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An effective Dirac equation for a binary of two fermions

E Marsch

Max-Planck-Institut für Sonnensystemforschung, 37191 Katlenburg-Lindau, Germany

E-mail: marsch@mps.mpg.de

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Abstract

Effective Dirac equations are, by following the work of Pilkuhn, derived for a binary of two fermions from the original two-fermion Dirac-type Hamiltonian written in a 16-component spinor representation. For spherical interaction potential (like the static Coulomb potential) the spin dynamics in the product spin space and spatial dynamics in the particle–antiparticle state space can be fully decoupled and separated. The case of atomic hydrogen is solved again as an example, and the standard results including recoil effects through the reduced mass and fine structure induced by spin–orbit coupling are recovered for the energy spectrum.

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1. Introduction

The precise calculation of the energy spectra of binaries including their fine structure is a main topic of relativistic quantum mechanics. The state of this field has been described in a recent textbook by Pilkuhn [1], and previously in a review paper [2]. The classical example of such a binary system is the hydrogen atom. If one only considers the static Coulomb coupling between the proton and electron but accounts for their spins, one can solve this problem exactly, using the so-called Dirac–Coulomb Hamiltonian. In a previous publication by Marsch [4] the energy levels and wavefunctions of the two-fermion Hamiltonian for such a simple hydrogen-like binary bound by the Coulomb force were calculated exactly, following the same procedures that lead Gordon [3] to his solution of the Dirac equation. The eigenfunctions of the spin–orbit-coupling operators are four-component spinors forming a basis in the spin product state spanned by the spin singlet- and triplet-like eigenfunctions of the total angular momentum operator [5]. The four-component radial wavefunctions in the particle–antiparticle state can be expressed in terms of generalized hypergeometric functions which are determined through a matrix recursion relation [6].

Häckl *et al* [7] proposed a reduction of the 16-component spinor into an equivalent eight-component spinor by a fully relativistic elimination of two components, and by exploiting the common basis of the chirality and parity operators of the two-fermion Dirac equation. By a further transformation of the eight-component spinor by means of the spin-exchange operator of the two fermions, they were able to remove the spin of one fermion entirely, thus ending up with an effective Dirac equation for the binary which is discussed extensively in Pilkuhn's book [1] and in his two more recent papers [8, 9] on relativistic bound states and a Klein–Gordon equation for atoms.

Here we will point to some questions related to this approach and discuss alternative treatments of the problem, leading to other eight-component equations that preserve the original symmetries and still involve the full spin dynamics of the binary system of the two fermions with masses m_1 and m_2 and spins $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$, respectively corresponding to the vector of the standard Pauli [10] spin matrices. For $m_1 \neq m_2$, we obtain an effective Dirac equation that is linear in the momentum operator $\mathbf{p} = -\mathrm{i}\hbar\partial/\partial\mathbf{r}$ of relative motion (with $\mathbf{r}$ being the particles distance), and for $m_1 = m_2$ the result is a Kramers-like equation [11] which corresponds to the squared Dirac equation [12, 13] and is of second order in $\mathbf{p}$.

Two-body Dirac equations were proposed and used by Van Alstine and Crater [14] in the center-of-momentum (cms) coordinate system to provide Kramers- or Schrödinger-like wave equations (depending on p^2), which were then applied to binaries. Their approach is also important from the point of view that such equations are quite relevant for leptonic systems such as charmonium, or positronium for example [16], because exact results from reduced relativistic quantum mechanics can serve as benchmark cases for the solutions obtained by means of modern quantum field theory, which are mostly of a perturbative nature.

The relativistic quantum theory of two particles has a long history. In an early paper, Bekamjian and Thomas [15] defined two-body quantum mechanics on the basis of an exact unitary representation of the Poincaré group. In a later paper, Van Alstine and Crater [14] constructed, for example, the covariant two-fermion dynamics by means of quantization of the so-called relativistic constraint mechanics. Their model leads to a 16-component covariant wave equation. Another form of a relativistic wave equation for two fermions has most recently been derived by Giachetti and Sorace [17], who start from the covariant classical kinematics of a binary and then derive its quantization as a free two-fermion system in a framework of pure relativistic quantum mechanics. The resulting Hamiltonian, in which we use the standard Dirac matrices [12] $\hat{\boldsymbol{\alpha}}$ and $\hat{\beta}$ and include a general scalar interaction potential $V(r)$ depending on the relative distance $r = \sqrt{\mathbf{r}\cdot\mathbf{r}}$, can be written as follows:

$$\mathcal{H}_{12} = V(r) + \hat{\beta}_1 m_1 c^2 + \hat{\beta}_2 m_2 c^2 + \hat{\boldsymbol{\alpha}}_1 \cdot c\mathbf{p}_1 + \hat{\boldsymbol{\alpha}}_2 \cdot c\mathbf{p}_2. \tag{1}$$

