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The Dirac equation in orthogonal coordinate systems†: I. The local representation

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Abstract. A new approach to handle the Dirac equation in orthogonal curvilinear coordinate systems is presented. It is applicable at least for all coordinate systems which can be described by conformal mappings in a specified manner. The method is based on a space-dependent transformation of the wavefunction corresponding to a space-dependent set of Dirac matrices, a local representation. This transformation, which can be given in closed form, is chosen in such a way that the Dirac equation in the given coordinates assumes a very simple form, well suited for numerical and analytical examinations. The relationship between the different forms of the Dirac equation is then discussed. The special case of spherical coordinates is investigated in detail.

1. Introduction

Electrons and other spin-$\frac{1}{2}$ particles are described relativistically by the Dirac equation (Dirac 1928), a partial differential equation in the four space–time coordinates. In the absence of an electromagnetic potential, solutions like plane waves or spherical Bessel functions are known. Moreover, these solutions can be chosen to be eigenfunctions of any operator commuting with the Hamiltonian, such as momentum, angular momentum or parity. But there are only very few cases where stationary eigenfunctions and eigenvalues are known explicitly, if the electron interacts with an external potential. The best known example is the pure Coulomb potential. Frequently the potential possesses some geometrical symmetries, for instance invariance under arbitrary rotations around a fixed point, which in some cases can be used to reduce the Dirac equation to a system of ordinary differential equations. However, this is impossible even for such interesting potentials as those generated by two fixed point-like nuclei. Here the best one can do is to separate one coordinate in the stationary problem, for example the azimuthal angle φ. Then one is left with a partial differential equation in two coordinates, which has to be solved numerically.

The optimal set of coordinates to be chosen depends strongly on the potential examined. They should 'fit' it. Firstly the potential should take a simple form in the particular coordinates used; especially the singularities and symmetries should match.

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A second point in choosing new coordinates, which, of course, have to be mathematically still manageable, is a suitable asymptotic behaviour; then sometimes simple asymptotic expressions for the wavefunctions near the boundaries can be found. To formulate the problem in non-cartesian coordinates we can use the general relativistic formulation of the Dirac equation in a Minkowski space (Fock 1929, Schmutzer 1968), using the covariant derivative with space-dependent spinor-connections. For example, the spherical Dirac equation, in the presence of an external potential V, reads

$$\left[-\mathrm{i}\left(\gamma^0\frac{\partial}{\partial t}+\gamma^1\frac{1}{r}\frac{\partial}{\partial\theta}+\gamma^2\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}+\gamma^3\frac{\partial}{\partial r}\right)+m+\gamma^0V-\mathrm{i}\left(\frac{\cot\theta}{2r}\gamma^1+\frac{1}{r}\gamma^3\right)\right]\psi_{\mathrm{r}}=0. \quad (1.1)$$

We use the convention $\hbar=c=1$ throughout. Another way is the direct transformation of the coordinates, starting with the cartesian Dirac equation, where the spinor connections vanish. This generates space-dependent matrices, $\bar{\gamma}^\mu$, in front of the derivatives. Here the Dirac equation becomes (Rose 1961)

$$\left[-\mathrm{i}\left(\gamma^0\frac{\partial}{\partial t}+\bar{\gamma}^1\frac{1}{r}\frac{\partial}{\partial\theta}+\bar{\gamma}^2\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}+\bar{\gamma}^3\frac{\partial}{\partial r}\right)+m+\gamma^0V\right]\psi_{\mathrm{c}}=0 \quad (1.2)$$

with the matrices

$$\begin{aligned}\bar{\gamma}^1&=\cos\theta(\cos\varphi\,\gamma^1+\sin\varphi\,\gamma^2)-\sin\theta\,\gamma^3,\\ \bar{\gamma}^2&=-\sin\varphi\,\gamma^1+\cos\varphi\,\gamma^2,\\ \bar{\gamma}^3&=\sin\theta(\cos\varphi\,\gamma^1+\sin\varphi\,\gamma^2)+\cos\theta\,\gamma^3.\end{aligned} \quad (1.3)$$

In both cases we arrive at a rather complicated partial differential equation. Clearly, the two wavefunctions, ψ_{r} and ψ_{c}, are not identical. The connection between them is not trivial.

Subsequently we will show that there exists a third possibility combining the advantages of the previously mentioned ones. This leads to

$$\left[-\mathrm{i}\left(\gamma^0\frac{\partial}{\partial t}+\gamma^1\frac{1}{r}\frac{\partial}{\partial\theta}+\gamma^2\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}+\gamma^3\frac{\partial}{\partial r}\right)+m+\gamma^0V\right]\psi=0. \quad (1.4)$$

Moreover, we can give immediately the connecting transformation between the three wavefunctions,

$$\psi_{\mathrm{c}}=S\psi_{\mathrm{r}}=\mathrm{e}^{B}S\psi, \quad (1.5)$$

with a certain space-dependent unitary matrix S and a scalar-valued function B, which can be given in closed form. The method can be applied at least for all coordinate systems which can be obtained from the cartesian system in one or more steps by conformal mappings. This means that it is practicable for all coordinate systems normally encountered in applications, in particular for the 37 systems described by Moon and Spencer (1961). Such a unitary transformation corresponds to a new representation of the Dirac matrices. Because of the space dependence of S we will call it a local representation (Good 1955). We will show that the added flexibility of a space-dependent representation may lead to significant simplifications. Not only the Hamiltonian, but also other operators of physical interest appear in an astonishingly simple form. For example, the z component of the total angular momentum operator just becomes

$$\hat{J}_z=-\mathrm{i}\,\partial/\partial\varphi. \quad (1.6)$$

The expressions for orbital or spin angular momentum alone are much more complicated.

Because of this simplicity it can be expected that the numerical treatment of the Dirac equation as a partial differential equation needs far less expense, if we use the local representation. Furthermore, it will be much easier to find analytical expressions for eigenfunctions of an operator, if this operator has a simple structure. A trivial example is given by $\hat{J}_z$ where every bispinor of the form $\psi(r, \theta)\, e^{i\mu\varphi}$ yields an eigenfunction with eigenvalue μ. Finally, we think that these advantages are a motivation *per se* to study the Dirac equation in the local representation.

This paper is organised as follows. In § 2 we will fix the notation, develop the idea on which the method is based and find some of its properties. In § 3 the Dirac equation in local representation is derived for cylindrical coordinates. Next we will show how to calculate the transformation matrix in less trivial cases. It is proven that the method is applicable for all coordinate systems which can be obtained from conformal mappings in a certain sense. Finally we will study in § 5 the special case of spherical coordinates in detail. The application to the two-centre Dirac equation is postponed to the following paper.

