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The Dirac equation in orthogonal coordinate systems†: II. The two-centre Dirac equation

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Abstract. We study the relativistic two-centre problem for Dirac particles. A set of coordinates is introduced which allows a convenient description of the two asymptotic cases of very large and very small two-centre distances. Calculations become more practicable by means of the implantation of the local representation discussed in the preceding paper. The boundary conditions as well as symmetries of the wavefunctions are investigated in detail and a numerical procedure for the solution of the Dirac equation in Cassini coordinates is presented.

1. Introduction

The motion of an electron in the presence of two charged nuclei has been studied since the earliest days of quantum mechanics. In 1927 Heitler and London were able to explain the covalent binding for diatomic molecules. The first exact non-relativistic calculations were performed by Hylleraas (1931) and Teller (1930) using elliptical coordinates. While the Schrödinger equation with a potential generated by two point-like nuclei still separates in these coordinates, the Dirac equation remains a partial differential equation in two dimensions (Müller *et al* 1973, Müller and Greiner 1976). Therefore relativistic and spin effects can be examined only with very enlarged numerical expense. Today the valence bond is investigated mostly by non-relativistic approximations with atomic orbitals (LCAO MO) in a variational concept (McWeeny and Pickup 1968). Because of the low binding energies this leads to rather reliable results.

In the last years the two-centre problem has gained enhanced interest, because it supplies an opportunity to test QED in strong external electromagnetic fields (Reinhardt and Greiner 1977). Such fields can be realised in collisions of very heavy ions. Here a relativistic description of the electron motion is mandatory. A first step of the solution of this dynamical problem may be the discussion of the stationary two-centre Dirac equation with the two-centre distance $2a$ as an independent parameter. In this context accurate calculations become more and more necessary, so that precise theoretical predictions of various processes are possible. Up to now, the problem has

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been treated by an ansatz with spherical solutions of the united system (Rafelski and Müller 1976). This approximation works with sufficient accuracy only for small distances between the nuclear charges, as do the atomic orbitals for large a. To describe the electron in both the intermediate region and the asymptotic regions, the first step has to be the introduction of well suited coordinates. This means that one set of coordinate planes becomes spherical in both asymptotic cases. The singularities of the coordinates have to coincide with the position of the two centres. Such a system is obtained if one defines one coordinate by the potential of two point charges in two-dimensional electrodynamics. In the literature (Moon and Spencer 1961) they are known as Cassini coordinates.

Because electrostatics in the plane can be treated within the framework of the theory of analytical functions, the coordinate transformation is 'induced' by a conformal mapping. This is an important condition for the application of a transformation method described in the preceding paper. The complexity of these new variables shows up in the scaling factors, which appear unavoidably in the wave equation. In the case of the Dirac equation more trouble arises with additional space-dependent terms. These are avoided if we use the transformation method mentioned. Thereby the Dirac equation gains lucidity and practical calculations are simplified greatly.

In § 2 we will introduce these new coordinates and transform the Dirac equation. The result will be a Hamiltonian which embodies a partial differential operator. In § 3 we will derive the boundary conditions that the wavefunction has to fulfil. Moreover, we discuss symmetry properties of the Hamiltonian. This supplies the prerequisites for a numerical solution. In § 4 we will give a brief description of the computational scheme employed.

2. Dirac equation in Cassini coordinates

In this section we want to repeat the essential steps of the transformation of the Dirac equation to its local representation in the special case of Cassini coordinates. We will use the method presented in the preceding paper (Schlüter *et al* 1983, to be referred to as I). We will take over the notation of this paper. It may be advantageous if we derive the relations leading to the Dirac equation in some detail. Considering the intricate coordinates used, the result will be rather simple.

We start with the definition of these coordinates, called Cassini coordinates w and δ. Here the lines with constant w are Cassinian ovals (figure 1). These curves were first used by Giovanni Domenico Cassini (1625–1712) to describe the planetary motion around the sun (Cassini 1740). Today they are more important in the context of two-dimensional electrodynamics, where they are the equipotential lines for two equal point charges.

The Cassini coordinates can be expressed easily by a holomorphic function f of the complex variable

$$\zeta = z + \mathrm{i}\rho \tag{2.1}$$

with the cylindrical coordinates z and ρ (figure 2),

$$f(\zeta) = \tfrac{1}{2}\left(\log\frac{\zeta - a}{a} + \log\frac{\zeta + a}{a}\right) = \tfrac{1}{2}\left(\log\frac{r_1 r_2}{a^2} + \mathrm{i}(\theta_1 + \theta_2)\right) \tag{2.2}$$

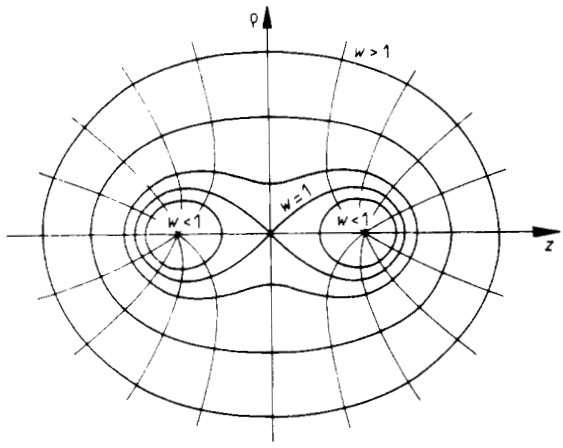

Figure 1. Cassinian ovals in the ρ, z plane. The line with $w = 1$ is the lemniscate.

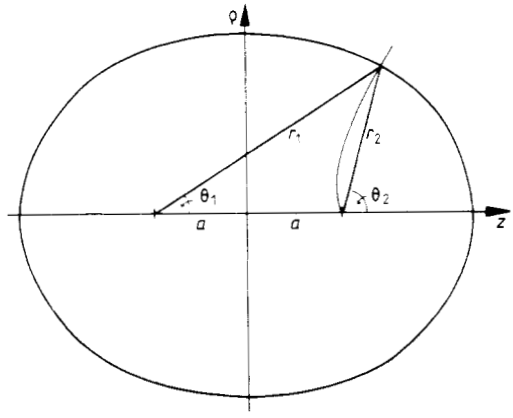

Figure 2. Explanation of the geometrical quantities r_1, r_2, θ_1 and θ_2, which define the Cassini coordinates by $w = (r_1 r_2)^{1/2}/a$ and $\delta = \frac{1}{2}(\theta_1 + \theta_2)$.

with

$$r_1^2 = \rho^2 + (z+a)^2, \qquad \theta_1 = \tan^{-1}[\rho/(z+a)],$$
$$r_2^2 = \rho^2 + (z-a)^2, \qquad \theta_2 = \tan^{-1}[\rho/(z-a)]. \tag{2.3}$$

The number $2a$ denotes the two-centre distance. The new coordinates will be defined by the real and imaginary part of f,

$$w = e^{\mathrm{Re}\, f} = (r_1 r_2)^{1/2}/a, \qquad \delta = \mathrm{Im}\, f = \tfrac{1}{2}(\theta_1 + \theta_2). \tag{2.4}$$

Hence the Cassinian ovals are the curves where the product $r_1 r_2$ is constant. A holomorphic function is angle preserving and so we get a new set of orthogonal coordinates with the real and imaginary part (Behnke and Sommer 1976). The important scaling factor reads

$$h_{\log w} = h_\delta = h = |\mathrm{d}\zeta/\mathrm{d}f| = w^2 a/\sqrt[4]{D}, \tag{2.5}$$

with the discriminant

$$D = w^4 + 2w^2 \cos 2\delta + 1. \tag{2.6}$$

As a consequence of the coordinate transformation the volume element will be modified,

$$d\tau = \rho \, d\rho \, dz \, d\varphi = (w^3 a^2/\sqrt{D})\rho \, dw \, d\delta \, d\varphi. \tag{2.7}$$

For the following calculations we need the expression

$$\rho(w, \delta) = (a/\sqrt{2})(\sqrt{D} - 1 - w^2 \cos 2\delta)^{1/2} \tag{2.8}$$

for the distance from the symmetry axis.