In this equation, and in the above-mentioned similar cases, the underlying assumptions of relativistic theory are obvious, and one can identify the representation of the Hilbert space and unitary representation of the Poincaré group. In (1) $\mathbf{p}_{1,2}$ is the fermion momentum in the inertial frame, c the speed of light in vacuo, and $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$ the distance vector between the loci of the two fermions. This quantum-mechanical approach is certainly useful for calculating relativistic corrections of the energy spectrum for unlike binaries such as the hydrogen atom or the muon–positron bound state. However, the static Coulomb potential used below clearly must be complemented by radiative effects of the electromagnetic interaction, when the two fermions have equal masses such as in positronium, muonium or charmonium, where genuine relativistic effects dominate. Of course, relativistic quantum mechanics has its limitations, and only modern quantum field theory [18] provides an adequate relativistic description of any fermionic binary.

In the present paper we analyze the possible solutions of the differential equations arising from the relativistic quantum mechanics of two fermions, both being governed by the binary Dirac equation (1), with a $1/r$-Coulomb potential binding the particles. The relevant Hamiltonian is given subsequently in (3), which in this form has been investigated before by Marsch [4], using Dirac's original method to derive (1). The Dirac matrices appearing in (1) can be decomposed into direct products, in which the operators α and β act in particle–antiparticle space and the Pauli matrix operator as usually acts in the spin space related to each fermion. We can thus rewrite the Dirac matrices in the following form:

$$\hat{\boldsymbol{\alpha}} = \alpha\boldsymbol{\sigma} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\boldsymbol{\sigma}, \qquad \hat{\beta} = \beta\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\sigma_0. \tag{2}$$

Here σ_0 is understood to be the 2×2 unit matrix, and the symbol $\boldsymbol{\sigma}$ denotes a three-component vector, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, consisting of the Pauli [10] matrices which have their standard form. Equation (2) implies the definition of α and β.

2. The two-fermion Dirac–Coulomb operator

The two-fermion problem is treated here in the center-of-momentum system (cms) and in relative coordinates. For a more comprehensive discussion of this subject see the book of Pilkuhn [1]. The nomenclature is as usual: e is the electric charge unit, and $\alpha_S = e^2/\hbar c$ is Sommerfeld's fine structure constant. One fermion is assumed to have charge number +1, the other -1. In the cms, $\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{0}$, and thus one can write $\mathbf{p}_{1,2} = \pm\mathbf{p}$. The Coulomb interaction is assumed as instantaneous, because the light travel time through a Bohr or Fermi radius is very much shorter than any typical dynamic evolution time of the particles, and therefore retardation effects are neglected here in lowest order. The simplest possible electrostatic binary Hamiltonian then reads

$$\mathcal{H} = -\frac{\alpha_S \hbar c}{r} + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + \alpha_1 \boldsymbol{\sigma}_1 \cdot c\mathbf{p} - \alpha_2 \boldsymbol{\sigma}_2 \cdot c\mathbf{p}. \tag{3}$$

The nomenclature used here was defined previously in [4] and is consistent with that adopted in the textbook by Strange [19] on the relativistic quantum mechanics of multi-electron atoms. The operator in equation (3) represents the binary's mass Casimir operator of the underlying representation of the Poincaré group, as shown by Giachetti and Sorace [17]. The angular momentum operator corresponding to the relative momentum of the particles orbiting around each other is

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}. \tag{4}$$

Before continuing the calculations, we analyze the internal symmetries of the binary system. The orbital momentum operator $\mathbf{L}$ commutes with the Coulomb potential, $\left[\mathbf{L}, \frac{1}{r}\right] = \mathbf{0}$, but not with the spin terms. As usually we denote the commutator by $[,]$ and anti-commutator as $\{,\}$. The single-spin operators of the two fermions forming the binary are $\mathbf{S}_{1,2} = \frac{1}{2}\hbar\boldsymbol{\sigma}_{1,2}$. The total angular momentum operator, defined as

