_\sigma^{-1} U_\sigma^{-1},$$

where

$$\sum_{k=1}^4 \Omega_{mk} \sigma_k V_\sigma = V_\sigma \sigma_m.$$

This shows us that we can take the operator  $V$  obtained from Eq. (C4), replace the  $\sigma'$ 's by the  $\sigma$ 's and multiply in the order  $UV$ ; i.e.

$$V_\sigma' U_\sigma = U_\sigma V_\sigma. \quad (\text{C6})$$

The reader can verify this for special rotations. The use of this process is helpful in reducing the algebraic manipulations.

Applying it to the space rotations, we get

$$\begin{aligned}
U(\{\xi, \eta, \zeta\}) &= U(\{0, \eta, 0\}) \cdot U(\{\xi, 0, 0\}) \cdot U(\{0, \zeta, 0\}) \\
&= [-i \sin \frac{1}{2}\eta \cdot \sigma_3 + \cos \frac{1}{2}\eta \cdot \sigma_4] [-i \sin \frac{1}{2}\xi \cdot \sigma_1 \\
&\quad + \cos \frac{1}{2}\xi \cdot \sigma_4] [-i \sin \frac{1}{2}\zeta \cdot \sigma_3 + \cos \frac{1}{2}\zeta \cdot \sigma_4] \\
&= -i \sin \frac{1}{2}\xi (\sin \frac{1}{2}\eta \sin \frac{1}{2}\zeta + \cos \frac{1}{2}\eta \cos \frac{1}{2}\zeta) \sigma_1 \\
&\quad - i \sin \frac{1}{2}\xi (\sin \frac{1}{2}\eta \cos \frac{1}{2}\zeta - \cos \frac{1}{2}\eta \sin \frac{1}{2}\zeta) \sigma_2 \\
&\quad - i \cos \frac{1}{2}\xi (\cos \frac{1}{2}\eta \sin \frac{1}{2}\zeta + \sin \frac{1}{2}\eta \cos \frac{1}{2}\zeta) \sigma_3 \\
&\quad + \cos \frac{1}{2}\xi (\cos \frac{1}{2}\eta \cos \frac{1}{2}\zeta - \sin \frac{1}{2}\eta \sin \frac{1}{2}\zeta) \sigma_4.
\end{aligned}$$

An inspection shows that these coefficients are identical with those of Eq. (43) of the text.

#### APPENDIX D. THE NORMALIZATION OF THE DIRAC WAVE FUNCTIONS FOR THE ENERGY LEVELS OF THE HYDROGENIC ATOM (§17)

The normalization of the hydrogenic atom wave functions has been carried out by Bechert.<sup>62</sup> The following procedure is based on a method given by Kramers.<sup>63</sup>

The normalization integral is<sup>62a</sup>

$$\begin{aligned}
\iint |\psi|^2 dx dy dz &= \int_0^\infty |rf|^2 dr \\
&\quad + \int_0^\infty |rG|^2 dr = 1. \quad (D1)
\end{aligned}$$

From the differential equations (80) for  $f(r)$  and  $G(r)$  we have

$$\begin{aligned}
\frac{d(rf)}{dr} &= -\frac{J+\frac{1}{2}}{r}(rf) - \frac{i}{\hbar c} \left( E + \frac{Ze^2}{r} - m_0c^2 \right) (rG), \\
\frac{d(rG)}{dr} &= \frac{J+\frac{1}{2}}{r}(rG) - \frac{i}{\hbar c} \left( E + \frac{Ze^2}{r} + m_0c^2 \right) (rf). \quad (D2)
\end{aligned}$$

The functions defined by these equations may be considered to be functions of  $E$  in addition to their dependence on  $r$ . If we treat  $E$  and  $r$  as independent variables and write

$$f_E = (\partial f / \partial E), \quad G_E = (\partial G / \partial E)$$

we get, by partial differentiation of these equations with respect to  $E$ ,

$$\begin{aligned}
\frac{\partial}{\partial r}(rf_E) &= -\frac{J+\frac{1}{2}}{r}(rf_E) \\
&\quad - \frac{i}{\hbar c} \left( E + \frac{Ze^2}{r} - m_0c^2 \right) (rG_E) - \frac{i}{\hbar c} (rG), \\
\frac{\partial}{\partial r}(rG_E) &= \frac{J+\frac{1}{2}}{r}(rG_E) \\
&\quad - \frac{i}{\hbar c} \left( E + \frac{Ze^2}{r} + m_0c^2 \right) (rf_E) - \frac{i}{\hbar c} (rf). \quad (D3)
\end{aligned}$$

From these relations and their complex conjugates, we find

$$\frac{\partial}{\partial r} [(rf)^*(rG_E) + (rf_E)(rG)^*] = -\frac{i}{\hbar c} [|rf|^2 + |rG|^2],$$

and so from (D1)

$$\int_0^\infty \frac{\partial}{\partial r} [(rf)^*(rG_E) + (rf_E)(rG)^*]_{\epsilon=\epsilon_n, J} dr = -\frac{i}{\hbar c}.$$

On integrating the left-hand side we find

$$\lim_{r \rightarrow \infty} [(rf)^*(rG_E) + (rf_E)(rG)^*]_{\epsilon=\epsilon_n, J} = -\frac{i}{\hbar c} \quad (D4)$$

since the functions vanish at the lower limit  $r \rightarrow 0$ .