2. The local representation

The Dirac equation in cartesian coordinates $x_c^\mu = (t, x, y, z)$ reads, in the presence of an electromagnetic potential A_c^μ,

$$[\gamma^\mu(i\hat{D}_\mu^c - eA_\mu^c) - m]\psi_c = 0 \tag{2.1}$$

with the derivative

$$\hat{D}_\mu^c = \partial/\partial x_c^\mu. \tag{2.2}$$

Greek indices run from 0 to 3, Latin indices through 1, 2, 3. The summation convention is used for Greek indices only. Here $\{\gamma^\mu\}$ denotes a set of four constant 4×4 matrices, which obey the well known anticommutator relations

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} = 2\,\mathrm{diag}(+1, -1, -1, -1) \tag{2.3}$$

as well as the hermiticity condition

$$\gamma^{\mu\,+} = \gamma^0\gamma^\mu\gamma^0. \tag{2.4}$$

Therefore the adjoint spinor is

$$\bar{\psi}_c = \psi_c^+\gamma^0. \tag{2.5}$$

For further reference we introduce the following abbreviations for some products of γ-matrices:

$$\begin{aligned} &\alpha_k = \gamma^0\gamma^k, \qquad &&\Sigma_k = \tfrac{1}{2}i\sum_{lm}\varepsilon_{klm}\gamma^l\gamma^m, \\ &\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3, \qquad &&\rho^\mu = i\gamma^5\gamma^\mu. \end{aligned} \tag{2.6}$$

Together with the 4×4 unit matrix and the four γ-matrices they form a set of 16 linearly independent matrices. All products, commutators or anticommutators of these matrices can be obtained directly from (2.3); this means that the result can be expressed as a linear combination of our basic matrices. We mention that most

calculations can be done without reference to a specific representation of the γ-matrices.

Different representations are closely interrelated. This is the proposition of:

Pauli's fundamental theorem (Pauli 1936). Two sets $\{\gamma^\mu\}$ and $\{\bar{\gamma}^\mu\}$ of Dirac matrices, each fulfilling the anticommutator relations (2.3), are connected by a similarity transformation, unique up to a factor. If, besides this, both sets obey (2.4), the transformation matrix can be chosen unitary. More definitely: from

$$\begin{aligned} &\{\gamma^\mu, \gamma^\nu\} = \{\bar{\gamma}^\mu, \bar{\gamma}^\nu) = 2g^{\mu\nu}, \\ &\gamma^{\mu\,+} = \gamma^0\gamma^\mu\gamma^0, \qquad \bar{\gamma}^{\mu\,+} = \bar{\gamma}^0\bar{\gamma}^\mu\bar{\gamma}^0, \end{aligned} \tag{2.7}$$

it follows that there exists a unitary matrix S, such that

$$\bar{\gamma}^\mu = S\gamma^\mu S^{-1}, \tag{2.8}$$

and this matrix is unique up to a phase.

Now we want to introduce into the Dirac equation new orthogonal space coordinates $x^\mu = (x^0, x^1, x^2, x^3)$. We demand that $\{x^i\}$ depends on $\{x_c^i\}$ only, i.e. it has to be independent of $x_c^0 = x^0 = t$. Moreover, we assume for simplicity that the three orthogonal unit vectors ($\boldsymbol{e}_i^c$ denote the cartesian unit vectors)

$$\boldsymbol{e}_i = \frac{1}{h_i}\sum_j \frac{\partial x_c^j}{\partial x^i}\boldsymbol{e}_j^c \tag{2.9}$$

form a right-handed system. Here we have denoted the scale factors as

$$h_i = \left(\sum_j (\partial x_c^j/\partial x^i)^2\right)^{1/2}; \tag{2.10}$$

then the three-dimensional volume element changes according to

$$\mathrm{d}\tau = \mathrm{d}x_c^1\,\mathrm{d}x_c^2\,\mathrm{d}x_c^3 = h_1h_2h_3\,\mathrm{d}x^1\,\mathrm{d}x^2\,\mathrm{d}x^3. \tag{2.11}$$

The components V^i of any three-vector

$$\boldsymbol{V} = \sum_i \boldsymbol{e}_i^c V_c^i = \sum_i \boldsymbol{e}_i V^i \tag{2.12}$$

in the new system are

$$V^i = \frac{1}{h_i}\sum_j \frac{\partial x_c^j}{\partial x^i} V_c^j. \tag{2.13}$$

The components of the derivative become simply

$$\hat{D}_j = (h_j)^{-1}\,\partial/\partial x^j. \tag{2.14}$$

Thus the Dirac equation reads ($A^0 = A_c^0$, $\hat{D}_0 = \hat{D}_0^c$)

$$[\bar{\gamma}^\mu(\mathrm{i}\hat{D}_\mu - eA_\mu) - m]\psi_c = 0. \tag{2.15}$$

Here the matrices

$$\bar{\gamma}^0 = \gamma^0, \qquad \bar{\gamma}^j = h_j\sum_k \frac{\partial x^j}{\partial x_c^k}\gamma^k = \frac{1}{h_j}\sum_k \frac{\partial x_c^k}{\partial x^j}\gamma^k, \tag{2.16}$$

appear, which in general will depend on the x^i, for the basis vectors $\boldsymbol{e}_i$ will do so.

However, since the $\boldsymbol{e}_j$ are orthogonal, the $\bar{\gamma}$'s obey the same anticommutator relations and hermiticity conditions, namely

$$\{\bar{\gamma}^\mu, \bar{\gamma}^\nu\} = 2g^{\mu\nu}, \qquad \bar{\gamma}^{\mu+} = \bar{\gamma}^0\bar{\gamma}^\mu\bar{\gamma}^0, \tag{2.17}$$

with the old, cartesian $g^{\mu\nu}$.

Therefore we know from Pauli's fundamental theorem that there exists a unitary matrix S, generally space-dependent, which transforms them back into the old γ's, cf (2.8).

Now it seems obvious to make the following ansatz:

$$\psi_c = e^B S\psi, \tag{2.18}$$

where e^B denotes a non-zero complex factor, independent of t, which is up to now completely arbitrary. Inserting this into the Dirac equation, we get, after multiplication from the left with $e^{-B}S^{-1}$,

$$[\gamma^\mu(i\hat{D}_\mu - eA_\mu + i\Gamma_\mu) - m]\psi = 0 \tag{2.19}$$

with an additional term

$$\Gamma_\mu = e^{-B}S^{-1}(\hat{D}_\mu e^B S) = \hat{D}_\mu B + S^{-1}\hat{D}_\mu S. \tag{2.20}$$

Thus we have the old γ-matrices in the Dirac equation, now multiplied with the components $\hat{D}_\mu$ and A_μ in the new coordinate system. After the discussion of an example in the next paragraph we will show that in many important cases a B can be found such that the term $\gamma^\mu\Gamma_\mu$ vanishes. If we choose $B = 0$, we get an equation similar to (1.1), the Dirac equation formulated according to general relativity. So S is the unitary matrix transforming ψ_c into ψ_r, cf (1.5), and $S^{-1}\hat{D}_\mu S$ have to be the spinor connections. We will come back to this point in § 4. Clearly the behaviour under gauge transformations is not affected. An ansatz like (2.18) implies a transition to a new representation of γ-matrices. Here S depends generally on the coordinates x^i, thus we have a space-dependent or 'local' representation. It has the advantage, at least for $\gamma^\mu\Gamma_\mu = 0$, that the Dirac equation takes a much simpler form.