Studying the relativistic electron problem, we take as the starting point the time-dependent Dirac equation, written in cylindrical coordinates, in the local representation (I, (3.9)). This formulation of the Dirac equation was described as an illustrative example in I. Later on we want to consider merely the stationary problem for the symmetric two-centre potential induced by point-like nuclei without retardation,

$$\begin{aligned} &\left[-i\left((\gamma^1 \frac{\partial}{\partial \rho} + \gamma^2 \frac{1}{\rho} \frac{\partial}{\partial \varphi} + \gamma^3 \frac{\partial}{\partial z}\right) - \varepsilon \gamma^0 + m\right]\psi_z = 0 \\ &\varepsilon = E - V_{tc}(\rho, z), \qquad V_{tc} = -Z\alpha(1/r_1 + 1/r_2). \end{aligned} \tag{2.9}$$

The bound states have to be normalised according to

$$\int d\varphi \, d\rho \, dz \, \psi_z^+ \psi_z = 1. \tag{2.10}$$

For the next steps it is necessary to know precisely in which manner the Dirac equation has to be transformed to its new local representation, if a holomorphic function induces the change of coordinates. This is explained in §§ 2 and 4 of I.

Now we carry out the transformation in the (ρ, z) plane. After the introduction of the new system we get in analogy to (I, (2.16)) the matrices

$$\begin{aligned} &\tilde{\gamma}^3 = \cos\alpha \, \gamma^3 + \sin\alpha \, \gamma^1, \qquad \tilde{\gamma}^1 = -\sin\alpha \, \gamma^3 + \cos\alpha \, \gamma^1, \\ &\tilde{\gamma}^2 = \gamma^2, \qquad \tilde{\gamma}^0 = \gamma^0 \end{aligned} \tag{2.11}$$

with, remembering (I, (4.10)),

$$\begin{aligned} \cos\alpha &= \frac{(\sqrt{D} + 1 + w^2 \cos 2\delta)^{1/2}(\sqrt{D} - 1)}{\sqrt{2} w^2 \sqrt[4]{D}} \operatorname{sgn}(\cos\delta), \\ \sin\alpha &= \frac{(\sqrt{D} - 1 - w^2 \cos 2\delta)^{1/2}(\sqrt{D} + 1)}{\sqrt{2} w^2 \sqrt[4]{D}}. \end{aligned} \tag{2.12}$$

The unitary space-dependent matrix (I, (4.16)) which will rotate (2.11) back to the constant old representation γ^μ, reads

$$S_2(\alpha) = \exp(-\tfrac{1}{2} i \alpha \Sigma_2) = \cos(\tfrac{1}{2}\alpha) - i \sin(\tfrac{1}{2}\alpha)\Sigma_2. \tag{2.13}$$

Now the condition for the vanishing of $\gamma^\mu \Gamma_\mu$ has to be fulfilled. We have to find the solution of (I, (4.23)), the first-order differential equations

$$\frac{1}{h} \frac{\partial}{\partial \log w} \beta + \frac{1}{h} \frac{\partial}{\partial \delta} \frac{\alpha}{2} = 0, \qquad \frac{1}{h} \frac{\partial}{\partial \delta} \beta - \frac{1}{h} \frac{\partial}{\partial \log w} \frac{\alpha}{2} = 0. \tag{2.14}$$

In § 4 of I the relation of this system to the Cauchy–Riemann differential equations for the function $\log(\mathrm{d}\zeta/\mathrm{d}f)$ is explained. By means of (I, (4.29)) we can write down the solution β immediately,

$$\beta = -\tfrac{1}{2}\log|\mathrm{d}\zeta/\mathrm{d}f| = -\tfrac{1}{2}\log h. \tag{2.15}$$

We summarise the whole transformation in the equation

$$\psi_c = \frac{1}{\sqrt{\rho}} S_3(\varphi)\psi_z = \frac{1}{\sqrt{\rho}}\left(\frac{\sqrt[4]{D}}{w^2 a}\right)^{1/2} S_3(\varphi)S_2(\alpha)\psi \tag{2.16}$$

with $S_3(\varphi) = \exp(-\mathrm{i}\tfrac{1}{2}\varphi\Sigma_3)$. ψ_c embodies the wavefunction in the ordinary cartesian representation. The resulting Dirac equation in the local representation retains only the complicated scaling factors and the potential, now formulated in Cassini coordinates, is

$$V_{tc}(w, \delta) = -Z\alpha(\sqrt{2}/aw^2)(\sqrt{D} + 1 + w^2)^{1/2}. \tag{2.17}$$

Figure 3 shows some equipotential lines. In spite of the complicated angle dependence via the discriminant D the potential fluctuates very little if δ varies in the range $(0, \pi)$. Even in the worst case ($w = 1$) it deviates from the mean value by only $\pm 17.2\%$. For $w < 0.25$ and $w > 4$ this deviation becomes less than $\pm 1.5\%$. We recall that the Cassini curves (w = constant) are just the equipotential lines in two-dimensional electrostatics, which apparently do not differ very much from those in the three-dimensional case.

The bound states have to be normalised with the following integral:

$$\int \frac{aw}{\sqrt[4]{D}}\mathrm{d}w\ \mathrm{d}\delta\ \mathrm{d}\varphi\ \psi^{\dagger}\psi = 1. \tag{2.18}$$

The Hamiltonian used in further examination now reads, remembering (2.8) and (2.17),

$$\hat{H} = -\mathrm{i}\frac{\sqrt[4]{D}}{aw}\left(\alpha_3\frac{\partial}{\partial w} + \alpha_1\frac{1}{w}\frac{\partial}{\partial\delta}\right) - \mathrm{i}\alpha_2\frac{1}{\rho}\frac{\partial}{\partial\varphi} + V_{tc} + m\gamma^0, \tag{2.19}$$

the ugly terms $\cos\alpha$ and $\sin\sigma$ of (2.12) do not appear. In this rather brief derivation we were able to obtain the Hamiltonian even for such complicated coordinates. We think that this is the most appropriate way to study the two-centre Dirac equation.

