wave equation and is altered from the Schrödinger form (1.2) upon which the probability interpretation in the nonrelativistic theory is based. This we do in analogy with the Schrödinger equation, taking ψ^* times (1.11), ψ times the complex conjugate equation, and subtracting:

$$\psi^*\left[\Box + \left(\frac{mc}{\hbar}\right)^2\right]\psi - \psi\left[\Box + \left(\frac{mc}{\hbar}\right)^2\right]\psi^* = 0$$

$$\nabla^\mu(\psi^*\nabla_\mu\psi - \psi\nabla_\mu\psi^*) = 0$$

or

$$\frac{\partial}{\partial t}\left[\frac{i\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)\right] + \operatorname{div}\frac{\hbar}{2im}[\psi^*(\nabla\psi) - \psi(\nabla\psi^*)] = 0 \quad (1.12)$$

We would like to interpret $(i\hbar/2mc^2)\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)$ as a probability density ρ. However, this is impossible, since it is not a positive definite expression. For this reason we follow the path of history[1] and temporarily discard Eq. (1.11) in the hope of finding an equation of first order in the time derivative which admits a straightforward probability interpretation as in the Schrödinger case. We shall return to (1.11), however. Although we shall find a first-order equation, it still proves impossible to retain a positive definite probability density for a single particle while at the same time providing a physical interpretation of the negative-energy root of (1.10). Therefore Eq. (1.11), also referred to frequently as the Klein-Gordon equation, remains an equally strong candidate for a relativistic quantum mechanics as the one which we now discuss.

1.3 The Dirac Equation

We follow the historic path taken in 1928 by Dirac[2] in seeking a relativistically covariant equation of the form (1.2) with positive definite probability density. Since such an equation is linear in the time derivative, it is natural to attempt to form a hamiltonian linear in the space derivatives as well. Such an equation might assume a form

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar c}{i}\left(\alpha_1\frac{\partial\psi}{\partial x^1} + \alpha_2\frac{\partial\psi}{\partial x^2} + \alpha_3\frac{\partial\psi}{\partial x^3}\right) + \beta mc^2\psi \equiv H\psi \quad (1.13)$$

[1] E. Schrödinger, *Ann. Physik*, **81**, 109 (1926); W. Gordon, *Z. Physik*, **40**, 117 (1926); O. Klein, *Z. Physik*, **41**, 407 (1927).

[2] P. A. M. Dirac, *Proc. Roy. Soc.* (*London*), **A117**, 610 (1928); *ibid.*, **A118**, 351 (1928); "The Principles of Quantum Mechanics," *op. cit.*

The coefficients α_i here cannot simply be numbers, since the equation would not be invariant even under a spatial rotation. Also, if we wish to proceed at this point within the framework stated in Sec. 1.1, the wave function ψ cannot be a simple scalar. In fact, the probability density $\rho = \psi^*\psi$ should be the time component of a conserved four-vector if its integral over all space, at fixed t, is to be an invariant.

To free (1.13) from these limitations, Dirac proposed that it be considered as a matrix equation. The wave function ψ, in analogy with the spin wave functions of nonrelativistic quantum mechanics, is written as a column matrix with N components

$$\psi = \begin{bmatrix} \psi_1 \\ \cdot \\ \cdot \\ \cdot \\ \psi_N \end{bmatrix}$$

and the constant coefficients α_i, β are $N \times N$ matrices. In effect then, Eq. (1.13) is replaced by N coupled first-order equations

$$\begin{aligned} i\hbar \frac{\partial \psi_\sigma}{\partial t} &= \frac{\hbar c}{i} \sum_{\tau=1}^{N} \left(\alpha_1 \frac{\partial}{\partial x^1} + \alpha_2 \frac{\partial}{\partial x^2} + \alpha_3 \frac{\partial}{\partial x^3} \right)_{\sigma\tau} \psi_\tau + \sum_{\tau=1}^{N} \beta_{\sigma\tau} mc^2 \psi_\tau \\ &= \sum_{\tau=1}^{N} H_{\sigma\tau} \psi_\tau \end{aligned} \tag{1.14}$$

Hereafter we adopt matrix notation and drop summation indices, in which case Eq. (1.14) appears as (1.13), to be now interpreted as a matrix equation.

If this equation is to serve as a satisfactory point of departure, first, it must give the correct energy-momentum relation

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

for a free particle, second, it must allow a continuity equation and a probability interpretation for the wave function ψ, and third, it must be Lorentz covariant. We now discuss the first two of these requirements.