An observable $\hat{O}_c$ of the original, cartesian representation is transformed according to

$$\hat{O}_c \to \hat{O} = e^{-B}S^{-1}\hat{O}_c e^B S. \tag{2.21}$$

We mention that the derivative $\hat{D}_i$, defined in (2.2) and (2.14), has to be distinguished from the momentum operator $\hat{p}_i$. As an example we consider the Hamiltonian assuming $\gamma^\mu\Gamma_\mu = 0$.

$$\hat{H}_c = \sum_k \alpha_k(-i\hat{D}_k^c + eA_k^c) + eA_0^c + \gamma^0 m \to \hat{H} = \sum_k \alpha_k(-i\hat{D}_k + eA_k) + eA_0 + \gamma^0 m. \tag{2.22}$$

What will happen to bilinear expressions, especially to the current density

$$j_c^\mu = \bar{\psi}_c\gamma^\mu\psi_c, \tag{2.23}$$

if it expressed in terms of ψ? Firstly, there occurs for all μ a factor $e^{2\,\mathrm{Re}(B)}$; besides this factor j^0 will remain unchanged. It will be suitable to look for the components of $\boldsymbol{j}$ in the new coordinate system, because they will take a simple form too:

$$j_0 = \bar{\psi}\gamma^0\psi\, e^{2\,\mathrm{Re}(B)}, \qquad j^i = \bar{\psi}_c\boldsymbol{\gamma}\cdot\mathbf{e}_i\psi_c = \bar{\psi}\gamma^i\psi\, e^{2\,\mathrm{Re}(B)}. \tag{2.24}$$

The normalisation condition now becomes

$$\int \mathrm{d}\tau\, \psi_c^+ \psi_c = \int \mathrm{d}\tau\, \mathrm{e}^{2\,\mathrm{Re}(B)} \psi^+ \psi = 1, \tag{2.25}$$

where $\mathrm{d}\tau$ is given in (2.11).

3. The Dirac equation in cylindrical coordinates

As a first illustrative example we will examine the Dirac equation in cylindrical coordinates:

$$x = \rho \cos\varphi, \qquad y = \rho \sin\varphi, \qquad z = z. \tag{3.1}$$

Inserting this transformation into the Dirac equation (2.1) we get

$$\left[\gamma^0\left(\mathrm{i}\frac{\partial}{\partial t} - eA_0\right) + (\cos\varphi\,\gamma^1 + \sin\varphi\,\gamma^2)\left(\mathrm{i}\frac{\partial}{\partial\rho} - eA_\rho\right)\right.$$
$$\left. + (-\sin\varphi\,\gamma^1 + \cos\varphi\gamma^2)\left(\mathrm{i}\frac{1}{\rho}\frac{\partial}{\partial\varphi} - eA_\varphi\right) + \gamma^3\left(\mathrm{i}\frac{\partial}{\partial z} - eA_z\right) - m\right]\psi_c = 0 \tag{3.2}$$

corresponding to (2.15). Here $A_\rho = \boldsymbol{A}\cdot\boldsymbol{e}_\rho$ and $A_\varphi = \boldsymbol{A}\cdot\boldsymbol{e}_\varphi$ are the components of the vector potential in cylindrical coordinates. Thus we have the space-dependent matrices

$$\tilde\gamma^1 = \cos\varphi\,\gamma^1 + \sin\varphi\,\gamma^2, \qquad \tilde\gamma^2 = -\sin\varphi\,\gamma^1 + \cos\varphi\,\gamma^2, \qquad \tilde\gamma^0 = \gamma^0, \qquad \tilde\gamma^3 = \gamma^3. \tag{3.3}$$

A matrix S, transforming them back into the γ^μ, is easily found:

$$S = \exp(-\tfrac{1}{2}\mathrm{i}\varphi\Sigma_3) = \cos(\tfrac{1}{2}\varphi) - \mathrm{i}\sin(\tfrac{1}{2}\varphi)\,\Sigma_3. \tag{3.4}$$

Σ_3 is just the generator for rotations around the z axis. Hence the ansatz

$$\psi_c = \mathrm{e}^B \exp(-\tfrac{1}{2}\mathrm{i}\varphi\Sigma_3)\psi \tag{3.5}$$

will lead to (2.19) in cylindrical coordinates with the additional term

$$\gamma^\mu\Gamma_\mu = \gamma^1\left(\frac{\partial}{\partial\rho}B + \exp(\tfrac{1}{2}\mathrm{i}\varphi\Sigma_3)\frac{\partial}{\partial\rho}\exp(-\tfrac{1}{2}\mathrm{i}\varphi\Sigma_3)\right)$$
$$+ \gamma^2\left(\frac{1}{\rho}\frac{\partial}{\partial\varphi}B + \exp(\tfrac{1}{2}\mathrm{i}\varphi\Sigma_3)\frac{1}{\rho}\frac{\partial}{\partial\varphi}\exp(-\tfrac{1}{2}\mathrm{i}\varphi\Sigma_3)\right) \tag{3.6}$$

where we assumed that B depends on ρ and φ only. Equation (3.6) becomes

$$\gamma^\mu\Gamma_\mu = \gamma^1(\partial B/\partial\rho + 1/2\rho) + \gamma^2(\rho^{-1}\,\partial B/\partial\varphi). \tag{3.7}$$

This term will vanish if we choose

$$B = -\tfrac{1}{2}\log\rho, \qquad \mathrm{e}^B = 1/\sqrt{\rho}. \tag{3.8}$$

In this case the Dirac equation simply reads

$$\left[\gamma^0\left(\mathrm{i}\frac{\partial}{\partial t} - eA_0\right) + \gamma^1\left(\mathrm{i}\frac{\partial}{\partial\rho} - eA_\rho\right) + \gamma^2\left(\mathrm{i}\frac{1}{\rho}\frac{\partial}{\partial\varphi} - eA_\varphi\right) + \gamma^3\left(\mathrm{i}\frac{\partial}{\partial z} - eA_z\right) - m\right]\psi = 0. \tag{3.9}$$

This new wavefunction has to be normalised according to

$$\int \mathrm{d}z\ \mathrm{d}\rho\ \mathrm{d}\varphi\ \psi^{+}\psi = 1. \tag{3.10}$$

We observe that the density function ρ is just cancelled by the factor e^{2B}. Clearly, the Hamiltonian is now

$$\hat{H} = \alpha_1\left(-\mathrm{i}\frac{\partial}{\partial\rho} + eA_\rho\right) + \alpha_2\left(-\mathrm{i}\frac{1}{\rho}\frac{\partial}{\partial\varphi} + eA_\varphi\right) + \alpha_3\left(-\mathrm{i}\frac{\partial}{\partial z} + eA_z\right) + eA_0 + \gamma^0 m. \tag{3.11}$$

If the electromagnetic potential is independent of the azimuthal angle φ, the operator $-\mathrm{i}\,\partial/\partial\varphi$ commutes with $\hat{H}$.

Because of (2.21) the z component of the angular momentum operator becomes

$$\hat{J}_z = \sqrt{\rho}\exp(\tfrac{1}{2}\mathrm{i}\varphi\Sigma_3)\left(-\mathrm{i}\frac{\partial}{\partial\varphi} + \tfrac{1}{2}\Sigma_3\right)\frac{1}{\sqrt{\rho}}\exp(-\tfrac{1}{2}\mathrm{i}\varphi\Sigma_3) = -\mathrm{i}\frac{\partial}{\partial\varphi}. \tag{3.12}$$

Normally one would expect that $-\mathrm{i}\,\partial/\partial\varphi$ has the eigenvalues $0, \pm 1, \ldots$, while for the electron as a spin-$\frac{1}{2}$ particle the eigenvalues of $\hat{J}_z$ should be $\pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$. The explanation is as follows. The coordinate space (ρ, φ, z) is not unique; any interval $\varphi_L < \varphi < \varphi_L + 2\pi$, $\varphi_L \in \mathbb{R}$ is possible. The original wavefunction ψ_c has to be continuous everywhere, i.e.

$$\psi_c(\varphi = \varphi_L) = \psi_c(\varphi = \varphi_L + 2\pi). \tag{3.13}$$

Once an interval, i.e. a value of φ_L, is chosen, the matrix S of (3.4) is well defined. However, different intervals will lead to different unitary matrices. Paying attention to

$$S(\varphi_L) = -S(\varphi_L + 2\pi), \tag{3.14}$$

despite the fact that φ_L and $\varphi_L + 2\pi$ denote the same point, it becomes clear that we have to require

$$\psi(\varphi = \varphi_L) = -\psi(\varphi = \varphi_L + 2\pi). \tag{3.15}$$

With these boundary conditions $\hat{J}_z = -\mathrm{i}(\partial/\partial\varphi)$ is a hermitian operator, having the eigenvalues

$$\mu = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \ldots. \tag{3.16}$$

The eigenfunctions are

$$\hat{J}_z\psi(\rho, z)\,\mathrm{e}^{\mathrm{i}\mu\varphi} = \mu\psi(\rho, z)\,\mathrm{e}^{\mathrm{i}\mu\varphi}, \tag{3.17}$$

and each component of the spinor wavefunction possesses the same factor $\mathrm{e}^{\mathrm{i}\mu\varphi}$.