3. Symmetries and boundary conditions

The symmetric two-centre problem obviously has two geometrical symmetries, the parity and the cylindrical symmetry. We can get the corresponding operators $\hat{P}$ and $\hat{J}_z$ in our local representation using the unitary transformation matrices $S_2(\alpha)$, $S_3(\varphi)$, cf (2.16), and the known standard operators (Rose 1961)

$$\hat{J}_z^c = -\mathrm{i}\partial/\partial\varphi + \tfrac{1}{2}\Sigma_3, \qquad \hat{P}_c = \hat{I}_s\gamma^0, \tag{3.1}$$

in (I, (2.21)). The factor e^B is invariant under the space inversion $\hat{I}_s$ and rotations around the z axis as can easily be seen.

Alternatively we can see in analogy to the spherical case (I, § 5) that $-\mathrm{i}\,\partial/\partial\varphi$ in the Hamiltonian (2.19) is the commuting hermitian operator $\hat{J}_z$. The solutions naturally have to obey the boundary conditions (I, (3.15)) of the cylindrical case. The eigenvalues

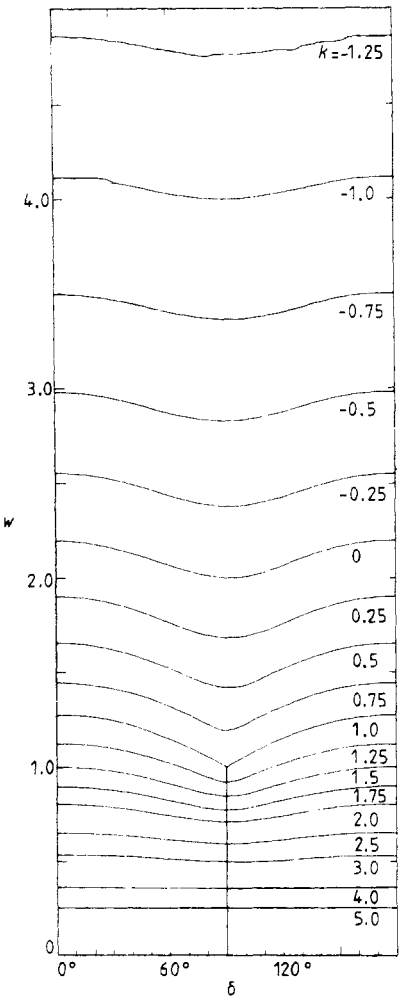

Figure 3. Equipotential lines for the Coulomb potential generated by two-point nuclei, each with charge number Z; the potential is given by $V = -Z\alpha 2^k/a$.

and functions are now well known from the cylindrical and the spherical problem (I, §§ 3, 5),

$$\hat{J}_c\psi(w,\delta)\,e^{i\mu\varphi} = \mu\psi(w,\delta)\,e^{i\mu\varphi}, \qquad \mu = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \ldots. \tag{3.2}$$

Furthermore, especially for the consideration of the parity, we will replace $\hat{J}_z$ by its eigenvalue, the magnetic quantum number μ, to get rid of the φ dependence in the Dirac equation.

It is more difficult to find the transformed parity operator $\hat{P}$ without the help of (I, (2.21)). Obviously all coefficients in (2.19) do not change the sign under space inversion because the angle coordinate appears as $\cos 2\delta$ only. But the angle derivative $\partial/\partial\delta$ becomes negative. So we have to find a 4×4 matrix which commutes with all matrices appearing in the Hamiltonian (2.19) with the exception of α_1; here it must anticommute. Moreover $\hat{P}$ has to satisfy

$$\hat{P}^2 = 1, \qquad \hat{P}^+ = P. \tag{3.3}$$

One finds easily that $\pm i\gamma^0\Sigma_1$ fulfils these conditions and it will replace γ^0 in (3.1). The undetermined sign should be fixed consistent with the standard formulation. The result is

$$\hat{P} = \pm i\gamma^0\Sigma_1\hat{I}_s(\delta \to \pi - \delta, \varphi \to \varphi \pm \pi) \tag{3.4}$$

with the eigenvalue equation

$$\hat{P}\psi_\pm(w, \delta, \varphi) = \pm\psi_\pm(w, \delta, \varphi). \tag{3.5}$$

In (3.4) the upper or lower sign is to be taken throughout. It has to be chosen in such a way that φ does not leave the interval $(0, 2\pi)$. This is necessary for the uniqueness of $S_3(\varphi)$. This problem is discussed in more detail in (I, § 3).

The remarkable fact that we get the same parity behaviour as in the spherical case is a consequence of the similar form of the Dirac equation. Also there the space inversion has no effect on the scaling factors and only the corresponding angle derivative changes its sign.

There exists no analogue to Dirac's $\hat{K}$ operator in spherical coordinates. This means more precisely that there is no operator of the form

$$\hat{B} = \sum_{n=0}^{N}\sum_{m=0}^{M} B_{nm}(r)(\partial/\partial\delta)^n(\partial/\partial\varphi)^m, \qquad N \geqslant 1, \tag{3.6}$$

which commutes with $\hat{H}$. The simple proof is given in appendix 1.

For the further examinations it is advantageous to reduce the Hamiltonian to a two-dimensional partial differential operator,

$$\hat{H}^{(\mu)} = -i\frac{\sqrt[4]{D}}{wa}\left(\alpha_3\frac{\partial}{\partial w} + \alpha_1\frac{1}{w}\frac{\partial}{\partial\delta}\right) + \frac{\mu}{\rho}\alpha_2 + V_{tc}(w, \delta) + \gamma^0 m. \tag{3.7}$$

At this point we mention that a representation, where α_1 and α_3 are purely imaginary while α_2 is real, will obviously be ideal for analytical and numerical purposes. In the spherical case we have already introduced such matrices cf (I, (5.25)). With a skilfully chosen representation the type of the partial differential equation can also be determined easily. We multiply the eigenvalue equation (3.7) from the left with $i\alpha_3$ and take a set of α-matrices for which the product $\alpha_3\alpha_1$ is diagonal. The purely imaginary diagonal elements (i, −i, i, −i) mean that our partial differential equation is of elliptical type (Courant and Hilbert 1968).

Now we will proceed to the boundary conditions. It will turn out that the wavefunction has to vanish at the boundaries of the domain of integration (figure 3). This is also valid along the cut $(0 < w < 1, \delta = \pi/2)$ and is mainly a result of the factor e^B which contains a term $\sqrt{\rho}$ for all coordinate systems with cylindrical symmetry. These results are a consequence of the asymptotic behaviour of the wavefunction near the boundaries which will be investigated subsequently. This knowledge greatly facilitates the numerical calculations.