From Eqs. (83) we see that  $rf$  is a pure imaginary, while  $rG$  is real, which permits us to write

$$\begin{aligned}
&(rf)^*(rG_E) + (rf_E)(rG)^* \\
&= (rG)^2 \left( \frac{f_E}{G} - \frac{f}{G} \frac{G_E}{G} \right) = (rG)^2 \frac{\partial}{\partial E} \left( \frac{f}{G} \right) \\
&= \frac{(rG)^2}{m_0c^2} \left\{ \frac{\partial}{\partial \epsilon} \left[ i \left( \frac{1-\epsilon}{1+\epsilon} \right)^{\frac{1}{2}} \frac{\Lambda_1 - \Lambda_2}{\Lambda_1 + \Lambda_2} \right] \right\} \quad (D5)
\end{aligned}$$

from Eqs. (83) and (85).

In this expression we must consider  $\Lambda_1$  and  $\Lambda_2$  as functions of  $\epsilon$  and  $r$  defined by the Eqs. (86) and the series (87). For  $\epsilon$  not equal to one of the values of Eq. (94) the series will be infinite of the form

$$\begin{aligned}
\Lambda_1(\epsilon, r) &= 1 + c_1' r + c_2' r^2 + \dots, \\
\Lambda_2(\epsilon, r) &= d_0' + d_1' r + d_2' r^2 + \dots, \\
c_k' &= (2\lambda)^k c_k, \quad d_k' = (2\lambda)^k d_k,
\end{aligned}$$

<sup>62</sup> K. Bechert, *Ann. d. Physik* **6**, 700 (1930).

<sup>63</sup> H. A. Kramers, "Theorien des Aufbaues der Materie" in *Hand- und Jahrbuch der chemischen Physik* (Akademische Verlagsgesellschaft, 1933-38), §66.



and it must be remembered that  $c_k$ ,  $d_k$  and  $\lambda$  are functions of  $\epsilon$ . Further

From Eqs. (88) we have as  $\epsilon \rightarrow \epsilon_{n, J}$

$$\Lambda_1(\epsilon, r) \rightarrow \Lambda_1(\epsilon_{n, J}, r) = \mathfrak{F}(-n'+1, 2\gamma+1; \rho),$$

$$\Lambda_2(\epsilon, r) \rightarrow \Lambda_2(\epsilon_{n, J}, r) =$$

$$-\frac{(\gamma+n')+(J+\frac{1}{2})\epsilon_{n, J}}{n'\epsilon_{n, J}} \mathfrak{F}(-n', 2\gamma+1; \rho).$$

We are interested in the asymptotic forms of these functions and their derivatives for  $r \rightarrow \infty$ . These can be found from the theory of the confluent hypergeometric functions,<sup>64</sup> and are given explicitly by Kramers:<sup>65</sup>

$$r \rightarrow \infty,$$

$$\Lambda_1(\epsilon_{n, J}, r) \approx (-)^{n'-1} \frac{\Gamma(2\gamma+1)}{\Gamma(2\gamma+n')} \rho^{n'-1},$$

$$\left\{ \frac{\partial}{\partial \epsilon} \Lambda_1(\epsilon, r) \right\}_{\epsilon=\epsilon_{n, J}} \approx \{ (-)^{n'}(n'-1)! Z\alpha(1-\epsilon^2)^{-\frac{1}{2}}$$

$$\times \Gamma(2\gamma+1) e^\rho \rho^{-2\gamma-n'} \}_{\epsilon=\epsilon_{n, J}},$$

$$\Lambda_2(\epsilon_{n, J}, r) \approx (-)^{n'+1} \frac{\gamma+n'+(J+\frac{1}{2})\epsilon_{n, J}}{n'\epsilon_{n, J}}$$

$$\times \frac{\Gamma(2\gamma+1)}{\Gamma(2\gamma+n'+1)} \rho^{n'},$$

$$\left\{ \frac{\partial}{\partial \epsilon} \Lambda_2(\epsilon, r) \right\}_{\epsilon=\epsilon_{n, J}} \approx \left\{ (-)^{n'+1} \frac{\gamma+n'+(J+\frac{1}{2})\epsilon}{n'\epsilon} (n'!) \right.$$

$$\left. \times Z\alpha(1-\epsilon^2)^{-\frac{1}{2}} \Gamma(2\gamma+1) e^\rho \rho^{-2\gamma-1-n'} \right\}_{\epsilon=\epsilon_{n, J}}$$

$\Gamma$  indicates the ordinary gamma-function.

It is important to note that the substitution  $\epsilon = \epsilon_{n, J}$  is made *after* the differentiation is performed.