4. Derivation of the transformation matrix

In the general case it will be rather difficult to find a unitary matrix S and a function B such that the Dirac equation takes the simple form

$$[\gamma^\mu(\mathrm{i}\hat{D}_\mu - eA_\mu) - m]\psi = 0, \tag{4.1}$$

or, written in detail,

$$\left[\mathrm{i}\left(\gamma^0 \frac{\partial}{\partial t}+\sum_j \gamma^j \frac{1}{h_j} \frac{\partial}{\partial x^j}\right)-e\left(\gamma^0 A^0-\sum_j \gamma^j A^j\right)-m\right]\psi=0. \tag{4.2}$$

Here the A^j denote the components of $\boldsymbol{A}$ in the coordinate system $\{x_i\}$, cf (2.13), expressed by the new variables. Therefore, we want to restrict the coordinate transformations to a certain class. This class consists of transformations which can be written as a product of transformations in two coordinates. The single transformations have to be induced by conformal mappings; the precise meaning of this will be discussed below. Sometimes it is useful to insert a transformation in one variable, leaving S and B unchanged; only a scale factor will be modified. Such a modification serves as a preparation of the coordinate couple for further conformal mappings, cf (4.5) below.

The most important property of conformal mappings is their preservation of angles and orientation (Behnke and Sommer 1976). They are described by holomorphic functions. In particular, this implies that the lines with $\mathrm{Re}\, f(\zeta)=\text{constant}$ are orthogonal to those with constant imaginary part for any holomorphic function $f(\zeta)$. So, combining x_i and x_j to the complex variable

$$\zeta = x_i + \mathrm{i}x_j, \tag{4.3}$$

we get a new orthogonal coordinate system through

$$x_i' = \mathrm{Re}\, f(\zeta), \qquad x_j' = \mathrm{Im}\, f(\zeta), \tag{4.4}$$

which has the same orientation as the old one. However, we will say that the coordinate transformation is induced by the conformal mapping f only, if the scale factors coincide:

$$h_i = h_j = h. \tag{4.5}$$

This relation is not destroyed by the coordinate transformation, for we have

$$h_i' = h_j' = h' = \frac{h}{|df/\mathrm{d}\zeta|} = \left|\frac{\mathrm{d}\zeta}{\mathrm{d}f}\right| h \tag{4.6}$$

with the inverted mapping $\zeta(f)$. The condition (4.5) simplifies the following calculations greatly. It is not very stringent. If one starts with the cartesian coordinates x and y or with the cylindrical coordinates ρ and z, it is fulfilled with $h=1$. All coordinate systems, practically used, can be obtained in this way; Moon and Spencer (1961) give a description of not less than 37 coordinate systems of such a kind.

Subsequently we will show how to calculate the two unknowns S and B, if our stack of transformations is augmented by one step.

Let us assume that we have after n transformations a coordinate system x_i with the scale factors h_i and that the Dirac equation has the form of (4.1). The wavefunction ψ depends on ψ_c, the wavefunction in the original, cartesian, representation, by

$$\psi_c = \mathrm{e}^B S \psi. \tag{4.7}$$

Now we will consider the transformation, induced by a conformal mapping,

$$(x_i, x_j, x_k) \to (x_i', x_j', x_k' = x_k), \tag{4.8}$$

leaving x_k invariant. Without loss of generality we require that the three numbers i, j, k are an even permutation of 1, 2, 3, i.e. $\varepsilon_{ijk} = +1$. So, from now on i, j, k are fixed numbers.

Because of our condition that the three unit vectors $\boldsymbol{e}_i$, as well as the $\boldsymbol{e}'_i$, form a right-handed system, the two vectors $\boldsymbol{e}'_i$ and $\boldsymbol{e}'_j$ can be written as a linear combination of $\boldsymbol{e}_i$ and $\boldsymbol{e}_j$ of the following type:

$$\boldsymbol{e}'_i = \cos\alpha\,\boldsymbol{e}_i + \sin\alpha\,\boldsymbol{e}_j, \qquad \boldsymbol{e}'_j = -\sin\alpha\,\boldsymbol{e}_i + \cos\alpha\,\boldsymbol{e}_j. \tag{4.9}$$

Here $\cos\alpha$ and $\sin\alpha$ are calculated simply to be

$$\cos\alpha = \frac{h'}{h}\frac{\partial x'_i}{\partial x_i}, \qquad \sin\alpha = -\frac{h'}{h}\frac{\partial x'_j}{\partial x_i}. \tag{4.10}$$

Because of (4.6) they can be combined into

$$\mathrm{e}^{-\mathrm{i}\alpha} = \frac{1}{|\mathrm{d}f/\mathrm{d}\zeta|}\frac{\mathrm{d}f}{\mathrm{d}\zeta} \tag{4.11}$$

or

$$\mathrm{e}^{\mathrm{i}\alpha} = \frac{1}{|\mathrm{d}\zeta/\mathrm{d}f|}\frac{\mathrm{d}\zeta}{\mathrm{d}f}. \tag{4.12}$$

Inserting this in the Dirac equation (4.1) we get

$$[\bar{\gamma}^\mu(\mathrm{i}\hat{D}'_\mu - eA'_\mu) - m]\psi = 0 \tag{4.13}$$

with the new vector components A'_μ and the derivative

$$\hat{D}'_l = (h'_l)^{-1}\,\partial/\partial x^{l'}. \tag{4.14}$$

The new space-dependent Dirac matrices result as

$$\begin{aligned} &\bar{\gamma}^0 = \gamma^0, \qquad \bar{\gamma}^k = \gamma^k, \\ &\bar{\gamma}^i = \cos\alpha\gamma^i + \sin\alpha\,\gamma^j, \qquad \bar{\gamma}^j = -\sin\alpha\,\gamma^i + \cos\alpha\,\gamma^j, \end{aligned} \tag{4.15}$$

fulfilling the ordinary anticommutation relations (2.7). The similarity transformation, which rotates them back into the old γ^μ, cf (2.8), is the unitary matrix

$$S_k(\alpha) = \cos(\tfrac{1}{2}\alpha) - \mathrm{i}\sin(\tfrac{1}{2}\alpha)\,\Sigma_k = \exp(-\tfrac{1}{2}\mathrm{i}\alpha\Sigma_k), \tag{4.16}$$

i.e. we have

$$\bar{\gamma}^\mu = S_k(\alpha)\gamma^\mu S_k(-\alpha). \tag{4.17}$$

Thus we make the ansatz

$$\psi = \mathrm{e}^\beta S_k(\alpha)\psi' \tag{4.18}$$

with a hitherto unknown function β, depending like α on x_i and x_j only. The equation for ψ' becomes

$$[\gamma^\mu(\mathrm{i}\hat{D}'_\mu - eA'_\mu + \mathrm{i}\Gamma'_\mu) - m]\psi' = 0 \tag{4.19}$$

with

$$\Gamma'_\mu = \hat{D}'_\mu\beta + S_k(-\alpha)\hat{D}'_\mu S_k(\alpha). \tag{4.20}$$