Firstly we will consider the Hamiltonian for small and for large w. Therefore it is convenient to evaluate the space dependent coefficients in our partial differential equation. Fortunately the expression $\sqrt[4]{D}$ is the generating function for a special class of orthogonal Gegenbauer polynomials (Erdélyi *et al* 1953). We examine this term and the other coefficients of interest in appendix 2. Here we need only the lowest order terms of the expansions.

$$\sqrt[4]{D} = \begin{cases} 1 + O(w^2) & (w \to 0) \\ w + O(1/w) & (w \to \infty), \end{cases}$$

$$a/\rho = \begin{cases} 2/(w^2|\sin 2\delta|) + O(1) & (w \to 0) \\ 1/(w \sin \delta) + O(1/w^3) & (w \to \infty), \end{cases} \tag{3.8}$$

$$V_{tc} = \begin{cases} -(Z\alpha/a)(2/w^2) + O(1) & (w \to 0) \\ -(Z\alpha/a)(2/w) + O(1/w^3) & (w \to \infty). \end{cases}$$

In both limiting cases the potential becomes independent of the angle δ, cf figure 3. Inserting these expansions in (3.7) for the case $w \to 0$, the Dirac equation in Cassini coordinates reads, omitting the residual terms,

$$\left(-i\alpha_3 \frac{1}{wa} \frac{\partial}{\partial w} - i\alpha_1 \frac{1}{aw^2} \frac{\partial}{\partial \delta} + \alpha_2 \frac{2\mu}{aw^2|\sin 2\delta|} - \frac{2Z\alpha}{aw^2} + \gamma^0 m\right)\psi = E\psi \qquad (w \to 0). \tag{3.9}$$

With the substitutions $r = aw^2/2$ and $\theta = 2\delta$ or $\theta = 2\delta - \pi$ for the two centres of charge number Z respectively, the spherical Dirac equation for the hydrogen problem in its local representation is obtained. This is illustrated in figure 4(a). Here some circles around one of the two centres as well as some radii are drawn. For decreasing distances ($r \to 0$) these circles coincide better and better with the coordinate lines w = constant. Simultaneously the radii for which the polar angle θ is fixed become identical with the δ-lines. Moreover, these θ-curves are equally spaced ($\theta = 2\delta$).

For large values of w we do the same,

$$\left(-i\alpha_3 \frac{1}{a} \frac{\partial}{\partial w} - i\alpha_1 \frac{1}{wa} \frac{\partial}{\partial \delta} + \alpha_2 \frac{\mu}{wa \sin \delta} - \frac{2Z\alpha}{aw} + \gamma^0 m\right)\psi = E\psi \qquad (w \to \infty). \tag{3.10}$$

With the substitutions $r = aw$ and $\theta = \delta$ we get again the spherical Dirac equation for a Coulomb potential, now with the charge number $2Z$. We refer to figure 4(b). Here the same, *mutatis mutandis*, as in the opposite asymptotic case (figure 4(a)) holds true.

So, as a first simple consequence of the considerations of these two cases, we can adopt the general asymptotic behaviour of the spherical wavefunctions. It is pleasing that the Cassini coordinates in the asymptotic regions are related to the spherical coordinates in such a simple way.

For exceedingly large or small two-centre distances the main contribution of the wavefunction lies totally in one of the asymptotic regions. This means that it may be described very well by spherical states.

Our next problem will be the asymptotic behaviour of the solutions near the remaining boundaries, that is for small angles δ, $\delta \to \pi$ and along the cut. For small and large w this can be deduced easily from the previous results. In both cases we get essentially the same power behaviour of the angle variable and we expect that the wavefunctions vanish in the intermediate region in the same way as they do in the spherical case. For small δ we make the following power ansatz:

$$\psi = \tilde{\psi}\delta^{\alpha}. \tag{3.11}$$

We are interested in the lowest order only, and so we can restrict ourselves to two terms in the Hamiltonian (3.7), the angle derivative and the singular coefficient $1/\rho(w, \delta)$,

$$[-i\alpha_1(\sqrt[4]{D}/aw^2)\partial/\partial\delta + \alpha_2\mu/\rho]\psi = 0. \tag{3.12}$$

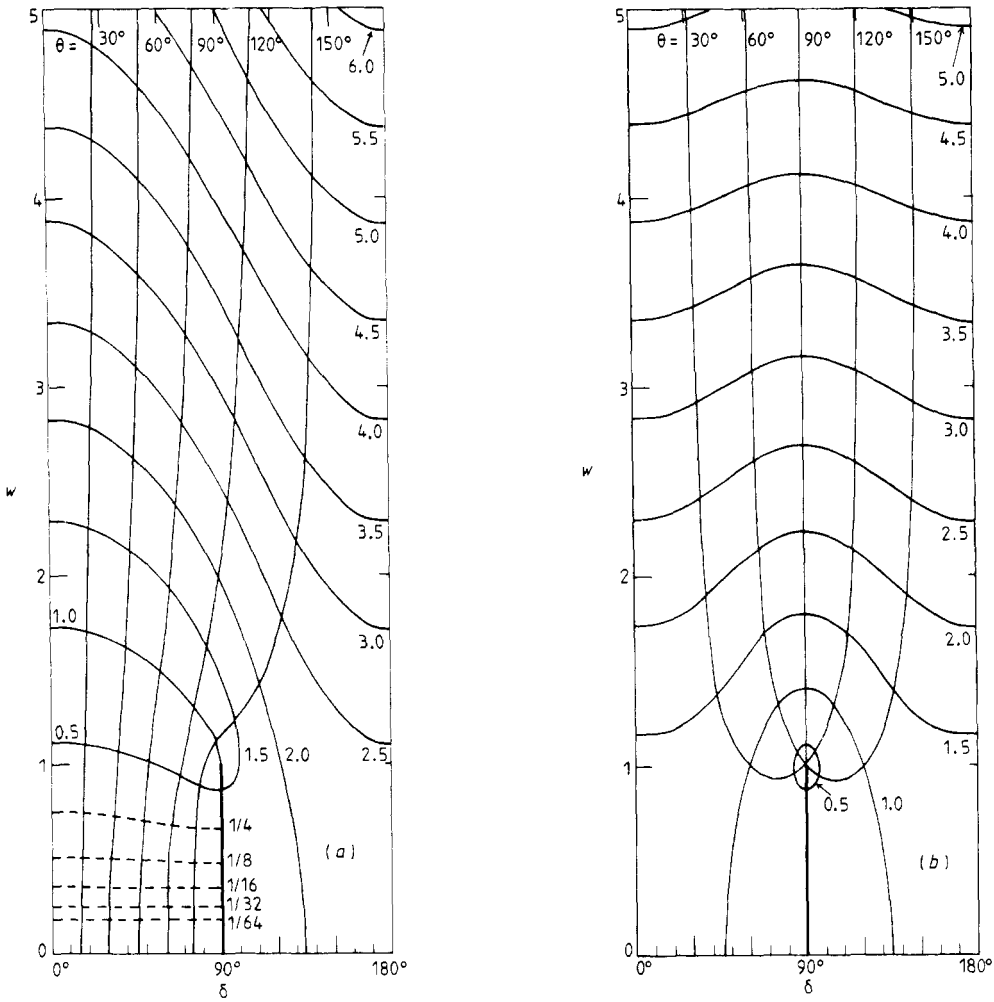

Figure 4. Coordinate lines for spherical coordinates r, θ in the w, δ plane. In (a) the origin is one of the two centres, in (b) it is the point in the middle between the two centres. The more-or-less horizontal lines correspond to circles. The radius in units of a is given by the numbers.