The analysis can be simplified by noting that as  $r \rightarrow \infty$

$$\left( \frac{\Lambda_1 - \Lambda_2}{\Lambda_1 + \Lambda_2} \right)_{\epsilon=\epsilon_{n, J}} \rightarrow -1.$$

<sup>64</sup> Whittaker and Watson, *Modern Analysis*, fourth edition (Cambridge University Press, 1927), chap. 16, §16.1 *et seq.* In the notation used here  $\mathfrak{F}(\xi, \eta; x) = {}_1F_1\{\xi; \eta; x\}$ .

<sup>65</sup> Kramers, reference 63, p. 313.

$$(rG)_{\epsilon=\epsilon_{n, J}} \approx (-)^{n'+1} N_1 \left\{ (1+\epsilon)^{\frac{\gamma+n'+(J+\frac{1}{2})\epsilon}{n'\epsilon}} \right.$$

$$\left. \times \frac{\Gamma(2\gamma+1)}{\Gamma(2\gamma+n'+1)} e^{-\frac{1}{2}\rho} \rho^{n'} \right\}_{\epsilon=\epsilon_{n, J}}.$$

The reduction of Eq. (D5) can now be readily carried out, and the result found

$$r \rightarrow \infty$$

$$\left[ (rG)^2 \frac{\partial}{\partial E} \left( \frac{f}{G} \right) \right]_{E=E_{n, J}} \approx -iN_1^2(n'-1)! \frac{2Z\alpha}{m_0c^2}$$

$$\times \frac{[\Gamma(2\gamma+1)]^2}{\Gamma(2\gamma+n'+1)} \left[ \frac{\gamma+n'+(J+\frac{1}{2})\epsilon}{n'\epsilon(1-\epsilon^2)} \right]_{\epsilon=\epsilon_{n, J}}.$$

If we equate this to  $-i/\hbar c$  we find the normalization factor quoted in the text.

#### APPENDIX E. THE DIRAC TRANSFORMATION FUNCTION (§18)

As the work proceeds on exactly similar lines to Appendix C we give only an abbreviated discussion.

##### Rotation about the $x$ axis

$$\eta = \zeta = 0,$$

$$\beta_1' = \beta_1, \quad \beta_4' = \beta_4,$$

$$\beta_2' = \beta_2 \cos \xi + \beta_3 \sin \xi,$$

$$\beta_3' = -\beta_2 \sin \xi + \beta_3 \cos \xi.$$

As  $U$  must commute with both  $\beta_1$  and  $\beta_4$ , it must be of the form

$$U = u_8 i \beta_2 \beta_3 + u_{13} i \beta_3 \beta_1 \beta_4 + u_{14} i \beta_1 \beta_2 \beta_4 + u_{16} I.$$

From the equations

$$\beta_2' U = U \beta_2, \quad \beta_3' U = U \beta_3,$$

we find

$$\frac{i u_8}{u_{16}} = \frac{u_{13}}{u_{14}} = -\frac{\sin \frac{1}{2} \xi}{\cos \frac{1}{2} \xi}.$$

The solution for which  $U \rightarrow I$  as  $\xi \rightarrow 0$  becomes

$$U = (i \sin \frac{1}{2} \xi) i \beta_2 \beta_3 + (\cos \frac{1}{2} \xi) I.$$

The analysis for the general space rotation continues just as in Appendix C with the result given in the text.

### Special Lorentz transformation (cf. text)

Here  $(\beta = v/c)$

$$\beta_1' = (\beta_1 + i\beta\beta_4)(1 - \beta^2)^{-\frac{1}{2}}, \quad \beta_2' = \beta_2, \quad \beta_3' = \beta_3, \\ \beta_4' = (\beta_4 - i\beta\beta_1)(1 - \beta^2)^{-\frac{1}{2}}.$$

The commutation of  $U$  with  $\beta_2$  and  $\beta_3$  requires that it be of the form

$$U = u_5 i\beta_1\beta_4 + u_{11} i\beta_1\beta_2\beta_3 + u_{12} i\beta_2\beta_3\beta_4 + u_{16} I.$$

The relations

$$\beta_1' U = U\beta_1, \quad \beta_2' U = U\beta_2$$

lead at once to

$$\frac{u_5}{u_{16}} = \frac{i u_{12}}{u_{11}} = -\frac{\beta}{1 + (1 - \beta^2)^{\frac{1}{2}}}.$$

If we let  $\cosh \vartheta = (1 - \beta^2)^{-\frac{1}{2}}$ ,  $\sinh \vartheta = \beta(1 - \beta^2)^{-\frac{1}{2}}$  we find

$$\frac{u_5}{u_{16}} = \frac{i u_{12}}{u_{11}} = -\frac{\sinh \frac{1}{2}\vartheta}{\cosh \frac{1}{2}\vartheta}.$$

The solution for which  $U \rightarrow I$  as  $\beta \rightarrow 0$  is

$$U = (-\sinh \frac{1}{2}\vartheta) i\beta_1\beta_4 + (\cosh \frac{1}{2}\vartheta) I.$$

### APPENDIX F. SAUTER'S METHOD OF SOLUTION OF THE DIRAC EQUATION

A general method for solving the Dirac equation without specializing the operators by the introduction of matrices has been developed by Sauter.<sup>66</sup> In §12 we remarked that the 16 operators are linearly independent, and form a complete set.