Because of

$$S_k(-\alpha)(\mathrm{d}/\mathrm{d}\alpha)S_k(\alpha) = -\tfrac{1}{2}\mathrm{i}\Sigma_k \tag{4.21}$$

the additional term can be evaluated to be

$$\gamma^\mu \Gamma'_\mu = [\hat{D}'_i\beta + \hat{D}'_j\alpha/2]\gamma^i + [\hat{D}'_j\beta - \hat{D}'_i\alpha/2]\gamma^j. \tag{4.22}$$

It vanishes if and only if the two terms vanish, that is, if the following two partial differential equations are fulfilled simultaneously:

$$\hat{D}'_i\beta + \hat{D}'_j\alpha/2 = 0, \qquad \hat{D}'_j\beta - \hat{D}'_i\alpha/2 = 0. \tag{4.23}$$

If there exists a solution, it can be chosen real, since α is real too. In this case (4.19) has the same form as the Dirac equation we started with,

$$[\gamma^\mu(i\hat{D}'_\mu - eA'_\mu) - m]\psi' = 0, \tag{4.24}$$

and the relation between ψ' and the cartesian wavefunction ψ_c is given by

$$\psi_c = e^{B'}S'\psi' = e^{B+\beta}SS_k(\alpha)\psi', \tag{4.25}$$

which is of the same form as (4.7). A solution of the system (4.23) is easily found. Substituting the definition (4.14) of $\hat{D}'_i$ the differential equations (4.23) become

$$\frac{\partial}{\partial x'_i}\beta + \frac{\partial}{\partial x'_j}\frac{\alpha}{2} = 0, \qquad \frac{\partial}{\partial x'_j}\beta - \frac{\partial}{\partial x'_i}\frac{\alpha}{2} = 0. \tag{4.26}$$

This looks like the Cauchy–Riemann differential equations for a holomorphic function $g(f)$ with

$$g(f) = \beta - i\alpha/2. \tag{4.27}$$

Such a function actually exists (cf (4.12)),

$$g(f) = -\tfrac{1}{2}\log(d\zeta/df), \tag{4.28}$$

so it is clear that

$$\beta = -\tfrac{1}{2}\log\left|\frac{d\zeta}{df}\right| = +\tfrac{1}{2}\log\left|\frac{df}{d\zeta}\right| = \tfrac{1}{2}\log\frac{h}{h'}, \qquad e^\beta = \left(\frac{h}{h'}\right)^{1/2}. \tag{4.29}$$

Under such a transformation the volume element is changed according to

$$d\tau = h^2 h_k\, dx_i\, dx_j\, dx_k \to h'^2 h'_k\, dx'_i\, dx'_j\, dx'_k = e^{-4\beta}h^2 h'_k\, dx'_i\, dx'_j\, dx'_k. \tag{4.30}$$

Thus a part of the density function is cancelled by the factor $e^{2\beta}$ in the normalisation integral. But also the transformations in only one coordinate, sometimes necessary to prepare two components of the coordinates for a further transformation by a conformal mapping, cf (4.5), have some influence on the volume element. Through the combination of these two effects it may be possible that the density function reduces to unity, as has been observed in the case of cylindrical coordinates. Later on we will see that the same happens in the case of spherical coordinates.

This in fact, completes our discussion. In every step of our stack of transformations we can find a unitary matrix, $S_k(\alpha)$, and a function β, such that the additional term $\gamma^\mu\Gamma'_\mu$ vanishes. Thus, in this case, a local representation can be found, in which the Dirac equation has the simple form (4.1). The total transformation operator $e^B S$ is just the product of matrices of the form $e^\beta S_k(\alpha)$. It connects the wavefunctions ψ and $\psi_c = e^B S\psi$, cf (4.7). What is the meaning of the 'intermediate' expression $e^B\psi = S^{-1}\psi_c$?

The answer is given in appendix 1, where we will show that this function is identical with the wavefunction obeying the covariantly formulated Dirac equation, which has been derived by Fock (1929) for any orthogonal coordinate system, i.e.

$$\left(\gamma^{\mu}(\mathrm{i}\hat{D}_{\mu} - eA_{\mu}) - m + \mathrm{i}\sum_{l}\gamma^{l}[\tfrac{1}{2}\hat{D}_{l}\log(h_1h_2h_3/h_l)]\right)\psi_{\mathrm{r}} = 0. \tag{4.31}$$

This proves the proposition stated in (1.5) and elucidates the meaning of S.

5. Discussion of the Dirac equation in spherical coordinates

In this section we will discuss—as an example—in detail the Dirac equation in spherical coordinates

$$x = r\sin\theta\cos\varphi, \qquad y = r\sin\theta\sin\varphi, \qquad z = r\cos\theta, \tag{5.1}$$

with

$$r \in (0, \infty), \qquad \theta \in (0, \pi). \tag{5.2}$$

We start with the Dirac equation in cylindrical coordinates, as derived in § 3. Defining the complex variable $\zeta = z + i\rho$, we get, using the complex logarithm,

$$f(\zeta) = f(z + \mathrm{i}\rho) = \log(\zeta) = s + \mathrm{i}\theta = \log r + \mathrm{i}\theta. \tag{5.3}$$

So we arrive at an intermediate coordinate system (s, θ). To find α and β, which are identical with those for (r, θ), we have to calculate the logarithm of the derivative, cf (4.27), (4.28),

$$\beta - \mathrm{i}\frac{\alpha}{2} = g(f) = -\tfrac{1}{2}\log\frac{\mathrm{d}\zeta}{\mathrm{d}f} = -\tfrac{1}{2}\log\frac{\mathrm{d}}{\mathrm{d}f}\mathrm{e}^{f} = -\tfrac{1}{2}f = -\tfrac{1}{2}\log r - \mathrm{i}\frac{\theta}{2}; \tag{5.4}$$

and therefore

$$\alpha = \theta, \qquad \beta = -\tfrac{1}{2}\log r, \qquad \mathrm{e}^{\beta} = 1/\sqrt{r}. \tag{5.5}$$

Thus choosing

$$\psi_{\mathrm{c}} = \frac{1}{r(\sin\theta)^{1/2}}S_3(\varphi)S_2(\theta)\psi \tag{5.6}$$

the Dirac equation reads

$$\left[\gamma^0\left(\mathrm{i}\frac{\partial}{\partial t} - eA_0\right) + \gamma^1\left(\mathrm{i}\frac{1}{r}\frac{\partial}{\partial\theta} - eA_\theta\right) + \gamma^2\left(\mathrm{i}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi} - eA\varphi\right)\right.$$
$$\left. + \gamma^3\left(\mathrm{i}\frac{\partial}{\partial r} - eA_r\right) - m\right]\psi = 0. \tag{5.7}$$

The wavefunction has to be normalised according to

$$\int \mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\varphi\,\psi^{+}\psi = 1. \tag{5.8}$$