We have to expand the expressions $\sqrt[4]{D}$ and $1/\rho(w, \delta)$ for small δ to get the power behaviour near the boundary,

$$\sqrt[4]{D} = (w^2+1)^{1/2} + O(\delta^2), \qquad a/\rho = (w^2+1)^{1/2}/(w^2\delta) + O(\delta). \quad (3.13)$$

Equation (3.12) now becomes, omitting the residual terms,

$$(w^2+1)^{1/2}/(aw^2)[-i\alpha_1\partial/\partial\delta + (\mu/\delta)\alpha_2]\psi = 0. \quad (3.14)$$

The first result is the requested independence of w of our power ansatz.

The magnetic quantum number has the main influence. If different representations of the Clifford algebra are considered, we observe that the chosen matrices α_1 and α_2 play an important role for the asymptotics of the different spinor components. Using the representation defined in (I, (5.25)) a purely real differential equation (3.14)

results, which reduces to

$$(\alpha+\mu)\tilde{\psi}_1=0, \qquad (\alpha-\mu)\tilde{\psi}_2=0, \qquad (\alpha+\mu)\tilde{\psi}_3=0, \qquad (\alpha-\mu)\tilde{\psi}_4=0. \quad ((3.15)$$

So it results that

$$\alpha=|\mu|. \tag{3.16}$$

Besides this we have

$$\begin{aligned} &\tilde{\psi}_1=\tilde{\psi}_3=0 \qquad \text{for } \mu>0 \\ &\tilde{\psi}_2=\tilde{\psi}_4=0 \qquad \text{for } \mu<0. \end{aligned} \tag{3.17}$$

The alternative possibility, $\alpha=-|\mu|$, leads to non-normalisable solutions. With the help of the parity (3.4) we can transfer these results to the region near $\delta=\pi$,

$$\tilde{\psi}_1(w,\pi)=\pm\tilde{\psi}_2(w,0), \qquad \tilde{\psi}_2(w,\pi)=\pm\tilde{\psi}_1(w,0), \tag{3.18}$$

and analogously for the remaining components. The different signs correspond to positive and negative parity. A similar investigation can be done for the case $\delta\to\pi/2$ and $0<w<1$. The resulting simple boundary conditions will be useful for a numerical treatment of the Dirac equation.

4. The numerical treatment of the Dirac equation in Cassini coordinates

It seems to be impossible even in these coordinates to get an analytical solution of the Dirac equation in the case of two point-like charges. Therefore we have to solve this partial differential equation in two dimensions numerically. The procedure proposed will be a semi-discrete Galerkin method which belongs to the class of variational methods. It reduces the problem to a system of ordinary differential equations.

First of all we will look at the domain of integration for our differential equation (figure 3). For $w<1$ the cut at $\delta=\pi/2$ divides it into two separate parts corresponding to the neighbourhoods of the distinct nuclei. As a consequence of defining the coordinate w dimensionless (lemniscate $w=1$) it follows that for different two-centre distances $2a$ a bound state with definite quantum numbers has its main contribution in different intervals of w. Especially for large a the spatial expectation value of the wavefunction is far down in one of the strips for $w<1$; for very small a it is far outside the lemniscate. We have mentioned earlier that in these asymptotic regions an approximation by means of the corresponding spherical states would be very accurate. The knowledge of these functions will be used later for the construction of angular basis functions. The lemniscate is the natural borderline for the validity of the 'atomic' and 'molecular' basis.

Treating the symmetrical problem we recognise by parity arguments that we can restrict our calculations to the half plane $(\pi/2, \pi)$. The starting point is the following approximate ansatz for the wavefunction, we begin with $w<1$

$$\psi^{(\mu)}(w,\delta)=\sum_{i=1}^{m}\hat{U}_i^{(\mu)}(\delta)\psi_i(w) \qquad (w<1) \tag{4.1}$$

with a certain magnetic quantum number μ. The bispinors $\psi_i(w)$ are the expansion coefficients, which are to be calculated for the given 4×4 basis matrices $\hat{U}_i^{(\mu)}$. The

index i is closely related to the equally spaced tracks

$$\delta_i = [\pi/(2m+2)]i + \pi/2, \qquad i = 1, 2, \ldots, m. \tag{4.2}$$

The reason for these relationships and the nature of the coefficients $\psi_i(w)$ will become clear later.

We can dispense with the tracks δ_0 and δ_{m+1}, because the wavefunction vanishes there. So we replace the infinite-dimensional solution space $S^{(\mu)}$ of δ-dependent spinor functions by a finite-dimensional subspace, or more precisely by a sequence of finite-dimensional subspaces $S_m^{(\mu)}$ with the running index m denoting the dimension. In general $\hat{U}_i^{(\mu)}$ is a diagonal 4×4 matrix containing the so-called roof functions $u_i(\delta)$ as elements. They are frequently used in finite element methods which are related to our numerical proceedings (Strang and Fix 1973).

These continuous functions $u_i(\delta)$ are zero unless $\delta \in (\delta_{i-1}, \delta_{i+1})$ where they have to fulfil the conditions

$$U_i(\delta_j) = \begin{cases} 0, & j \neq i, \\ 1, & j = i. \end{cases} \tag{4.3}$$

Two linear independent functions have to be taken in the definition of a set of roof functions. We use the pair $\sin\frac{1}{2}x \sin^{\mu} x$ and $\cos\frac{1}{2}x \sin^{\mu} x$ for the approximating function

$$f^{(\mu)}(x) = (a \cos\tfrac{1}{2}x + b \sin\tfrac{1}{2}x)\sin^{\mu} x, \qquad x = 2\delta - \pi, \tag{4.4}$$

between the grid points. The numbers a and b are real parameters, determined according to the conditions (4.3) for the intervals (δ_{i-1}, δ_i), (δ_i, δ_{i+1}) and every index i. Considering the spin-angular distribution of the spherical 1s-eigenstate (I, § 5), we recognise that it can be described exactly by the basic functions (4.4) for $x = \theta$. So they are well suited in the case of large two-centre distances. The functions (4.4) can fulfil the boundary condition of the angle interval in two different ways ($a = 0$ or $a \neq 0$). Here we have to remember the results in § 3. As a consequence we are forced to choose the appropriate roof functions in the diagonal of $\hat{U}_i^{(\mu)}(\delta)$ for the edge grid points of the angle interval.

Until now we have presumed a vanishing wavefunction on both sides of the angle interval $(\pi/2, \pi)$, as it is required for $w < 1$. For $w > 1$ we will continue with the 'molecular' part of our approximation. The main characteristic is the loss of the boundary condition for $\delta = \pi/2$. The parity condition will be some compensation on this side of our half plane. The approximating functions have to be modified to describe angle distributions according to the analytically known spherical solutions in the asymptotic regions for large w. So we propose that the functions

$$F^{(\mu)}(\delta) = (a \cos\tfrac{1}{2}\delta + b \sin\tfrac{1}{2}\delta)\sin^{\mu}\delta \tag{4.5}$$

replace the $f^{\mu}(\delta)$.

The matrix $\hat{U}_i^{\mu}$ will differ from the diagonal form for $w > 1$ in order to satisfy the parity relations. This effect becomes visible only on the new left edge grid point ($\delta_0 = \pi/2$), where the wavefunction may become non-zero now. Therefore we have to extend our expansion (4.1) in this region by one additional term. We relinquish a further discussion of more technical details of our ansatz and only summarise the basic idea in one sentence. By means of the known spherical asymptotics of our solution we can construct a suitable basis, divided in two main parts, so that its expansion coefficients embody the approximate wavefunction on the grid points.