$$\mathbf{J} = \mathbf{L} + \mathbf{S}_1 + \mathbf{S}_2, \tag{5}$$

does commute with $\mathcal{H}$. We [4] denote the eigenfunction of $\mathbf{J}$ in the four-dimensional spin state space by Υ. Note that according to the angular momentum operator algebra the following relations hold for the spins: $[\mathbf{L} + \mathbf{S}_{1,2}, (\mathbf{S}_{1,2} \cdot \mathbf{p})] = \mathbf{0}$, and similarly $[\mathbf{L} + \mathbf{S}_{1,2}, (\mathbf{S}_{1,2} \cdot \mathbf{r})] = \mathbf{0}$. Furthermore, the operator relations hold $[\alpha_1, \alpha_2] = [\beta_1, \beta_2] = [\beta_1, \alpha_2] = [\alpha_1, \beta_2] = 0$ and $\{\alpha_{1,2}, \beta_{1,2}\} = 0$, and finally $\alpha_{1,2}^2 = 1$ and $\beta_{1,2}^2 = 1$. For the Dirac equation, the associated

Hilbert space is two dimensional and describes particles and antiparticles. In the simplest matrix representation we then obtain

$$\alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6}$$

For the two-fermion Dirac equation (3) the operators $\alpha_{1,2}$ and $\beta_{1,2}$ act in a four-dimensional Hilbert space and thus are represented by 4×4 matrices. The eigenvectors of (6) simply are

$$\phi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \phi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{7}$$

which form an orthonormal set. The operator α interchanges particle and antiparticle. The two operators in (6) act as follows:

$$\alpha\phi_\pm = \phi_\mp, \qquad \beta\phi_\pm = \pm\phi_\mp. \tag{8}$$

It is now a straightforward task [4] to represent the Hamiltonian (3) as a 4×4 matrix. The stationary eigenvalue problem, $\mathcal{H}\Psi = E\Psi$, attains the form

$$\begin{pmatrix} (m_1+m_2)c^2 & \boldsymbol{\sigma}_1 \cdot c\mathbf{p} & -\boldsymbol{\sigma}_2 \cdot c\mathbf{p} & 0 \\ \boldsymbol{\sigma}_1 \cdot c\mathbf{p} & (-m_1+m_2)c^2 & 0 & -\boldsymbol{\sigma}_2 \cdot c\mathbf{p} \\ -\boldsymbol{\sigma}_2 \cdot c\mathbf{p} & 0 & (m_1-m_2)c^2 & \boldsymbol{\sigma}_1 \cdot c\mathbf{p} \\ 0 & -\boldsymbol{\sigma}_2 \cdot c\mathbf{p} & \boldsymbol{\sigma}_1 \cdot c\mathbf{p} & (-m_1-m_2)c^2 \end{pmatrix} \Psi(\mathbf{r}) = \left(E + \frac{\alpha_S \hbar c}{r}\right)\Psi(\mathbf{r}). \tag{9}$$

Let us consider from now on the free-particles problem and put for the time being $\alpha_S = 0$. We normalize the energy to the total rest energy with mass $M = m_1 + m_2$, i.e. $y = E/Mc^2$, and introduce the helicities:

$$S_{1,2}(\hat{\mathbf{p}}) = \boldsymbol{\sigma}_{1,2} \cdot \hat{\mathbf{p}}, \tag{10}$$

which obey the relation $S_{1,2}^2 = 1$, and of course $[S_1, S_2] = 0$. This results from the well-known algebra of the Pauli matrices: $\boldsymbol{\sigma} \times \boldsymbol{\sigma} = 2\mathrm{i}\boldsymbol{\sigma}$, and $(\boldsymbol{\sigma} \cdot \mathbf{p})^2 = p^2$. Here $\hat{\mathbf{p}} = \mathbf{p}/p$ is a unit vector. The solution of (9) is a plane wave, and the eigen spinor is here written as a row vector normalized to unity in the four-dimensional particle/antiparticle state space and reads

$$\Psi^\dagger(\mathbf{r}) = \exp(-\mathrm{i}\mathbf{p} \cdot \mathbf{r})\Upsilon^\dagger(a_1(p), a_2(p)S_1(\hat{\mathbf{p}}), a_3(p)S_2(\hat{\mathbf{p}}), a_4(p)S_1(\hat{\mathbf{p}})S_2(\hat{\mathbf{p}})). \tag{11}$$

The coefficients $a_j(p)$ of the spinor components are given by the following expressions:

$$a_{1,4}(p) = \mp\sqrt{\frac{y \pm 1}{y \mp 1}}A(p), \quad a_{2,3}(p) = \mp\frac{2y\tilde{p}}{\sqrt{y^2-1}(y \mp R)}A(p), \quad A(p) = \frac{\tilde{p}y}{\sqrt{y^4 - R^2}}. \tag{12}$$