For the densities of the charge and the current in the new, spherical coordinates we

refer to (2.24),

$$\rho(r,\theta)=\frac{1}{r(\sin\theta)^{1/2}}\psi^{+}\psi,$$

$$j_r(\rho,\theta)=\frac{1}{r(\sin\theta)^{1/2}}\psi^{+}\alpha_3\psi, \qquad j_\theta(r,\theta)=\frac{1}{r(\sin\theta)^{1/2}}\psi^{+}\alpha_1\psi, \tag{5.9}$$

$$j_\varphi(r,\theta)=\frac{1}{r(\sin\theta)^{1/2}}\psi^{+}\alpha_2\psi.$$

Next we will derive expressions for some operators, namely angular momentum and parity, and study the structure of the eigenfunctions. The Hamiltonian is now

$$\hat{H}=-\mathrm{i}\left[\frac{1}{r}\left(\alpha_1\frac{\partial}{\partial\theta}+\alpha_2\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\right)+\alpha_3\frac{\partial}{\partial r}\right]+\gamma^0 m+V, \tag{5.10}$$

if the vector part of A_μ vanishes. We also introduced the potential energy

$$V=eA_0. \tag{5.11}$$

As in the case of cylindrical coordinates, the z component of the angular momentum is

$$\hat{J}_z=-\mathrm{i}\,\partial/\partial\varphi. \tag{5.12}$$

The wavefunction has to obey the same boundary condition, namely (3.15). $\hat{J}_z$ will commute with $\hat{H}$, if V is independent of φ. Again, the eigenfunctions of $\hat{J}_z$ are $\mathrm{e}^{\mathrm{i}\mu\varphi}$, corresponding to the eigenvalues $\mu=\pm\frac{1}{2},\pm\frac{3}{2},\ldots$, multiplied by any four-component spinor independent of φ. To clarify the eigensolutions there are other important operators, especially Dirac's $\hat{K}$ operator and the parity $\hat{P}$. In space-independent representation Dirac's operator is defined by

$$\hat{K}_c=\gamma^0(\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{L}}_c+1). \tag{5.13}$$

Inserting the orbital angular momentum

$$\hat{\boldsymbol{L}}_c=-\mathrm{i}(\boldsymbol{e}_\varphi\,\partial/\partial\theta-\boldsymbol{e}_\theta(\sin\theta)^{-1}\,\partial/\partial\varphi) \tag{5.14}$$

we get after some algebra according to (2.21)

$$\hat{K}=-\mathrm{i}\gamma^0(\Sigma_2\,\partial/\partial\theta-(\sin\theta)^{-1}\,\Sigma_1\,\partial/\partial\varphi). \tag{5.15}$$

Here the matrices are just the cartesian Σ_1 and Σ_2, instead of $\boldsymbol{\Sigma}\cdot\boldsymbol{e}_\varphi$ and $\boldsymbol{\Sigma}\cdot\boldsymbol{e}_\theta$. The Hamiltonian is then simply

$$\hat{H}=-\mathrm{i}[\alpha_3\,\partial/\partial r+(\gamma^3/r)\hat{K}]+\gamma^0 m+V. \tag{5.16}$$

The operators $\hat{H}$ and $\hat{K}$ will commute if the potential depends on r only. This operator $\hat{K}$ could have been found just by looking at the differential equation. Clearly the parentheses in (5.10) contain the total angle dependence. So we have to find only a regular matrix to be multiplied with this term such that the product commutes with $\hat{H}$. This matrix turns out to be γ^3, but it is unique only up to a factor, determined in consistency with the standard notation. In appendix 2 it is shown that the eigenvalues are $-\kappa=\pm1,\pm2,\ldots$ which are related to j, the angular momentum and the parity quantum number l by

$$j=|\kappa|-\tfrac{1}{2}, \qquad l=j+\tfrac{1}{2}\,\mathrm{sgn}(\kappa). \tag{5.17}$$

Actually the parity is

$$\pi = (-1)^l = \mathrm{sgn}(\kappa)(-1)^k. \tag{5.18}$$

In the original representation it is the eigenvalue of

$$\hat{P}_c = \gamma^0 \hat{I}_s \tag{5.19}$$

with the space-inversion operator $\hat{I}_s$,

$$\hat{I}_s \psi(\boldsymbol{r}) = \psi(-\boldsymbol{r}). \tag{5.20}$$

In spherical coordinates $\hat{I}_s$ operates on the angles:

$$\hat{I}_s: \quad \begin{array}{l} \theta \to \pi - \theta \\ \varphi \to \begin{cases} \varphi + \pi & \text{for } \varphi \in (\varphi_L, \varphi_L + \pi) \\ \varphi - \pi & \text{for } \varphi \in (\varphi_L + \pi, \varphi_L + 2\pi) \end{cases} \\ r \to r. \end{array} \tag{5.21}$$

Transforming this into the local representation, we have to observe the fact that $\hat{I}_s$ acts also on $e^B S$:

$$\hat{P} = \pm i\gamma^0 \Sigma_1 \hat{I}_s. \tag{5.22}$$

Here the upper sign refers to $\varphi \in (\varphi_L, \varphi_L + \pi)$, the lower to $\varphi \in (\varphi_L + \pi, \varphi_L + 2\pi)$, cf (5.21).

To calculate the wavefunctions we have to choose a specific representation. We will not use the standard representation,

$$\gamma_s^0 = \sigma_3 \otimes \mathbb{1}, \qquad \gamma_s^k = i\sigma_2 \otimes \sigma_k, \tag{5.23}$$

with the Pauli matrices σ_k,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{5.24}$$

the 2×2 unit-matrix $\mathbb{1}$ and the direct product $\otimes$. We found the following set of matrices more convenient,

$$\gamma_w^0 = \sigma_3 \otimes \mathbb{1}, \qquad \gamma_w^1 = i\sigma_2 \otimes \sigma_2, \qquad \gamma_w^2 = i\sigma_2 \otimes \sigma_1, \qquad \gamma_w^3 = -i\sigma_1 \otimes \mathbb{1}. \tag{5.25}$$

The other Dirac matrices are defined by (2.6). The matrices (5.25) are related to the matrices γ_s^μ by the similarity transformation

$$\gamma_w^\mu = U_{sw} \gamma_s^\mu U_{sw}^{-1} \tag{5.26}$$

with

$$U_{sw} = U_{sw}^+ = U_{sw}^{-1} = \begin{pmatrix} \sigma & 0 \\ 0 & -\sigma_2 \end{pmatrix}. \tag{5.27}$$

With these matrices the eigenvalue equation, as a partial differential equation in θ and r ($-i\,\partial/\partial\varphi$ replaced by μ), is purely real and so the solutions without the factor $e^{i\mu\varphi}$ can be chosen real too. To get the solutions of

$$\hat{K}\psi = -\kappa\psi, \qquad \hat{J}_z\psi = \mu\psi, \tag{5.28}$$

we will not transform the solutions of the space-independent representation, but we will start directly with the differential equation,

$$1 \otimes [\mathrm{i}\sigma_2\, \partial/\partial\theta - \sigma_1 \mu/(\sin\theta)]\psi = -\kappa\psi. \tag{5.29}$$

Here we have replaced $-\mathrm{i}\,\partial/\partial\varphi$ by its eigenvalue μ. So the upper two and lower two components fulfil the same differential equation. Thus they must coincide up to a factor that may depend on r,

$$\psi = \begin{pmatrix} u(r) \\ v(r) \end{pmatrix} \otimes \varphi_\kappa^\mu(\theta)\, \mathrm{e}^{\mathrm{i}\mu\varphi} = \begin{pmatrix} u(r)\varphi_\kappa^\mu(\theta) \\ v(r)\varphi_\kappa^\mu(\theta) \end{pmatrix} \mathrm{e}^{\mathrm{i}\mu\varphi}. \tag{5.30}$$