In order that the correct energy-momentum relation emerge from Eq. (1.13), each component ψ_σ of ψ must satisfy the Klein-Gordon second-order equation, or

$$-\hbar^2 \frac{\partial^2 \psi_\sigma}{\partial t^2} = (-\hbar^2 c^2 \nabla^2 + m^2 c^4) \psi_\sigma \tag{1.15}$$

Iterating Eq. (1.13), we find

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \sum_{i,j=1}^{3} \frac{\alpha_j \alpha_i + \alpha_i \alpha_j}{2} \frac{\partial^2 \psi}{\partial x^i \, \partial x^j} + \frac{\hbar m c^3}{i} \sum_{i=1}^{3} (\alpha_i \beta + \beta \alpha_i) \frac{\partial \psi}{\partial x^i} + \beta^2 m^2 c^4 \psi$$

We may resurrect (1.15) if the four matrices α_i, β obey the algebra:

$$\begin{aligned} \alpha_i \alpha_k + \alpha_k \alpha_i &= 2\delta_{ik} \\ \alpha_i \beta + \beta \alpha_i &= 0 \\ \alpha_i^2 = \beta^2 &= 1 \end{aligned} \tag{1.16}$$

What other properties do we require of these four matrices α_i, β, and can we explicitly construct them? The α_i and β must be hermitian matrices in order that the hamiltonian $H_{\sigma\tau}$ in (1.14) be a hermitian operator as desired according to the postulates of Sec. 1.1. Since, by (1.16), $\alpha_i^2 = \beta^2 = 1$, the eigenvalues of α_i and β are ± 1. Also, it follows from their anticommutation properties that the trace, that is, the sum of the diagonal elements, of each α_i and β is zero. For example,

$$\alpha_i = -\beta \alpha_i \beta$$

and by the cyclic property of the trace

$$\operatorname{Tr} AB = \operatorname{Tr} BA$$

one has

$$\operatorname{Tr} \alpha_i = + \operatorname{Tr} \beta^2 \alpha_i = + \operatorname{Tr} \beta \alpha_i \beta = - \operatorname{Tr} \alpha_i = 0$$

Since the trace is just the sum of eigenvalues, the number of positive and negative eigenvalues ± 1 must be equal, and the α_i and β must therefore be even-dimensional matrices. The smallest even dimension, $N = 2$, is ruled out, since it can accommodate only the three mutually anticommuting Pauli matrices σ_i plus a unit matrix. The smallest dimension in which the α_i and β can be realized is $N = 4$, and that is the case we shall study. In a particular explicit representation the matrices are

$$\alpha_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix} \qquad \beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1.17}$$

where the σ_i are the familiar 2×2 Pauli matrices and the unit entries in β stand for 2×2 unit matrices.

To construct the differential law of current conservation, we first introduce the hermitian conjugate wave functions $\psi^\dagger = (\psi_1^* \cdots \psi_4^*)$

and left-multiply (1.13) by $\psi^\dagger$:

$$i\hbar\psi^\dagger \frac{\partial\psi}{\partial t} = \frac{\hbar c}{i} \sum_{k=1}^{3} \psi^\dagger \alpha_k \frac{\partial}{\partial x^k} \psi + mc^2\psi^\dagger\beta\psi \tag{1.18}$$

Next we form the hermitian conjugate of (1.13) and right-multiply by ψ:

$$-i\hbar \frac{\partial\psi^\dagger}{\partial t} \psi = -\frac{\hbar c}{i} \sum_{k=1}^{3} \frac{\partial\psi^\dagger}{\partial x^k} \alpha_k\psi + mc^2\psi^\dagger\beta\psi \tag{1.19}$$

where $\alpha_i^\dagger = \alpha_i$, $\beta_i^\dagger = \beta$. Subtracting (1.19) from (1.18), we find

$$i\hbar \frac{\partial}{\partial t} \psi^\dagger\psi = \sum_{k=1}^{3} \frac{\hbar c}{i} \frac{\partial}{\partial x^k} (\psi^\dagger\alpha^k\psi)$$

or

$$\frac{\partial}{\partial t} \rho + \operatorname{div} \mathbf{j} = 0 \tag{1.20}$$

where we make the identification of probability density

$$\rho = \psi^\dagger\psi = \sum_{\sigma=1}^{4} \psi_\sigma^*\psi_\sigma \tag{1.21}$$

and of a probability current with three components

$$j^k = c\psi^\dagger\alpha^k\psi \tag{1.22}$$

Integrating (1.20) over all space and using Green's theorem, we find

$$\frac{\partial}{\partial t} \int d^3x \psi^\dagger\psi = 0 \tag{1.23}$$

which encourages the tentative interpretation of $\rho = \psi^\dagger\psi$ as a positive definite probability density.