Normalization requires that $\Psi^\dagger\Psi = 1$, which is fulfilled since $a_1^2 + a_2^2 + a_3^2 + a_4^2 = 1$, whereby the subsequent dispersion equation (13) is exploited. The eigenvalue problem for $E(p)$ yields, through the vanishing determinant of the matrix in (9), this dispersion relation, i.e. the normalized momentum $\tilde{p} = p/Mc$ as a function of normalized energy:

$$\tilde{p} = \sqrt{\frac{(y^2-1)(y^2-R^2)}{(2y)^2}}, \tag{13}$$

where we introduced the abbreviation symbol $R = (m_2 - m_1)/M$. For bound states dealt with in [4] we have $y < 1$. Then we may write $\tilde{p} = \mathrm{i}\kappa$, where κ must be positive to ensure that the wavefunction decays to zero at infinity. For free particles dealt with in this section $\tilde{p}$ is real, and

we can solve the resulting fourth-order polynomial for y and obtain for $E(p)$ the four energy combinations: $E_1 + E_2$, $-E_1 + E_2$, $E_1 - E_2$, $-E_1 - E_2$. Here $E_{1,2}(p) = \sqrt{(m_{1,2}c^2)^2 + (cp)^2}$ simply is the total energy of a free relativistic fermion in the cms frame.

Any reduced version of the original equation (3) must reproduce the above energy spectrum for zero interaction. Furthermore, one must also require that the genuine symmetries are obeyed and not broken by a reduction of the spinor components. For example, the individual angular momenta, $\mathbf{J}_{1,2} = \mathbf{L} + \mathbf{S}_{1,2}$, do not commute with (3), since in the binary both spins are intrinsically linked through their common spin–orbit coupling. One may introduce the spin permutation operator [1] as $\mathcal{P} = 1/2(1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)$, which obeys $\mathcal{P}^2 = 1$. Operator algebra yields $\mathcal{P}\boldsymbol{\sigma}_{1,2}\mathcal{P} = \boldsymbol{\sigma}_{2,1}$. Note that this operator also does not commute with the Hamiltonian, since it interchanges the spins, and thus leads to a wrong mixed association with the α-operators in (3).

3. Three versions of the reduced operator for two free fermions

In this section, while following closely the work of Pilkuhn [1], we will establish three novel forms of the eight-component spinor wave equation, which result from linear transformations of the original wave equation (3). Again, we set $\alpha_S = 0$, but return in the next section to the hydrogen-like atom problem. In the following it eases the notation to define the dimensionless symbols: $\mu_\pm = (m_1 \pm m_2)/M = \mu_1 \pm \mu_2$, with $\mu_+ = 1$ by definition, and similarly $\sigma_\pm = \sigma_1 \pm \sigma_2$, where

$$\sigma_{1,2}(\mathbf{p}) = (\boldsymbol{\sigma}_{1,2} \cdot \mathbf{p})/(Mc). \tag{14}$$

By definition we have $\sigma_{1,2}^2 = p^2/(Mc)^2$ and $\sigma_+\sigma_- = \sigma_-\sigma_+ = 0$. Inspection of the structure of the original matrix (9) suggests combining similar blocks and introducing two-component spinors by respectively pairing two of the four components of $\Psi^\dagger = \left(\psi_1^\dagger, \psi_2^\dagger, \psi_3^\dagger, \psi_4^\dagger\right)$ in various suitable combinations. The simplest version is obtained by introducing

$$\zeta = \begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \qquad \xi = \begin{pmatrix}\psi_3\\ \psi_4\end{pmatrix}, \tag{15}$$

which leads to the following set, in which the matrices of (6) are again used:

$$\begin{aligned}(-y + (\mu_1\beta + \mu_2) + \sigma_1\alpha)\zeta &= \sigma_2\xi\\ (-y + (\mu_1\beta - \mu_2) + \sigma_1\alpha)\xi &= \sigma_2\zeta.\end{aligned} \tag{16}$$