This suggests writing the solution of the wave equation in the form

$$\psi = f_1 I + f_2 \alpha_1 + \cdots + f_{16} \alpha_1 \alpha_2 \alpha_3 \alpha_4 \quad (F1)$$

with 16 space functions  $f_1, \dots, f_{16}$ .

This can be reduced to an expression in terms of four functions by considering the operator

<sup>66</sup> F. Sauter, *Zeits. f. Physik* **63**, 803 (1930); **64**, 295 (1930). See also A. Proca, *J. de phys.* **1**, 235 (1930); **3**, 172 (1932). Eddington, reference 38, chap. 2 *et seq.*

$$\Gamma = I + \alpha_4 - i\alpha_1\alpha_2 - i\alpha_1\alpha_2\alpha_4. \quad (F2)$$

It is easily verified that

$$\Gamma = \alpha_4 \Gamma = -i\alpha_1\alpha_2 \Gamma = -i\alpha_1\alpha_2\alpha_4 \Gamma, \\ \alpha_3 \Gamma = \alpha_3 \alpha_4 \Gamma = -i\alpha_1\alpha_2\alpha_3 \Gamma = -i\alpha_1\alpha_2\alpha_3\alpha_4 \Gamma, \\ \alpha_1 \Gamma = \alpha_1 \alpha_4 \Gamma = -i\alpha_2 \Gamma = -i\alpha_2\alpha_4 \Gamma, \\ \alpha_1\alpha_3 \Gamma = \alpha_1\alpha_3\alpha_4 \Gamma = -i\alpha_2\alpha_3 \Gamma = -i\alpha_2\alpha_3\alpha_4 \Gamma. \quad (F3)$$

With the help of these formulas we find from (F1)

$$\psi \Gamma = (\chi_1 I + \chi_2 \alpha_1 \alpha_3 + \chi_3 \alpha_3 + \chi_4 \alpha_1) \Gamma, \quad (F4)$$

where  $\chi_1, \chi_2, \chi_3, \chi_4$  are linear combinations of the  $f_1, \dots, f_{16}$ . For example

$$\chi_1 = f_2 + f_5 + i f_6 + i f_{13}.$$

If  $\psi$  is a solution of the Dirac equation

$$(i\hbar \partial / \partial t - \mathcal{H}_D) \psi = 0, \quad (F5)$$

so is  $\psi \Gamma$ . By substitution of (F4) one obtains

$$0 = (i\hbar \partial / \partial t - \mathcal{H}_D) \psi \Gamma = [(i\hbar \partial / \partial t - \epsilon\phi + m_0 c^2) \chi_1 \\ + c \Pi_- \chi_4 + c \Pi_3 \chi_3] \Gamma + [(i\hbar \partial / \partial t - \epsilon\phi + m_0 c^2) \chi_2 \\ + c \Pi_+ \chi_3 - c \Pi_3 \chi_4] \alpha_1 \alpha_3 \Gamma + [(i\hbar \partial / \partial t - \epsilon\phi - m_0 c^2) \chi_3 \\ + c \Pi_- \chi_2 + c \Pi_3 \chi_1] \alpha_3 \Gamma + [(i\hbar \partial / \partial t - \epsilon\phi - m_0 c^2) \chi_4 \\ + c \Pi_+ \chi_1 - c \Pi_3 \chi_2] \alpha_1 \Gamma. \quad (F6)$$

This equation can be satisfied only if each of the expressions in square brackets vanishes separately, since the operators are linearly independent. This brings us back just to Eqs. (64).

The argument now is that if by any means one can obtain a solution in the general form (F1), he can write out  $\psi \Gamma$  and interpret at once in terms of the  $\chi$ 's.

As an example, consider Sauter's treatment<sup>67</sup> of the Dirac electron in a field  $\epsilon\phi = V(x)$ .  $\mathbf{A} = 0$ . Substituting

$$\psi = e^{(i/\hbar)(p_2 y + p_3 z - E t)} X(x) \quad (F7)$$

Dirac's equation goes over into

$$\left( \frac{E - V}{c} + i\hbar \alpha_1 \frac{d}{dx} + \alpha_2 p_2 + \alpha_3 p_3 + \alpha_4 m_0 c \right) X(x) = 0,$$

<sup>67</sup> F. Sauter, *Zeits. f. Physik* **69**, 742 (1931).

which we multiply from the left side with  $-i\alpha_1/\hbar$  to obtain:

$$\left[ \frac{d}{dx} - \frac{i}{\hbar c} (E - V)\alpha_1 + \frac{k}{\hbar} - \alpha_5 \right] X(x) = 0. \quad (\text{F8})$$