Our basic mathematical procedure to reduce the two-dimensional partial differential equation to an ordinary linear system of first order is the method of Galerkin–Bubnow, cf Strang and Fix (1973). Using this procedure, we look for a weak solution $\psi_E^{(\mu)}$ of the differential equation. Generally this is an element of some solution space $\tilde{S}^{(\mu)}$ such that

$$(\chi, (\hat{H}^{(\mu)} - E)\psi_E^{(\mu)}) = 0 \tag{4.6}$$

for every function $\chi \in \tilde{V}^{(\mu)}$, the test space. The scalar product has been defined in (2.18) in the context of the normalisation of bound states of the Dirac equation. We want to use this variational method for the angular coordinate only in order to get a system of ordinary differential equations. To implement this idea we take the angle-dependent part of this scalar product and define

$$\langle \chi | \psi \rangle = \int \frac{\mathrm{d}\delta}{\sqrt[4]{D}} \chi^{+}(\delta)\psi(\delta). \tag{4.7}$$

In the case of the semi-discrete Galerkin–Bubnow method we choose for $\tilde{V}^{(\mu)}$ the space $S_m^{(\mu)}$. Moreover, we require that the angular dependence of the weak solution $\psi_E^{(\mu)}$ can be described by the same functions. The result is a linear system of first order differential equations,

$$(w\mathbb{A}\,\mathrm{d}/\mathrm{d}w + \mathbb{B} + \mu\mathbb{G} - Z\alpha\mathbb{W} + ma\mathbb{D})\Psi_E^{(\mu)}(w) = Ea\mathbb{F}\Psi_E^{(\mu)}(w) \tag{4.8}$$

with

$$\begin{aligned}
\mathbb{A}_{ij} &= \langle \hat{U}_j^{(\mu)} | -\mathrm{i}\alpha_3 \sqrt[4]{D} | \hat{U}_i^{(\mu)} \rangle, & \mathbb{B}_{ij} &= \langle \hat{U}_j^{(\mu)} | -\mathrm{i}\alpha_1 \sqrt[4]{D}\,\partial/\partial\delta | \hat{U}_i^{(\mu)} \rangle, \\
\mathbb{G}_{ij} &= w^2 \langle \hat{U}_j^{(\mu)} | \alpha_2/\rho | \hat{U}_i^{(\mu)} \rangle, & \mathbb{W}_{ij} &= \sqrt{2}\langle \hat{U}_j^{(\mu)} | (\sqrt{D} + 1 + w^2)^{1/2} | \hat{U}_i^{(\mu)} \rangle, \\
\mathbb{D}_{ij} &= w^2 \langle \hat{U}_j^{(\mu)} | \gamma^0 | \hat{U}_i^{(\mu)} \rangle, & \mathbb{F}_{ij} &= w^2 \langle \hat{U}_j^{(\mu)} | \hat{U}_i^{(\mu)} \rangle.
\end{aligned} \tag{4.9}$$

Here we observe that the listed matrix elements are again 4×4 matrices. $\Psi_E^{(\mu)}(w)$ contains all the expansion coefficients $\psi_i(w)$ of $\psi_E^{(\mu)}(w, \delta)$, cf (4.1). We want to point out the independence of the matrices $\mathbb{A}$ and $\mathbb{B}$ of the variable w. This simplifies considerably the numerical treatment of the system (4.8) by any multistep integration method, which is used frequently for such calculations.

A decomposition of, for instance, $\mathbb{A}$ in the direct product as

$$\mathbb{A}_{ij} = \langle u_j | \sqrt[4]{D} | u_i \rangle \otimes (-\mathrm{i}\alpha_3) \tag{4.10}$$

(u_i, u_j are the pure roof functions) fails because of the different behaviour of the spinor components at the boundaries. Nevertheless the matrices contain some symmetries, which lead to numerical advantages. The approximating function $f^{(\mu)}(\delta)$, and therefore the roof functions $u_i(\delta)$ too, as well as the weighting functions in (4.9), e.g. $1/\rho(w, \delta)$, have invariance properties under space inversion, where we have to distinguish between the atomic and molecular regions. But we do not want to discuss the technical consequences in detail. The matrices $\mathbb{A}$ through $\mathbb{W}$ have band character caused by the roof functions. The elements can be calculated using a Gauss integration of low order. For the two matrices $\mathbb{A}$ and $\mathbb{B}$ it is even possible to obtain analytical values, a further advantage of these matrices.

After this brief description of the integration method of the partial differential equation, we now turn to the problem of finding eigenvalues and eigenfunctions. For this purpose we want to transfer an effective method for eigenvalue problems of ordinary differential equations which is known as the matching method. It is a member

of the family of the multiple shooting methods (Stoer and Bulirsch 1973, Keller 1968). In the case of radial relativistic wavefunctions the energy expectation value is the starting point for the set-up of a well convergent procedure, as proposed by Mayers (1957). Starting with a regular asymptotic solution at the left side ($r \to 0$) we get a 'left solution'. Analogously we calculate a 'right solution'.

If the starting value is not an eigenvalue the left solution diverges on the right side and *vice versa*. At a matching point, normally the classical turning point, the mismatching can be employed to yield a correction for the starting energy.

For the more complex problem of a partial differential equation we have to reconcile the ordinary matching method with the requirement that the wavefunction is continuous on a matching line (e.g. $w = w_c$).

In figure 5 we have introduced two starting lines, w_0 and w_∞, for the left and right solutions $\psi_L(w, \delta)$ and $\psi_R(w, \delta)$, which obey (4.8). Generally we do not know the correct spin-angle distributions to start our integrations in w_0 and w_∞. But they must exist for a certain eigenvalue E, so that we can connect the solutions ψ_R and ψ_L along w_c in such a way that the combined wavefunction becomes continuous and differentiable everywhere. Our procedure is divided into two steps, starting with an energy E_0. Firstly we determine the two spin-angle distributions by minimising the following mismatch function:

$$\Delta_\psi = \|\psi_L - \psi_R\| / \|\psi_L + \psi_R\| \,|_{w=w_c}. \tag{4.11}$$

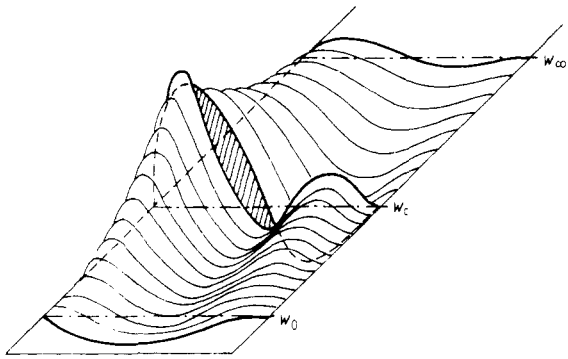

Figure 5. Schematic illustration of the matching method. A 'left (right) regular' solution is generated by integration from w_0 to w_c (w_∞ to w_c). The distribution of only one spinor component is shown. The energy correction follows from the discontinuity at $w = w_c$.