Insertion of the second in the first equation, while exploiting the matrix properties of α and β, yields a Dirac equation for particle 1 in the center-of-momentum frame. Similarly, combining the first and third, and the second and fourth components gives a Dirac equation for particle 2. Thus each particle obeys

$$\varepsilon_{1,2}\zeta_{1,2} = (\beta\mu_{1,2} + \alpha\sigma_{1,2}(\mathbf{p}))\zeta_{1,2}, \tag{17}$$

where we suppressed the indices for α and β. Squaring of (17) results in the cms mass–shell condition, $\varepsilon_{1,2}^2 - \mu_{1,2}^2 = (p/Mc)^2$, of a free particle. The total energy is $E = Mc^2(\varepsilon_1 + \epsilon_2)$, whereby the individual fractional energy is

$$\varepsilon_{1,2} = \left(y^2 - \mu_{2,1}^2 + \mu_{1,2}^2\right)\big/(2y). \tag{18}$$

The resulting spectrum is identical to what we found when solving the original four-component spinor eigenvalue problem (9). Apparently, both particles are entirely decoupled by this scheme. However, this approach is not convenient when the interaction is switched on. Moreover, somehow the original symmetry seems broken, since the Dirac operator (17)

already commutes with the one-particle angular momentum operator $\mathbf{J}_{1,2}$, whereas the full Hamiltonian (3) did not.

It then appears more appropriate [7] to make use of the common basis of the chirality operator $\mathcal{A} = \alpha_1\alpha_2$ and parity operator $\mathcal{B} = \beta_1\beta_2$, which commute with each other. The relations hold, $\mathcal{A}^2 = 1$ and $\mathcal{B}^2 = 1$, so that their eigenvalues simply are ± 1. This basis change is achieved by the following linear combinations:

$$\phi_{1,2} = (\psi_1 \pm \psi_4)/\sqrt{2}, \qquad \phi_{3,4} = (\psi_2 \pm \psi_3)/\sqrt{2}. \tag{19}$$

Here the basis ψ_j, with j running from 1 to 4, is in a standard form as already given in paper [4]. The eigenvalue problem (9) in the new basis attains the form

$$\begin{pmatrix} -y & \mu_+ & \sigma_-(\mathbf{p}) & 0 \\ \mu_+ & -y & 0 & \sigma_+(\mathbf{p}) \\ \sigma_-(\mathbf{p}) & 0 & -y & -\mu_- \\ 0 & \sigma_+(\mathbf{p}) & -\mu_- & -y \end{pmatrix} \cdot \begin{pmatrix} \phi_1(\mathbf{r}) \\ \phi_2(\mathbf{r}) \\ \phi_3(\mathbf{r}) \\ \phi_4(\mathbf{r}) \end{pmatrix} = 0. \tag{20}$$

We now try another combination of components:

$$\chi_+ = \begin{pmatrix} \phi_1 \\ \phi_4 \end{pmatrix}, \qquad \chi_- = \begin{pmatrix} \phi_2 \\ \phi_3 \end{pmatrix}. \tag{21}$$

The coupled set of equations for these two-component spinors reads

$$\begin{aligned} y\chi_+ &= (\mu_1\beta + \mu_2 + \alpha(\sigma_1 + \sigma_2\beta))\,\chi_- \\ y\chi_- &= (\mu_1\beta + \mu_2 + \alpha(\sigma_1 - \sigma_2\beta))\,\chi_+. \end{aligned} \tag{22}$$

Multiplying these equations, one obtains a new Kramers–Dirac-like equation as follows:

$$\hat{\varepsilon}(p)\chi_\pm = (\beta\hat{\mu}_\pm(\mathbf{p}) + \alpha\hat{\sigma}_\pm(\mathbf{p}))\chi_\pm. \tag{23}$$

Note that the spin- and mass-dependent operators do no longer contain the matrix β, and therefore commute with α. In detail we have the definitions

$$\hat{\varepsilon}(\tilde{p}) = \left(y^2 - \mu_1^2 - \mu_2^2 - 2\tilde{p}^2\right)/2, \tag{24}$$

$$\hat{\mu}_\pm(\mathbf{p}) = \mu_1\mu_2 \mp \sigma_1(\mathbf{p})\sigma_2(\mathbf{p}), \tag{25}$$

$$\hat{\sigma}_\pm(\mathbf{p}) = \mu_2\sigma_1(\mathbf{p}) \pm \mu_1\sigma_2(\mathbf{p}). \tag{26}$$