Here we have introduced the new symbol  $\alpha_5$  by the relations

$$k\alpha_5 = -i\alpha_1(\alpha_2 p_2 + \alpha_3 p_3 + \alpha_4 m_0 c),$$

$$k^2 = m_0^2 c^2 + p_2^2 + p_3^2.$$

We see that

$$\alpha_1 \alpha_5 + \alpha_5 \alpha_1 = 0, \quad \alpha_5^2 = 1.$$

The form of the differential equation (F8) suggests looking for a solution in the form:

$$X = [f(x) + \alpha_5 g(x)] \cdot (1 + \alpha_1). \quad (\text{F9})$$

If this is introduced in the differential equation one obtains

$$\left\{ \left[ \frac{df}{dx} - \frac{i}{\hbar c} (E - V)f + \frac{k}{\hbar} \right] + \left[ \frac{dg}{dx} + \frac{i}{\hbar c} (E - V)g + \frac{k}{\hbar} \right] \alpha_5 \right\} (1 + \alpha_1) = 0.$$

Multiplication on the left-hand side with  $(1 - \alpha_1)$  shows that

$$\frac{df}{dx} - \frac{i}{\hbar c} (E - V)f + \frac{k}{\hbar} g = 0,$$

$$\frac{dg}{dx} + \frac{i}{\hbar c} (E - V)g + \frac{k}{\hbar} f = 0. \quad (\text{F10})$$

The problem is thus reduced to only two linear differential equations. If they are solved we write down  $X \cdot \Gamma$  and obtain

$$X_1 = f + \frac{p_2 + im_0 c}{k} g, \quad X_2 = -i \frac{p_3}{k} g,$$

$$X_3 = i \frac{p_3}{k} g, \quad X_4 = f - \frac{p_2 + im_0 c}{k} g,$$

with  $\chi_k = e^{(i/\hbar)(p_2 y + p_3 z - Et)} X_k$ .

#### APPENDIX G. NOTES ON OTHER SOLUTIONS OF THE DIRAC EQUATION

For the convenience of the reader we append some notes on the correlation of our notation with standard treatments in the literature.

#### Coulomb field

Darwin<sup>68</sup> gives the radial functions as infinite series. The relation between Darwin's solutions and ours is:

$$f(r) = -iF_k(r), \quad G(r) = G_k(r), \quad k = J - \frac{1}{2},$$

$$g(r) = -iF_{-k-1}(r), \quad F(r) = G_{-k-1}(r), \quad k = -(J + \frac{3}{2}).$$

A constant factor has been omitted since Darwin does not normalize his wave functions.  $F_k$  and  $G_k$  are given by Eqs. (8, 9) of Darwin's article and  $F_{-k-1}$  and  $G_{-k-1}$  are obtained by formally substituting  $-k-1$  for  $k$ .

Gordon<sup>69</sup> puts the solutions in a form which is the basis of our treatment. Apart from an normalizing factor we have

$$f = i\psi_1/r, \quad G = \psi_2/r, \quad j' = -(J + \frac{1}{2}),$$

$$g = i\psi_1/r, \quad F = \psi_2/r, \quad j' = +(J + \frac{1}{2}).$$

The relation between Gordon's quantum number  $j'$  and our  $J$  is as indicated.

Kramers<sup>63</sup> has given some very convenient forms for the radial parts of the Coulomb wave function. The connection of his solutions which are given in Eqs. (214), (215) on page 311 of his monograph with our solutions may be verified by using the formula

$$x \cdot \mathfrak{F}'(a, b; x) = a[\mathfrak{F}(a+1, b; x) - \mathfrak{F}(a, b; x)].$$

Hulme<sup>70</sup> uses the same notation as Darwin but puts  $F(r)$  and  $G(r)$  in a form more adapted to use for the continuum ( $E > m_0 c^2$ ). He writes

$$F = (\mathfrak{F} + \mathfrak{G}) / (2(E/c + m_0 c)^{\frac{1}{2}}),$$

$$G = (\mathfrak{G} - \mathfrak{F}) / (2i(E/c - m_0 c)^{\frac{1}{2}})$$

with  $\mathfrak{F}$  and  $\mathfrak{G}$  given as integrals in the complex plane. (Eq. (17a) and (17b) of his article.) To normalize these functions such that

$$\int \psi^*(E, J, M) \psi(E' J' M') d\tau = (1/\hbar) \delta(E - E') \delta_{JJ'} \delta_{MM'},$$

they must be multiplied by a factor given by Eq. (22a) in his paper.

<sup>68</sup> C. G. Darwin, Proc. Roy. Soc. **A118**, 654 (1928).

<sup>69</sup> W. Gordon, Zeits. f. Physik **48**, 11 (1928).

<sup>70</sup> H. R. Hulme, Proc. Roy. Soc. **A133**, 381 (1931).