We think that this factorising is a further aesthetic advantage of the local representation. According to (5.29), the spinor function φ_κ^μ has to obey

$$(\mu\sigma_1 - \mathrm{i}\sigma_2 \sin\theta\, \mathrm{d}/\mathrm{d}\theta - \kappa \sin\theta)\varphi_\kappa^\mu(\theta) = 0. \tag{5.31}$$

Making use of the anticommutator relations of the Pauli matrices, we see immediately that

$$\sigma_3\varphi_\kappa^\mu \sim \varphi_{-\kappa}^\mu, \qquad \mathrm{i}\sigma_2\varphi_\kappa^\mu \sim \varphi_\kappa^{-\mu}, \qquad \sigma_1\varphi_\kappa^\mu \sim \varphi_{-\kappa}^{-\mu}. \tag{5.32}$$

Moreover, we have

$$\sigma_1\varphi_\kappa^\mu(\theta) \sim \varphi_\kappa^\mu(\pi - \theta). \tag{5.33}$$

These are very simple relations between solutions with different quantum numbers. The factors which arise here depend on the phases chosen. However, it will be sufficient to solve the differential equation (5.31) for the special case $\kappa > 0, \mu > 0$. This is done in appendix 2. The normalised solution is

$$\varphi_\kappa^\mu(\theta) = c_1 \sin^\mu\theta \begin{pmatrix} \sin\frac{1}{2}\theta\, P_n^{(\mu+1/2,\mu-1/2)}(\cos\theta) \\ \cos\frac{1}{2}\theta\, P_n^{(\mu-1/2,\mu-1/2)}(\cos\theta) \end{pmatrix} \qquad (\kappa > 0, \mu > 0) \tag{5.34}$$

with the abbreviation

$$n = |\kappa| - |\mu| - \tfrac{1}{2} = j - |\mu|. \tag{5.35}$$

The $P_n^{(\alpha,\beta)}$'s are Jacobi polynomials. A short list of them is given in appendix 2. These polynomials occur also in the theory of angular momentum describing matrix elements for finite rotations (Edmonds 1957). The normalisation constant is

$$c_1 = \frac{(-1)^{\mu+1/2}}{(2\pi)^{1/2}} \frac{[(\kappa - \mu - \frac{1}{2})!\,(\kappa + \mu - \frac{1}{2})!]^{1/2}}{2^\mu(\kappa - 1)!} \qquad (\kappa > 0, \mu > 0) \tag{5.36}$$

to be consistent with the standard wavefunctions, cf (5.42) below. The solutions are normalised according to

$$2\pi \int_0^\pi \varphi_\kappa^{\mu\,+} \varphi_{\kappa'}^\mu\, \mathrm{d}\theta = \delta_{\kappa\kappa'}. \tag{5.37}$$

Thus the phase factors are fixed for $\kappa > 0, \mu > 0$. In the remaining cases we make use of (5.32) and define the wavefunctions by

$$\begin{aligned} \sigma_1\varphi_\kappa^\mu &= \mathrm{sgn}(\kappa)^+(-1)^{\mu+1/2}\varphi_{-\kappa}^{-\mu}, \\ \mathrm{i}\sigma_2\varphi_\kappa^\mu &= \mathrm{sgn}(\kappa)^+(-1)^{\mu+1/2}\varphi_\kappa^{-\mu}, \\ \sigma_3\varphi_\kappa^\mu &= \varphi_{-\kappa}^\mu, \end{aligned} \tag{5.38}$$

valid for arbitrary κ, μ. It can be shown that the symmetry relation of (5.33) actually is

$$\varphi_\kappa^\mu(\pi-\theta)=(-1)^{l+\mu+1/2}\sigma_1\varphi_\kappa^\mu(\theta). \tag{5.39}$$

Indeed, with this property, the wavefunctions of (5.30) are eigenfunctions of the parity operator (5.22) with the eigenvalue given by (5.18).

If the potential energy depends on r only, the Hamiltonian $\hat{H}$, Dirac's operator $\hat{K}$ and $\hat{J}_z$ possesss common eigenvectors; these have to have the form described in (5.30). In this case the radial wavefunctions have to fulfil a certain differential equation, which we will derive now. Inserting (5.30) into the eigenvalue equation

$$\hat{H}\psi = E\psi \tag{5.40}$$

we get

$$\mathrm{d}u/\mathrm{d}r=-(\kappa/r)u+(1+E-V)v, \qquad \mathrm{d}v/\mathrm{d}r=(1-E+V)u+(\kappa/r)v. \tag{5.41}$$

This is just the differential equation for the wavefunction in the space-independent standard representation of (5.23),

$$\psi_c=\frac{1}{r}\begin{pmatrix} u(r)\chi_\kappa^\mu(\theta,\varphi) \\ \mathrm{i}v(r)\chi_{-\kappa}^\mu(\theta,\varphi)\end{pmatrix}. \tag{5.42}$$

Here we used the notation of Rose (1961). For bound states they have to be normalised according to

$$\int_0^\infty \mathrm{d}r\,(u^2+v^2)=1. \tag{5.43}$$

So all results which have been obtained by studying the radial Dirac equation in the space-independent standard representation can be taken over to our case without any change.

Conclusion

In the preceding sections we presented a new approach to handle the Dirac equation in curvilinear coordinate systems. It is applicable to all coordinate systems which can be expressed in a specified sense by conformal mappings. Our method is based on a space-dependent transformation of the wavefunction, corresponding to a space-dependent set of Dirac matrices, a local representation. This transformation, which can be given in closed form, is chosen in such a way that the Dirac equation in the given coordinates assumes a very simple form. In particular, the derivative operators are just multiplied by the old, constant γ-matrices; furthermore no undesirable additional potential terms arise. We proved the existence of such a transformation for all coordinate systems normally used in physics. It should be mentioned, however, that there may exist coordinates for which no such transformation can be constructed. For example, it is not evident whether the method is applicable for transformations involving all three components at once, since these cannot be described by a conformal mapping. Beside this, there are also rotational symmetric coordinates which cannot be described by a holomorphic function, for instance the coordinates introduced by the equipotential planes of the three-dimensional two-centre problem. In such cases it is not clear whether a local representation exists.

The local representation for a given coordinate system is particularly distinguished by simplifying the Hamiltonian $\hat{H}$ greatly when expressed in terms of these coordinates. Furthermore, not only the Hamiltonian but also other operators normally appearing in connection with these coordinates (e.g. the angular momentum operators in spherical coordinates) show up in a very simple form, even simpler than in the usual cartesian representation. In contrast to this, an operator generating a symmetry transformation not related to the coordinates (e.g. the linear momentum operators in spherical coordinates) will have a rather complicated structure. So it will be rather easy to find operators commuting with $\hat{H}$. Inversely, it is nearly trivial to disprove by induction the existence of an operator playing the role of $\hat{K}$ in the spherical case for a system exhibiting less symmetry like elliptical coordinates (ξ, η, φ). Here no operator of the form

$$\sum_{n=0}^{N} \sum_{m=0}^{M} A_{nm}(\boldsymbol{r})(\partial/\partial\eta)^n(\partial/\partial\varphi)^m, \qquad N \geqslant 1, \tag{6.1}$$

with the angular coordinates η and φ and arbitrary space-dependent 4×4 matrices A_{nm} (at least one, $A_{Nm} \neq 0$) can exist which commutes with $\hat{H}$.