We recall that the spin algebra yields $[\sigma_{1,2}, \sigma_{1,2}] = 0$, and therefore when squaring the operators in (25)–(26) the multiplication sequence does not matter. Exploiting $\alpha\beta + \beta\alpha = 0$, we can square equation (23) and obtain a quadratic equation in y^2. It reads $y^4 - 2y^2\left(\mu_1^2 + \mu_2^2 + 2\tilde{p}^2\right) + \left(\mu_1^2 - \mu_2^2\right)^2 = 0$. The solution gives the same old combination of free-particle energies as was derived in the previous section from (13). So, the full asymptotic spectrum results from (23), which formally looks like a Dirac equation, yet which through $\hat{\varepsilon}(\tilde{p})$ and $\hat{\mu}_\pm(\mathbf{p})$ is in fact of second order in $\tilde{p}$, as in the Kramers (Klein–Gordon) equation. It should be emphasized that there is no problem in going to the limit of equal masses in this equation. Furthermore, both spins still appear, and thus $\mathbf{J}_{1,2}$ is not conserved, but $\mathbf{J}$ of (5) is. Thus the equation keeps the original symmetry, also when interchanging the indices, yet it does not commute with $\mathcal{P}$.

There is a third way of combining the elements of the originally four-component spinor [1]. We may better choose

$$\psi_- = \begin{pmatrix} \phi_1 \\ \phi_3 \end{pmatrix}, \qquad \psi_+ = \begin{pmatrix} \phi_2 \\ \phi_4 \end{pmatrix}. \tag{27}$$

This leads to a particularly transparent form of the reduced equations:

$$\begin{aligned}(y-\alpha\sigma_-)\,\psi_- &= (\mu_2+\mu_1\beta)\psi_+\\ (y-\alpha\sigma_+)\,\psi_+ &= (\mu_2+\mu_1\beta)\psi_-.\end{aligned} \tag{28}$$

Multiplying these equations, one can exploit the fact that $\sigma_+\sigma_- = 0$ and thus remove the quadratic term in p entirely. Thus one obtains an effective Dirac equation, which really is linear in the momentum $\mathbf{p}$ and reads as follows:

$$\varepsilon\psi_\pm = (\beta\mu + \alpha\,\Sigma_\pm(\mathbf{p}))\,\psi_\pm. \tag{29}$$

Here we have newly introduced the spin matrix that is defined as

$$\Sigma_\pm(\mathbf{p}) = \begin{pmatrix}\hat\sigma_\pm(\mathbf{p})/\mu_+ & 0\\ 0 & -\hat\sigma_\mp(\mathbf{p})/\mu_-\end{pmatrix} = \begin{pmatrix}\frac{\mu_2\sigma_1\pm\mu_1\sigma_2}{\mu_2+\mu_1} & 0\\ 0 & \frac{\mu_2\sigma_1\mp\mu_1\sigma_2}{\mu_2-\mu_1}\end{pmatrix}, \tag{30}$$

which uses the symbol defined in (26) and thus has the property that $(\alpha\,\Sigma_\pm)^2 = p^2/(Mc)^2$. It also obeys $[\Sigma_\pm, \beta] = 0$. Both signs in (30) are equivalent and therefore we will only use the plus sign in the following. We introduced a symbol for the effective reduced mass: $\mu = \mu_1\mu_2/y$. Squaring equation (29) gives the mass–shell condition: $\varepsilon^2 = \mu^2 + p^2/(Mc)^2$, where the energy variable is defined as

$$\varepsilon = \left(y^2 - \mu_1^2 - \mu_2^2\right)/(2y). \tag{31}$$

Solving for y yields the four previously obtained free solutions, so that the asymptotic behavior is okay. Note, however, that the limit $m_1 = m_2$ cannot be obtained as $\Sigma_\pm$ formally diverges in this limit, and the inversion of the set of equations (28) becomes impossible. In the interesting extreme limits of $m_1 \gg m_2$ or $m_2 \gg m_1$, the operator simply goes into σ_2, respectively σ_1. As a result, we obtain in case of one particle being the dominant in mass the simple Dirac equation for the other particle involving its spin only, yet with the important recoil effect of the heavier particle included in ε and μ. Strictly speaking, however, as for all the other three versions of the effective Dirac equations, we have to calculate the spin states in the direct product space formed by the spins of the two particles of the binary. In the above limiting cases, in lowest order of the mass ratio one may consider, respectively, the individual angular momentum $\mathbf{J}_{1,2}$ to be conserved. Generally, however, both spins appear, and thus only $\mathbf{J}$ of (5) remains strictly conserved. Thus equation (29) fully keeps the original symmetry, also when formally interchanging the indices, yet it does not commute with $\mathcal{P}$, since $[\mathcal{P}, \hat\sigma_\pm] \neq 0$.