Furry<sup>71</sup> neglects terms of the order  $(Z\alpha)^2$  and approximates Hulme's solutions for high energies. With these approximate solutions he constructs linear combinations which reduce to plane waves at large distances. (Eqs. (4) and (5) of Furry's article.)

Rose<sup>72</sup> gives a collection of wave functions in the continuous spectrum of the Coulomb field. He uses a system of units with  $m_0$ ,  $c$  and  $\hbar$  all equal to unity.

### Other types of field

Huff<sup>73</sup> has treated the case of the homogeneous magnetic field. With the field in the direction of the  $z$  axis and the electron moving in the  $(x, y)$  plane, he obtains the solutions expressed in terms of parabolic cylinder functions  $D_\nu(\xi)$  (for definition see reference 64). Huff considers also the passage of electrons from a field free region into a region containing a homogeneous magnetic field.

Sauter<sup>67</sup> has studied the Dirac equations for a homogeneous electric field. His solution obtained in symbolic form is easily translated into more ordinary notation as is shown in Appendix F. The wave functions are

$$\chi_j = e^{(i/\hbar)(v p_2 + z p_3 - E t)} X_j(x)$$

and the  $X_j$  are connected to the functions  $f$  and  $g$  which are introduced by Sauter through Eq. (F9) of Appendix F. Sauter gives two representations for  $f$  and  $g$ . The one in Eqs. (14a, 14b) of his article makes use of hypergeometric functions, while the other (Eqs. (17a), (17b)) uses contour integrals in the complex plane. For electric fields which are not extremely high an approximate solution is given in Eqs. (21), (22), which makes use only of functions for which tables are available.

Plesset<sup>74</sup> has given a formal discussion of the solutions obtainable in various potential fields expressed as polynomials in the coordinates and their reciprocals.

Other references to the literature will be found in these papers.

### APPENDIX H. SPINOR ANALYSIS

In the discussion of this article we have treated the Dirac wave function as represented in the form

$$\psi = \chi_1 \mathbf{a}_1 + \chi_2 \mathbf{a}_2 + \chi_3 \mathbf{a}_3 + \chi_4 \mathbf{a}_4,$$

where  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4$  were introduced merely as "spin symbols" or "spin functions." We can give the formalism more of an intuitive geometrical character by imagining the  $\mathbf{a}$ 's as four linearly independent basis vectors, while  $\psi$  is a more general vector, in a 4-dimensional "spin space."

Interpreting the results of §18 geometrically, we say that to every Lorentz transformation in  $(x, y, z, t)$  there is coupled a transformation in spin space to a new set of basic vectors, the *Dirac vector*  $\psi$  is however unaffected by the rotation. Because of the appearance of the half-angles in the transformation formulas in spin space (§18) the correspondence between the transformations in  $(x, y, z, t)$  space, and those in spin space is not one-to-one, but is two-to-one. For a given Lorentz transformation one can use either  $\pm U$  for the specification of the associated transformation in spin space.

The nature of the transformation induced in spin space by the group of Lorentz transformations<sup>75</sup> may be made more apparent by introducing a new set of vectors in spin space defined by

$$\begin{aligned} \mathbf{a}_I &= 2^{-\frac{1}{2}}(\mathbf{a}_1 + \mathbf{a}_3), & \mathbf{a}_{II} &= 2^{-\frac{1}{2}}(\mathbf{a}_2 + \mathbf{a}_4), \\ \mathbf{a}_{III} &= 2^{-\frac{1}{2}}(-\mathbf{a}_1 + \mathbf{a}_3), & \mathbf{a}_{IV} &= 2^{-\frac{1}{2}}(-\mathbf{a}_2 + \mathbf{a}_4), \end{aligned} \quad (\text{H1})$$

with the conjugate vectors

$$\begin{aligned} \bar{\mathbf{a}}_I &= 2^{-\frac{1}{2}}(\bar{\mathbf{a}}_1 + \bar{\mathbf{a}}_3), & \bar{\mathbf{a}}_{II} &= 2^{-\frac{1}{2}}(\bar{\mathbf{a}}_2 + \bar{\mathbf{a}}_4), \\ \bar{\mathbf{a}}_{III} &= 2^{-\frac{1}{2}}(-\bar{\mathbf{a}}_1 + \bar{\mathbf{a}}_3), & \bar{\mathbf{a}}_{IV} &= 2^{-\frac{1}{2}}(-\bar{\mathbf{a}}_2 + \bar{\mathbf{a}}_4). \end{aligned}$$

The Dirac wave function  $\psi$  is written in terms of this set of spin vectors as

$$\psi = v_I \mathbf{a}_I + v_{II} \mathbf{a}_{II} + v_{III} \mathbf{a}_{III} + v_{IV} \mathbf{a}_{IV}, \quad (\text{H2})$$

<sup>71</sup> W. H. Furry, Phys. Rev. **46**, 391 (1934).

<sup>72</sup> M. E. Rose, Phys. Rev. **51**, 484 (1937).

<sup>73</sup> L. D. Huff, Phys. Rev. **38**, 501 (1931).