The notation (1.20) anticipates that the probability current $\mathbf{j}$ forms a vector if (1.22) is to be invariant under three-dimensional space rotations. We must actually show much more than this. The density and current in (1.20) must form a four-vector under Lorentz transformations in order to ensure the covariance of the continuity equation and of the probability interpretation. Also, the Dirac equation (1.13) must be shown to be Lorentz covariant before we may regard it as satisfactory.

1.4 Nonrelativistic Correspondence

Before delving into the problem of establishing Lorentz invariance of the Dirac theory, it is perhaps more urgent to see first that the equation makes sense physically.

We may start simply by considering a free electron and counting the number of solutions corresponding to an electron at rest. Equation (1.13) then reduces to

$$i\hbar \frac{\partial \psi}{\partial t} = \beta mc^2 \psi$$

since the de Broglie wavelength is infinitely large and the wave function is uniform over all space. In the specific representation of Eq. (1.17) for β, we can write down by inspection four solutions:

$$\psi^1 = e^{-(imc^2/\hbar)t} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad \psi^2 = e^{-(imc^2/\hbar)t} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$
$$\psi^3 = e^{+(imc^2/\hbar)t} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad \psi^4 = e^{+(imc^2/\hbar)t} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{1.24}$$

the first two of which correspond to positive energy, and the second two to negative energy. The extraneous negative-energy solutions which result from the quadratic form of $H^2 = p^2c^2 + m^2c^4$ are a major difficulty, but one for which the resolution leads to an important triumph in the form of antiparticles. We come to this point in Chap. 5. Here we confine ourselves to the "acceptable" positive-energy solutions. In particular, we wish to show that they have a sensible nonrelativistic reduction to the two-component Pauli spin theory. To this end we introduce an interaction with an external electromagnetic field described by a four-potential

$$A^\mu : (\Phi, \mathbf{A})$$

The coupling is most simply introduced by means of the gauge-invariant substitution

$$p^\mu \rightarrow p^\mu - \frac{e}{c} A^\mu \tag{1.25}$$

made in classical relativistic mechanics to describe the interaction of a point charge e with an applied field. In the present case

$$p^\mu \rightarrow i\hbar\, \partial/\partial x_\mu \equiv \mathsf{p}^\mu$$

according to (1.5), and (1.25) takes the Dirac equation (1.13) to

$$i\hbar \frac{\partial \psi}{\partial t} = \left(c\boldsymbol{\alpha} \cdot \left(\mathbf{p} - \frac{e}{c}\mathbf{A} \right) + \beta mc^2 + e\Phi \right) \psi \tag{1.26}$$

Equation (1.26) expresses the "minimal" interaction of a Dirac particle, considered to be a point charge, with an applied electromagnetic field. To emphasize its classical parallel, we write in (1.26) $H = H_0 + H'$, with $H' = -e\boldsymbol{\alpha} \cdot \mathbf{A} + e\Phi$. The matrix $c\boldsymbol{\alpha}$ appears here as the operator transcription of the velocity operator in the classical expression for the interaction energy of a point charge:

$$H'_{\text{classical}} = -\frac{e}{c}\mathbf{v} \cdot \mathbf{A} + e\Phi$$

This operator correspondence $\mathbf{v}_{\text{op}} = \mathbf{c}\boldsymbol{\alpha}$ is again evident in Eq. (1.22) for the probability current. It also follows if we make the relativistic extension of the Ehrenfest relations:[1]

$$\frac{d}{dt}\mathbf{r} = \frac{i}{\hbar}[H,\mathbf{r}] = \mathbf{c}\boldsymbol{\alpha} \equiv \mathbf{v}_{\text{op}}$$

and

$$\frac{d}{dt}(\boldsymbol{\pi}) = \frac{i}{\hbar}[H,\boldsymbol{\pi}] - \frac{e}{c}\frac{\partial}{\partial t}\mathbf{A}$$

$$\frac{d}{dt}(\boldsymbol{\pi}) = e\left[\mathbf{E} + \frac{1}{c}\mathbf{v}_{\text{op}} \times \mathbf{B} \right] \tag{1.27}$$

with $\boldsymbol{\pi} \equiv \mathbf{p} - (e/c)\mathbf{A}$ the operator corresponding to the kinetic momentum and

$$\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla\Phi \qquad \text{and} \qquad \mathbf{B} = \text{curl}\,\mathbf{A}$$

the field strengths. Equation (1.27) is the operator equation of motion for a point charge e. More general couplings in (1.26) would lead to specific dipole and higher multipole terms in analogy with the classical development.