4. The wavefunctions and spectrum of a hydrogen-like binary

We now return to the Dirac–Coulomb problem as formulated by operator (3). Its reduced version in its most convenient form for free particles was derived in the previous section. As discussed extensively by Pilkuhn [1] it suffices to introduce the potential linearly into (29). Originally, the replacement is $E \to E + \alpha_S\hbar c/r$. In the linear approximation, this corresponds in (29) to $\varepsilon \to \varepsilon + \alpha_S/x$, where we have normalized the distance coordinate to $\lambda_C = \hbar/(Mc)$, the Compton wavelength based on the total mass. In compliance with the spherical symmetry, the spin operator needs to be expressed in spherical coordinates. This is done, like e.g. in [4, 5] by introducing instead of (14) the spin–orbit coupling operator:

$$\sigma_{1,2}(\mathbf{p}) = S_{1,2}(\hat{\mathbf{r}})\frac{\mathrm{i}}{x}\left(-\frac{\partial}{\partial x}x + \hat K_{1,2}\right), \tag{32}$$

with the unit vector $\hat{\mathbf{r}} = \mathbf{r}/r$, and $\hat K_{1,2} = 1 + \mathbf{L}\cdot\boldsymbol{\sigma}_{1,2}/\hbar$. Like in (10), we here introduced the spatial helicity:

$$S_{1,2}(\hat{\mathbf{r}}) = \boldsymbol{\sigma}_{1,2}\cdot\hat{\mathbf{r}}. \tag{33}$$

As a consequence of this definition $S_{1,2}^2 = 1$. The operator $\mathbf{J}$ commutes with $\hat{K}_{1,2}$, which together can therefore have common eigenfunctions. Some operator algebra shows that the relation holds:

$$[\hat{K}_1, \hat{K}_2] = \frac{\mathrm{i}}{\hbar}\mathbf{L} \cdot (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2), \tag{34}$$

which indicates that the $\hat{K}$-Operators do generally not commute with each other. However, as it was shown [5] one can indeed construct common eigenfunctions for them. In the relevant subspaces spanned by singlet and mixed triplet spin states, the $\hat{K}$-operators do commute with each other and have common eigenfunctions here named again Υ_k for short. The related eigenvalue is called k. It can attain the values $k = \pm 1, \pm 2, \pm 3, \ldots$. Since it has frequently been used before that $\sigma_1(\mathbf{p})$ and $\sigma_2(\mathbf{p})$ commute, the original 4×4 product spin state must be reduced by one dimension [5] to ensure this property in spherical coordinates as well. Another consequence of that is for the singlet state only $k = 1$ is permitted. Finally, $\{\hat{K}_i, S_j\} = 0$ for any $i = 1, 2$ and $j = 1, 2$, whenever these operators act on an eigenfunction Υ_k. Therefore, we omit the index and make use of $\hat{K}\Upsilon_k = k\Upsilon_k$. As usually for the Coulomb potential, one makes the standard ansatz for the solution spinor:

$$\psi(\mathbf{x}) = \frac{1}{x}\phi(\mathbf{x}). \tag{35}$$

It is further convenient to introduce the spin helicity matrix,

$$S(\hat{\mathbf{x}}) = \begin{pmatrix} \frac{\mu_2 S_1 + \mu_1 S_2}{\mu_2 + \mu_1} & 0 \\ 0 & \frac{\mu_2 S_1 - \mu_1 S_2}{\mu_2 - \mu_1} \end{pmatrix}, \tag{36}$$

which possesses the property $(\alpha S)^2 = 1$. With these preparations we can write the effective Dirac equation (29) in the new concise form

$$\left(\varepsilon + \frac{\alpha_S}{x}\right)\phi(\mathbf{x}) = \left(\beta\mu + \alpha \mathrm{i} S(\hat{\mathbf{x}}) \left(-\frac{\partial}{\partial x} + \frac{\hat{K}}{x}\right)\right)\phi(\mathbf{x}), \tag{37}$$

of which the spatial part can be separated by making an ansatz for the spinor ϕ that is in analogy with the treatment of the normal Dirac equation and as in paper [4]:

$$\phi(\mathbf{x}) = \begin{pmatrix} (1 + S_1 S_2) F(x) \\ \mathrm{i}(S_1 + S_2) G(x) \end{pmatrix} \Upsilon_k. \tag{38}$$