<sup>74</sup> M. S. Plessett, Phys. Rev. **41**, 278 (1932).

<sup>75</sup> B. L. van der Waerden, *Nachrichten Gesellschaft der Wissenschaften zu Göttingen* (Gött. Nach. 1929), p. 100; also van der Waerden, *Die Gruppentheoretische Methode in der Quantenmechanik* (Springer, 1932). H. Weyl, *The Theory of Groups and Quantum Mechanics*, reference 27, p. 146 et seq.

where

$$\begin{aligned} v_I &= 2^{-\frac{1}{2}}(\chi_1 + \chi_3), & v_{II} &= 2^{-\frac{1}{2}}(\chi_2 + \chi_4), \\ v_{III} &= 2^{-\frac{1}{2}}(-\chi_1 + \chi_3), & v_{IV} &= 2^{-\frac{1}{2}}(-\chi_2 + \chi_4). \end{aligned} \quad (\text{H3})$$

The transformation properties of these vectors under the various transformations of the Lorentz group can be found by the methods of §18. We give a tabulation of the results for the basic transformations.

### General rotation in 3-dimensional space

$$\begin{aligned} \mathbf{a}_I' &= \mathbf{a}_I \cdot \cos \frac{1}{2}\xi \cdot e^{-i\frac{1}{2}(\eta+\tau)} - \mathbf{a}_{II} \cdot i \sin \frac{1}{2}\xi \cdot e^{i\frac{1}{2}(\eta-\tau)}, \\ \mathbf{a}_{II}' &= -\mathbf{a}_I \cdot i \sin \frac{1}{2}\xi \cdot e^{-i\frac{1}{2}(\eta-\tau)} + \mathbf{a}_{II} \cdot \cos \frac{1}{2}\xi \cdot e^{i\frac{1}{2}(\eta+\tau)}, \\ \mathbf{a}_{III}' &= \mathbf{a}_{III} \cdot \cos \frac{1}{2}\xi \cdot e^{-i\frac{1}{2}(\eta+\tau)} - \mathbf{a}_{IV} \cdot i \sin \frac{1}{2}\xi \cdot e^{i\frac{1}{2}(\eta-\tau)}, \\ \mathbf{a}_{IV}' &= -\mathbf{a}_{III} \cdot i \sin \frac{1}{2}\xi \cdot e^{-i\frac{1}{2}(\eta-\tau)} + \mathbf{a}_{IV} \cdot \cos \frac{1}{2}\xi \cdot e^{i\frac{1}{2}(\eta+\tau)}. \end{aligned}$$

### Special Lorentz transformations

(A) *Motion along the x axis with velocity  $\beta_x c$ .*—

$$\begin{aligned} \mathbf{a}_I' &= \mathbf{a}_I \cdot \cosh \frac{1}{2}\vartheta_x - \mathbf{a}_{II} \cdot \sinh \frac{1}{2}\vartheta_x, \\ \mathbf{a}_{II}' &= -\mathbf{a}_I \cdot \sinh \frac{1}{2}\vartheta_x + \mathbf{a}_{II} \cdot \cosh \frac{1}{2}\vartheta_x, \\ \mathbf{a}_{III}' &= \mathbf{a}_{III} \cdot \cosh \frac{1}{2}\vartheta_x + \mathbf{a}_{IV} \cdot \sinh \frac{1}{2}\vartheta_x, \\ \mathbf{a}_{IV}' &= \mathbf{a}_{III} \cdot \sinh \frac{1}{2}\vartheta_x + \mathbf{a}_{IV} \cdot \cosh \frac{1}{2}\vartheta_x. \end{aligned}$$

(B) *Motion along the y axis with velocity  $\beta_y c$ .*—

$$\begin{aligned} \mathbf{a}_I' &= \mathbf{a}_I \cdot \cosh \frac{1}{2}\vartheta_y - \mathbf{a}_{II} \cdot i \sinh \frac{1}{2}\vartheta_y, \\ \mathbf{a}_{II}' &= \mathbf{a}_I \cdot i \sinh \frac{1}{2}\vartheta_y + \mathbf{a}_{II} \cdot \cosh \frac{1}{2}\vartheta_y, \\ \mathbf{a}_{III}' &= \mathbf{a}_{III} \cdot \cosh \frac{1}{2}\vartheta_y + \mathbf{a}_{IV} \cdot i \sinh \frac{1}{2}\vartheta_y, \\ \mathbf{a}_{IV}' &= -\mathbf{a}_{III} \cdot i \sinh \frac{1}{2}\vartheta_y + \mathbf{a}_{IV} \cdot \cosh \frac{1}{2}\vartheta_y. \end{aligned}$$

(C) *Motion along the z axis with velocity  $\beta_z c$ .*—

$$\begin{aligned} \mathbf{a}_I' &= \mathbf{a}_I \cdot e^{-\frac{1}{2}\vartheta_z}, & \mathbf{a}_{II}' &= \mathbf{a}_{II} \cdot e^{\frac{1}{2}\vartheta_z}, \\ \mathbf{a}_{III}' &= \mathbf{a}_{III} \cdot e^{\frac{1}{2}\vartheta_z}, & \mathbf{a}_{IV}' &= \mathbf{a}_{IV} \cdot e^{-\frac{1}{2}\vartheta_z}. \end{aligned}$$