The norm is defined according to the earlier used scalar product (4.7)

$$\|\psi\|^2 = \langle\psi|\psi\rangle. \tag{4.12}$$

With these preparations we will look for the zeros of

$$\Delta_E(E_0) = \frac{(\psi|\hat{H} - E_0|\psi)}{(\psi|\psi)} = \frac{\langle\psi_L| - i\alpha_3\sqrt[4]{D}/\alpha w|\psi_R\rangle|_{w=w_c}}{(\psi|\psi)}. \tag{4.13}$$

ψ is the combined left and right solution with the minimised defect Δ_ψ. The w derivative in the Hamiltonian yields, operating on the discontinuous wavefunction ψ, the energy correction term Δ_E. So the next iteration step can be started with $E_1 = E_0 + \Delta_E(E_0)$, assuming that the expectation value represents a better approximation of the eigenvalue.

We hope that this short overview will suffice. A more complete description will be presented together with numerical results in a subsequent paper.

Up to now we can offer calculations of bound states with the magnetic quantum number $\mu = \frac{1}{2}$ in the potential of two point-like symmetric nuclei. In particular, we investigated the lead–lead system in detail. The half two-centre distances a have to be taken for the present out of the interval (10^4 fm, 10^{20} fm), because we have established first of all our 'atomic' basis. This is sufficient to give information about the accuracy and velocity of convergence of our procedure. The lower limit at $a \approx 10^4$ fm, depending on the state under consideration, becomes necessary, because for decreasing two-centre distances an increasing part of the electron density is localised outside the lemniscate, which cannot be described by our ansatz. For instance, the ground state of the symmetric lead system can be calculated with a relative accuracy of better than ten decimal places in the binding energy. For a distance of $a = 10^4$ fm we notice a slight deviation from the energy value calculated by diagonalising the Hamiltonian in the usual atomic basis, which we use as reference to compare with our data. The reason lies in the above-mentioned fact that a small part of the 1Σ wavefunction is unreachable.

In these calculations the discontinuity of the wavefunctions on the matching line can be reduced to 10^{-10} expressed by the mismatch $\Delta\psi$ of (4.11). Higher states such as 2Σ and 3Σ are also calculated with similar accuracies paying attention to the temporary borderline.

Clearly these results are of little physical interest. They prove, however, that the mathematical framework furnished in the preceding sections works and yields reliable results.

5. Conclusion

In this work we propose a new way to tackle the relativistic two-centre problem. It comprises two basic ideas. Firstly the chosen Cassini coordinates ensure in both asymptotic cases of physical interest a simple description of the electron motion based on the well known spherical behaviour. The coordinate transformation can be derived from an analytical function, which facilitates the application of the second idea. This is the implantation of our local representation, explained in detail in paper I.

The introduction of these two constituents into the Dirac equation with the two-centre potential has been carried out in § 2. A discussion of the geometrical symmetries in § 3 reduces the derived Hamiltonian to a partial differential operator in two dimensions. We restricted our work to the charge symmetric case which enables the utilisation of the parity conservation. The easily derived boundary condition, that the wavefunction has to vanish everywhere along the curve enclosing the domain of integration, is not sufficient to implement any numerical procedure. So more intensive investigations of the behaviour of regular, normalisable solutions near the boundaries became necessary, as described briefly in § 3. Notable results were the emergence of the spherical Dirac equation in the two asymptotic cases (w very small or very large) and the invariant power behaviour of the wavefunction for all w at the boundaries of the angular variable δ.

This was a legitimation and stimulation to introduce the special numerical method described in § 4. Paying attention to the natural borderline in the domain, the lemniscate, we have to establish two angle-dependent roof function bases, the 'atomic'

and the 'molecular' ones. Then the coordinate δ can be eliminated by a variational method, the Galerkin–Bubnow method. The derived differential equation of first order can be treated with commonly used methods like multistep procedures. Eigenenergies and eigenfunctions are found with a fast converging algorithm. It combines a matching step for two solutions with a certain starting energy, each regular in one of the two asymptotic regions, and a step for the determination of a new, corrected eigenvalue on the base of the energy expectation value.

After this brief repetition of the contents we want to discuss some important aspects for possible generalisations of the symmetric two-centre problem. We assumed preliminarily that the potential is generated by point-like nuclei. This permits the comparison in the asymptotic regions with analytically known values for energy and wavefunctions. The transition to extended nuclei, which are physically more realistic, can be achieved in analogy to the spherical case. There mostly the potential of uniformly charged spheres is taken to approximate this effect. It can be expressed by the Cassini coordinates. A slight deviation from homogeneously charged spherical nuclei leads to considerable simplifications in the analytical structure of the potential. In particular, we have to choose Cassinian ovals as nuclear surface, where the potential must be differentiable.

Another step of generalisation is the inclusion of charge asymmetry ($Z_1 \neq Z_2$). While in the symmetric case the conservation of parity can be used to reduce the numerical expense by half, we have to integrate in the full domain now. We point out that it may be advantageous to introduce modified Cassini coordinates defined by the holomorphic function

$$f(\zeta) = \tfrac{1}{2}\left(Q_1 \log \frac{\zeta - a}{a} + Q_2 \log \frac{\zeta + a}{a} \right) \tag{5.1}$$

instead of (2.2). Here the w-lines correspond to two-dimensional equipotential lines for two-point charges with values Q_1 and Q_2 respectively. For $Q_1 = 0$ these coordinates are identical with the spherical coordinates. Q_1 and Q_2 need not be chosen as Z_1 and Z_2. It may be better to adjust them so that the critical point of the coordinate system (double point of the 'lemniscate') coincides with the saddle point of the three-dimensional potential as in the symmetric case. However, we have to mention that probably the inverse of $f(\zeta)$—and consequently the scale factors and the potential—cannot be found analytically.

The Cassini coordinates can be generalised in one more direction. It is straightforward to introduce more than two collinearly arranged centres.

To investigate many-electron problems we need the relation between the electron densities and the generated screening potential. So it is important whether the Poisson equation in these complicated coordinates can be solved easily, similarly to the spherical case. This would be the prerequisite to perform Dirac–Fock calculations.

Our method of solving the Dirac equation in Cassini coordinates may also be an application in a totally different field. Recently the description of hadrons by the MIT bag model has gained increased attention. To allow for excited states or fission of hadrons, calculations with deformed bags have been performed. Here eigenenergies and eigensolutions of the Dirac equation are sought which are subject to the linear MIT boundary condition at the surface of the bag. A class of surfaces is given (e.g. expressed by Legendre polynomials up to a certain order) and the 'solutions' (quotation marks because they exist only for the eigenenergies) are found by superposition of spherical states (Vasak *et al* 1983). The problem is to obtain the eigenenergies. We

propose another method. If one considers bag shapes which correspond to Cassini curves w = constant, one has a rectangular domain of integration. These shapes should be very appropriate for describing fission processes. Then by outward integration a set of solutions can be found which generally will not fulfil the boundary condition. However, the methods developed for our problem, the two-centre problem, to find 'optimal' linear combinations and energy corrections can be transferred. This should be a rather fast convergent algorithm of finding solutions in a deformed bag.