A further advantage of the local representation becomes visible if we consider the Dirac equation as a partial differential equation which is to be treated numerically. Because of the simplicity of the differential equation the numerical expenditure is reduced greatly. It is not difficult to find the asymptotical behaviour of the wavefunction near the boundaries of the domain of integration. As an application of the method developed here we will discuss the two-centre Dirac equation extensively in the following paper. There we will introduce a suitable coordinate system, establish the Dirac equation in the local representation and present the numerical method used to calculate energy eigenvalues and wavefunctions. Finally we want to mention that our transformation presumably can be generalised to linear wave equations describing fermions or bosons with spin larger than $\frac{1}{2}$.

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Appendix 1. The connection between ψ_r and ψ

In this appendix we want to prove the asserted connection between the two wavefunctions ψ_r and ψ, cf (A1.1) below. The Dirac equation in any orthogonal coordinate system due to Fock (1929) is given by (4.31). It determines ψ_r. Alternatively ψ fulfils (4.1). The proof will be given by induction. The proposition is certainly true for cartesian coordinates. We assume that for some coordinate system $\{x\}$

$$\psi_r = \mathrm{e}^{B}\psi \tag{A1.1}$$

is true and we have to prove that a similar relation holds if we introduce new coordinates, $\{x\} \rightarrow \{x'\}$, cf (4.8),

$$\psi_r' = \mathrm{e}^{B'}\psi' = \mathrm{e}^{B}\,\mathrm{e}^{\beta}\psi', \tag{A1.2}$$

where ψ'_r and ψ' denote the wavefunctions in the new coordinates $\{x'\}$. We mention that the coordinate transformations are restricted by the conditions described in § 4.

The wavefunction ψ'_r obeys

$$\left(\gamma^\mu(\mathrm{i}\hat{D}'_\mu - eA'_\mu) - m + \mathrm{i}\sum_{l=i,j,k}\gamma^l[\tfrac{1}{2}\hat{D}'_l \log(h'_i h'_j h'_k/h'_l)]\right)\psi'_r = 0. \tag{A1.3}$$

For transformations involving only one variable the proposition is trivial. So we have to consider transformations induced by conformal mappings. Inserting (A1.2) we get

$$\left(\gamma^\mu(\mathrm{i}\hat{D}'_\mu - eA'_\mu) - m + \mathrm{i}\sum_{l=i,j,k}\gamma^l[\hat{D}'_l \tfrac{1}{2}\log(h'^2 h'_k/h'_l) + \hat{D}'_l B + \hat{D}'_l\beta]\right)\psi' = 0. \tag{A1.4}$$

The additional term becomes

$$\sum_l \gamma^l\left[\hat{D}'_l\left(\tfrac{1}{2}\log\frac{h^2 h_k}{h_l} + B\right) + \hat{D}'_l\left(\tfrac{1}{2}\log\frac{h'^2}{h^2}\frac{h_l}{h'_l} + \beta\right)\right]. \tag{A1.5}$$

The first part vanishes because of the assumption. We are left with

$$\gamma^i\hat{D}'_i[\tfrac{1}{2}\log(h'/h) + \beta] + \gamma^j\hat{D}'_j[\tfrac{1}{2}\log(h'/h) + \beta] + \gamma^k D'_k[\log(h'/h) + \beta] = 0 \tag{A1.6}$$

which follows from (4.29). So (A1.4) becomes identical to (4.24). This completes the proof.

Appendix 2. Solution of a differential equation

The task of this appendix is the solution of the differential equation (5.31). As already mentioned in § 5 it suffices to solve it for $\kappa > 0$, $\mu > 0$. Since it is a system of two first-order equations, there are two linearly independent solutions. An examination of the asymptotic behaviour for $\theta \to 0$, where the differential equation is singular, shows that one solution is proportional to θ^μ while any linearly independent solution diverges as $\theta^{-\mu}$ (Erdélyi 1956). Such a solution will not be normalisable, cf (5.37), since $\mu \geqslant \frac{1}{2}$. Hence there is at most one physical meaningful solution. The ansatz

$$\varphi^\mu_\kappa = \sin^\mu\theta\begin{pmatrix}\sin\frac{1}{2}\theta f_1(\theta)\\ \cos\frac{1}{2}\theta f_2(\theta)\end{pmatrix} \tag{A2.1}$$

leads to

$$(x+1)\,\mathrm{d}f_2/\mathrm{d}x + (\mu+\tfrac{1}{2})f_2 - \kappa f_1 = 0, \qquad (x-1)\,\mathrm{d}f_1/\mathrm{d}x + (\mu+\tfrac{1}{2})f_1 - \kappa f_2 = 0, \tag{A2.2}$$

where we substituted

$$x = \cos\theta. \tag{A2.3}$$

Eliminating f_2, this becomes

$$(1-x^2)\,\mathrm{d}^2 f_1/\mathrm{d}x^2 + [-1-(2\mu+2)x]\,\mathrm{d}f_1/\mathrm{d}x + [\kappa^2 - (\mu+\tfrac{1}{2})^2]f_1 = 0. \tag{A2.4}$$

This is just Jacobi's differential equation. It possesses as solutions Jacobi polynomials (Erdélyi *et al* 1953)

$$f_1(x) = c_1 P_n^{(\mu+1/2,\mu-1/2)}(x) \tag{A2.5}$$

with the abbreviation introduced in (5.35). The condition that $f_1(x)$ is a polynomial is equivalent to the condition that κ is an integer not less than $\mu + \frac{1}{2}$. The easiest way to determine f_2 is to observe (5.33) and use the symmetry property of the Jacobi polynomials (Abramowitz and Stegun 1965),

$$P_n^{(\alpha,\beta)}(-x) = (-1)^n P_n^{(\beta,\alpha)}(x). \tag{A2.6}$$

From this it follows that

$$f_2(x) = c_2 P_n^{(\mu-1/2,\mu+1/2)}(x). \tag{A2.7}$$

If n were not a non-negative integer, the solutions f_1 and f_2 could still be expressed by hypergeometric functions. However, this would lead to non-normalisable solutions diverging for $\theta \to \pi$. This fact gives the quantisation condition of κ mentioned above.

The constant c_2 can be found by specifying (A2.2) to $x = +1$

$$c_2 = c_1, \tag{A2.8}$$

where we used

$$P_n^{(\alpha,\beta)}(1) = \binom{n+\alpha}{n}. \tag{A2.9}$$

Therefore the unnormalised solution is

$$\varphi_\kappa^\mu(\theta) = c_1 \sin^\mu \theta \begin{pmatrix} \sin \frac{1}{2}\theta \, P_n^{(\mu+1/2,\mu-1/2)}(\cos\theta) \\ \cos \frac{1}{2}\theta \, P_n^{(\mu-1/2,\mu+1/2)}(\cos\theta) \end{pmatrix}. \tag{A2.10}$$

Using the orthogonality relation of the Jacobi polynomials, it is not difficult to show that $|c_1|$ is given by the expression (5.36).

Finally we give a short list of Jacobi polynomials, occurring for $\kappa = 1, 2, 3$ and $\mu = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$:

$$\begin{aligned} &P_0^{(1,0)} = P_0^{(2,1)} = P_0^{(3,2)} = 1, && P_1^{(1,0)} = \tfrac{1}{2}(3x+1), \\ &P_1^{(2,1)} = \tfrac{1}{2}(5x+1), && P_2^{(1,0)} = \tfrac{1}{2}(5x^2+2x-1). \end{aligned} \tag{A2.11}$$

The polynomials of the form $P_n^{(\mu-1/2,\mu+1/2)}$ follow directly from (A.2.6).

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