The most striking feature to be observed here is the fact that under each of these transformations the two pairs of spin vectors ( $\mathbf{a}_I, \mathbf{a}_{II}$ ) and ( $\mathbf{a}_{III}, \mathbf{a}_{IV}$ ) transform separately by a binary transformation. Since all of the transformations of the Lorentz group can be built up from these basic transformations, the result will hold good

for the complete group (but not including the reflections  $R_0$  and  $R_i$ ).

The reader can easily verify that for all of the transformations given above the relationships existing between the expressions for the two pairs of spin vectors can be expressed by the equations

$$\begin{aligned} \mathbf{a}_I' &= \alpha \mathbf{a}_I + \beta \mathbf{a}_{II}, & \mathbf{a}_{III}' &= \delta^* \mathbf{a}_{III} - \gamma^* \mathbf{a}_{IV}, \\ \mathbf{a}_{II}' &= \gamma \mathbf{a}_I + \delta \mathbf{a}_{II}, & \mathbf{a}_{IV}' &= -\beta^* \mathbf{a}_{III} + \alpha^* \mathbf{a}_{IV}, \end{aligned} \quad (\text{H4})$$

with  $\alpha\delta - \beta\gamma = 1$ . These relationships are preserved for the more general transformations of the group.

We can now see clearly that under the transformations induced by the Lorentz group, the 4-dimensional spin space is reducible to two 2-dimensional sub-spaces which transform separately by means of binary unimodular transformations, and that the transformations in the two separate sub-spaces are not identical, but are intimately related to each other.

The nature of these results can be emphasized by a change in notation. We set

$$\mathbf{e}_1 = \mathbf{a}_I, \quad \mathbf{e}_2 = \mathbf{a}_{II}, \quad \mathbf{u}^1 = \mathbf{a}_{III}, \quad \mathbf{u}^2 = \mathbf{a}_{IV}.$$

The raising of the index on the last two vectors expresses the fact that they transform contragrediently to the first pair, except that the dot beside the index indicates the transition to the complex conjugate transformation coefficients in Eqs. (H4).

If we define further

$$\xi^1 = v_I, \quad \xi^2 = v_{II}, \quad \eta_1 = v_{III}, \quad \eta_2 = v_{IV},$$

the Dirac wave function can be written as

$$\psi = \xi^1 \mathbf{e}_1 + \xi^2 \mathbf{e}_2 + \eta_1 \cdot \mathbf{u}^1 + \eta_2 \cdot \mathbf{u}^2.$$

The two parts

$$\xi^1 \mathbf{e}_1 + \xi^2 \mathbf{e}_2, \quad \eta_1 \cdot \mathbf{u}^1 + \eta_2 \cdot \mathbf{u}^2,$$

which transform separately under the Lorentz group are called *spinors*. The Dirac function  $\psi$  in 4-dimensional space is equivalent to two separate spinors.

It is of interest to examine the behavior of these spinors under the reflections  $R_0$  and  $R_i$  of §20. We find

$$R_0: \xi^1 \rightarrow -\eta_1, \quad \xi^2 \rightarrow -\eta_2, \quad \eta_1 \rightarrow -\xi^1, \quad \eta_2 \rightarrow -\xi^2,$$

$$R_t: \xi^1 \rightarrow \xi^{2*}, \quad \xi^2 \rightarrow -\xi^{1*}, \quad \eta_1 \rightarrow \eta_{2*}, \quad \eta_2 \rightarrow -\eta_{1*}.$$

In particular it is observed that  $R_0$  interchanges the roles of the two spinors, so that under the extended Lorentz group (i.e. the Lorentz transformations as defined in §18 with the addition of reflections) the 4-dimensional spin space is no longer strictly reducible into two separate sub-spaces.

For a more extensive development of the spinor calculus and its relationship to tensor analysis, with the formal re-working of the

Dirac equation and the Maxwell field equations in a consistent spinor notation, the reader is referred to the literature.<sup>76</sup> From the point of view of physical applications the spinor formulation loses some of its formal advantages due to the fact that it obscures the division of the Dirac function into "large" and "small" components, a division which assists materially in the discussion of physical problems.

<sup>76</sup> B. L. van der Waerden, reference 75. O. Laporte and G. Uhlenbeck, *Phys. Rev.* **37**, 1380 (1931). A. Einstein and W. Mayer, *Preuss. Akad. Wiss. Berlin, Ber.* **32**, 522 (1932); *Proc. König. Akad. Amsterdam* **36**, 497 (1933); **36**, 615 (1933). H. A. Kramers, reference 63, §61, §63. G. Rumer *Spinor Analysis* (NKTP, Moscow, 1936). (In Russian.)