This is a small selection of possible extensions which can universalise our method to a flexible program for the description of relativistic two-centre problems of spin-half particles. Numerical results like energy correlation diagrams will be published in a subsequent paper.

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Appendix 1. Proof of a theorem

The proposition stated in § 3 is a special case of a more general theorem.

Let us assume that the Dirac Hamiltonian has the form

$$\hat{H} = -\mathrm{i}\left(\alpha_1 \frac{1}{h_u}\partial_u + \alpha_2 \frac{1}{h_v}\partial_v + \alpha_3 \frac{1}{h_w}\partial_w\right) + \gamma^0 m + e\left(\sum_k \alpha_k A_k + A_0\right). \tag{A1.1}$$

This is just the local representation in the coordinates (u, v, w). In § 3 we have the special case $u = w$, $v = \delta$, $w = \varphi$. Besides this, we assume that the scale factor h_u depends on v $(\partial_v h_u \neq 0)$ but is independent of w $(\partial_w h_u \equiv 0)$. Then every differential operator

$$\hat{B} = \sum_{n=0}^{N} \sum_{m=0}^{M} B_{nm}(u, v, w)\partial_v^n \partial_w^m \tag{A1.2}$$

with space-dependent 4×4 matrices B_{nm} which commutes with $\hat{H}$ actually has the form

$$\hat{B} = \sum_{m=0}^{M} B_{0m}(u, v, w)\partial_w^m. \tag{A1.3}$$

Hence no derivative with respect to v occurs.

The following lemma will be useful:

$$[\alpha_1, B] = 0, \qquad [\alpha_1, \tilde{B}] = B\alpha_1 \qquad \Rightarrow \qquad B = 0 \tag{A1.4}$$

with any matrices B, $\tilde{B}$.

To prove this we multiply the second condition from the left and from the right respectively with α_1,

$$\tilde{B} - \alpha_1 \tilde{B} \alpha_1 = B, \qquad \alpha_1 \tilde{B} \alpha_1 - \tilde{B} = B, \tag{A1.5}$$

where we made use of the first condition. The proposition follows by addition.

To prove the theorem we look at the commutator

$$[\hat{H}, \hat{B}] = -\mathrm{i} \sum_{n,m} \alpha_1 \frac{1}{h_u} \partial_u B_{nm} \partial_v^n \partial_w^m + \mathrm{i} \sum_{n,m} B_{nm} \partial_v^n \partial_w^m \alpha_1 \frac{1}{h_u} \partial_u + R \tag{A1.6}$$

where R does not contain any u derivative. We sort according to powers of $\partial_u^k \partial_v^v \partial_w^u$. Since this commutator vanishes, in particular the terms in front of $\partial_u \partial_v^N \partial_w^m$ and $\partial_u \partial_v^{N-1} \partial_w^m$ must vanish ($N > 0$),

$$\begin{aligned} &(1/h_u)\alpha_1 B_{Nm} - (1/h_u) B_{Nm} \alpha_1 = 0, \\ &(1/h_u)\alpha_1 B_{N-1,m} - (1/h_u) B_{N-1,m} \alpha_1 - N(\partial_v (1/h_u) B_{Nm} \alpha_1 = 0. \end{aligned} \tag{A1.7}$$

These conditions lead to

$$[\alpha_1, B_{Nm}] = 0, \qquad [\alpha_1, B_{B-1,m}] = N h_u (\partial_v (1/h_u)) B_{Nm} \alpha_1. \tag{A1.8}$$

Now we can apply the lemma,

$$B_{Nm} = 0. \tag{A1.9}$$

The proof is completed by induction. Clearly the result does not depend on the local representation. It holds true also in the ordinary cartesian representation.

Apppendix 2. Asymptotic expressions for some terms

In this appendix we will derive Laurent expansions around $w = 0$ and $w = \infty$ for some terms in the Dirac equation in Cassini coordinates. In the asymptotic regions they are more convenient than the closed expressions for numerical as well as analytical investigation. The second and fourth roots of

$$D = 1 + 2 \cos 2\delta \, w^2 + w^4 \tag{A2.1}$$

are very easy to expand. They are just the generating functions for a special class of Gegenbauer polynomials (Erdélyi *et al* 1953),

$$\begin{aligned} \sqrt{D} &= \sum_{n=0}^{\infty} C_n^{-1/2}(-\cos 2\delta) w^{2n} \\ \sqrt[4]{D} &= \sum_{n=0}^{\infty} C_n^{-1/4}(-\cos 2\delta) w^{2n} \end{aligned} \qquad (w < 1) \tag{A2.2}$$

The inverses of these functions give

$$\begin{aligned} 1/\sqrt{D} &= \sum_{n=0}^{\infty} P_n(-\cos 2\delta) w^{2n} \\ 1/\sqrt[4]{D} &= \sum_{n=0}^{\infty} C_n^{1/4}(-\cos 2\delta) w^{2n}. \end{aligned} \qquad (w < 1) \tag{A2.3}$$

The series for $w > 1$ can be obtained easily from the expansion around $w = 0$ by use of the symmetry relation

$$D(1/w) = (1/w^4) D(w). \tag{A2.4}$$

The Gegenbauer polynomials can be calculated from the recurrence formula

$$(n+1)C_{n+1}^{\lambda}(x) = 2(n+\lambda)xC_n^{\lambda}(x) - (n+2\lambda-1)C_{n-1}^{\lambda}(x) \tag{A2.5}$$

and the starting values

$$C_0^{\lambda}(x) = 1, \qquad C_1^{\lambda}(x) = 2\lambda x. \tag{A2.6}$$

In the case $\lambda = -\frac{1}{2}$ we observe a remarkable behaviour. The polynomials $C_n^{-1/2}$ with order n larger than 1 always contain the factor $(1-x^2) = (1-\cos^2 2\delta) = \sin^2 2\delta$.

The potential energy (2.17) then becomes

$$V_{\mathrm{tc}} = -\frac{Z\alpha\sqrt{2}}{a}\frac{1}{w^2}\left(2 + (1+\cos 2\delta)w^2 + \sum_{n=2}^{\infty} C_n^{-1/2}(-\cos 2\delta)w^{2n}\right)^{1/2}. \tag{A2.7}$$

It obeys the interesting symmetry relation

$$(1/w)V_{\mathrm{tc}}(1/w) = w^2 V_{\mathrm{tc}}(w). \tag{A2.8}$$

The distance ρ from the symmetry axis is

$$\rho = \begin{cases} (a/\sqrt{2})w^2\left(\sum_{n=0}^{\infty} C_{n+2}^{-1/2}(-\cos 2\delta)w^{2n}\right)^{1/2} & \text{for } w < 1 \\ (a/\sqrt{2})w\left((1-\cos 2\delta)(1-w^2) + \sum_{n=2}^{\infty} C_n^{-1/2}(-\cos 2\delta)w^{-2n}\right)^{1/2} & \text{for } w > 1. \end{cases} \tag{A2.9}$$

Here we have to take care of a common factor $|\sin 2\delta|$ for $w < 1$ or $\sin\delta$ for $w > 1$. The Laurent expansions of V_{tc} and $1/\rho$ around $w = 0$ and $w = \infty$ can be obtained directly.

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