In taking the nonrelativistic limit of Eq. (1.26), it is convenient to work in the specific representation of Eq. (1.17) and to express the

[1] Pauli, Schiff, and Dirac, *op. cit.*

wave function in terms of two-component column matrices $\tilde{\varphi}$ and $\tilde{\chi}$:

$$\psi = \begin{bmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{bmatrix} \tag{1.28}$$

We then obtain for (1.26)

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{bmatrix} = c\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \begin{bmatrix} \tilde{\chi} \\ \tilde{\varphi} \end{bmatrix} + e\Phi \begin{bmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{bmatrix} + mc^2 \begin{bmatrix} \tilde{\varphi} \\ -\tilde{\chi} \end{bmatrix}$$

In the nonrelativistic limit the rest energy mc^2 is the largest energy in the problem and we write

$$\begin{bmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{bmatrix} = e^{-(imc^2/\hbar)t} \begin{bmatrix} \varphi \\ \chi \end{bmatrix} \tag{1.29}$$

where now φ and χ are relatively slowly varying functions of time which are solutions of the coupled equations

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \varphi \\ \chi \end{bmatrix} = c\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \begin{bmatrix} \chi \\ \varphi \end{bmatrix} + e\Phi \begin{bmatrix} \varphi \\ \chi \end{bmatrix} - 2mc^2 \begin{bmatrix} 0 \\ \chi \end{bmatrix} \tag{1.30}$$

The second of Eqs. (1.30) may be approximated, for kinetic energies and field interaction energies small in comparison with mc^2, to

$$\chi = \frac{\boldsymbol{\sigma} \cdot \boldsymbol{\pi}}{2mc} \varphi \tag{1.31}$$

Equation (1.31) reveals χ as the "small" components of the wave function ψ in comparison with the "large" components φ. Relative to φ, χ is reduced by $\sim v/c \ll 1$ in the nonrelativistic approximation. Inserting (1.31) into the first of Eqs. (1.30), we obtain a two-component spinor equation

$$i\hbar \frac{\partial \varphi}{\partial t} = \left(\frac{\boldsymbol{\sigma} \cdot \boldsymbol{\pi}\, \boldsymbol{\sigma} \cdot \boldsymbol{\pi}}{2m} + e\Phi \right) \varphi \tag{1.32}$$

This is further reduced by the identity for Pauli spin matrices

$$\boldsymbol{\sigma} \cdot \mathbf{a}\, \boldsymbol{\sigma} \cdot \mathbf{b} = \mathbf{a} \cdot \mathbf{b} + i\boldsymbol{\sigma} \cdot \mathbf{a} \times \mathbf{b}$$

or, here,

$$\begin{aligned} \boldsymbol{\sigma} \cdot \boldsymbol{\pi}\, \boldsymbol{\sigma} \cdot \boldsymbol{\pi} &= \boldsymbol{\pi}^2 + i\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \times \boldsymbol{\pi} \\ &= \boldsymbol{\pi}^2 - \frac{e\hbar}{c} \boldsymbol{\sigma} \cdot \mathbf{B} \end{aligned} \tag{1.33}$$

Then we have

$$i\hbar \frac{\partial \varphi}{\partial t} = \left[\frac{(\mathbf{p} - (e/c)\mathbf{A})^2}{2m} - \frac{e\hbar}{2mc} \boldsymbol{\sigma} \cdot \mathbf{B} + e\Phi \right] \varphi \tag{1.34}$$

which is recognized[1] as the Pauli equation. Equation (1.34) gives us confidence that we are on the right track in accepting Eqs. (1.13) and (1.26) as a starting point in constructing a relativistic electron theory. The two components of φ suffice to accommodate the two spin degrees of freedom of a spin one-half electron; and the correct magnetic moment of the electron, corresponding to the gyromagnetic ratio $g = 2$, automatically emerges. To see this explicitly, we reduce (1.34) further, keeping only first-order terms in the interaction with a weak uniform magnetic field $\mathbf{B} = \text{curl}\,\mathbf{A}$; $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$:

$$i\hbar \frac{\partial \varphi}{\partial t} = \left[\frac{\mathbf{p}^2}{2m} - \frac{e}{2mc}(\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B}\right]\varphi \qquad (1.35)$$

Here $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the orbital angular momentum, $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ is the electron spin, with eigenvalues $\pm\hbar/2$, and the coefficient of the interaction of the spin with $\mathbf{B}$ field gives the correct magnetic moment of the electron corresponding to a g value of 2.

Fortified by this successful nonrelativistic reduction of the Dirac equation, we go on and establish the Lorentz covariance of the Dirac theory, as required by special relativity. Next we must investigate further physical consequences of this theory; especially we must interpret those "negative-energy" solutions.

Problems

1. Write the Maxwell equations in Dirac form (1.13) in terms of a six-component field amplitude. What are the matrices corresponding to α and β? [See H. E. Moses, *Phys. Rev.*, **113**, 1670 (1959).]

2. Verify that the matrices (1.17) satisfy the algebra of (1.16).

3. Verify (1.33).

4. Verify (1.27).

[1] *Ibid.*