Note that the spinor is chosen to be invariant under the parity transformation $\beta\mathrm{P}$, since $\mathrm{P}S_{1,2} = -S_{1,2}$. Thus $\phi(\mathbf{x})$ carries the parity of Υ_k, which after [5] is $(-1)^l$, with l being the angular momentum quantum number. By paying careful attention to the anticommutation rules of the S- and $\hat{K}$-operators, we obtain by operating with the spin-helicity matrix on the spinor ϕ the result

$$\mathrm{i} S(\hat{\mathbf{x}}) \left(-\frac{\partial}{\partial x} + \frac{\hat{K}}{x}\right)\phi(\mathbf{x}) = \begin{pmatrix} \mathrm{i}(S_1 + S_2)\left(-\frac{\partial}{\partial x} + \frac{k}{x}\right) F(x) \\ -(1 + S_1 S_2)\left(-\frac{\partial}{\partial x} - \frac{k}{x}\right) G(x) \end{pmatrix} \Upsilon_k. \tag{39}$$

Exploiting this relation, we retain from (37) the familiar set of two coupled linear differential equations for the two spatial wavefunctions in matrix form:

$$\begin{pmatrix} \varepsilon + \frac{\alpha_S}{x} - \mu & -\frac{\partial}{\partial x} - \frac{k}{x} \\ \frac{\partial}{\partial x} - \frac{k}{x} & \varepsilon + \frac{\alpha_S}{x} + \mu \end{pmatrix} \cdot \begin{pmatrix} F(x) \\ G(x) \end{pmatrix} = 0. \tag{40}$$

The solution of this equation follows standard procedures [1] and need not be repeated here. The effective energy spectrum is given by the fine-structure formula:

$$\varepsilon/\mu = e(n, k) = \left(1 + \alpha_S^2 \Big/ \left(\sqrt{k^2 - \alpha_S^2} - |k| + n\right)^2\right)^{-1/2}. \tag{41}$$

We recall that, as discussed in [4, 5], there are two separate solutions concerning the spin–orbit-coupling quantum number k: the (in spatial angle) isotropic solution for a singlet para-hydrogen-like system, with $k = 1$ only, and the angularly nonuniform solution for the triplet ortho-hydrogen-like binary, with $k = 1$ and $k = \pm 2, \pm 3 \ldots$. One has $n = 1, 2, 3, \ldots$ as usually for the principal quantum number. To find the energy spectrum $E(n, k)$ of the binary one has to insert (41) into the quadratic equation (31) and solve for y. The result includes the recoil effect through the mass ratio μ_r/M with the reduced mass $\mu_r = m_1 m_2/(m_1 + m_2)$, and the Coulomb binding via the squared fine-structure constant α_S^2. The corresponding power series expansions in terms of these two basic parameters are discussed in the textbook [1].

Finally, let us consider the case $m_1 = m_2$, for which (30) cannot be used. Instead one may solve (23) for $\mu_1 = \mu_2 = 1/2$, and for the plus sign. We also have to replace y by $y + \alpha_S/x$. When applying the operator defined in (26),

$$\hat{\sigma}_+(\mathbf{p}) = (\mu_2\sigma_1(\mathbf{p}) + \mu_1\sigma_2(\mathbf{p})) = (\mu_2 S_1(\hat{\mathbf{x}}) + \mu_1 S_2(\hat{\mathbf{x}}))\frac{\mathrm{i}}{x}\left(-\frac{\partial}{\partial x}x + \hat{K}\right), \tag{42}$$

on the function (38), while observing that $\mu_1 + \mu_2 = 1$, the right-hand side of (39) is reproduced. Concerning the two operators of (24) and (25), we may simplify them by considering that the momentum in the Coulomb bound state is only small, $p/(Mc) \approx \mu_r/M\alpha_S = \mu_1\mu_2\alpha_S$, and $x \approx M/\mu_r$. Consistently, we can therefore neglect all terms quadratic in α_S, and thus obtain the p-independent quantities: $\hat{\varepsilon} = (y^2 - 1/2)/2$ and $\hat{\mu} = 1/4$. The energy spectrum can then be written in the same way as previously, with the ratio $\hat{\varepsilon}/\hat{\mu} = \varepsilon/\mu$ given by $e(n, k)$ of formula (41). For all possible mass ratios the general result is $y^2 = \mu_1^2 + \mu_2^2 + 2\mu_1\mu_2\varepsilon/\mu$, or finally in the original energy units

$$E(n, k) = Mc^2\sqrt{1 + 2\frac{\mu_r}{M}(e(n, k) - 1)}. \tag{43}$$

5. Conclusion

An effective Dirac equation using an eight-component spinor representation was derived for a binary of two fermions from the two-fermion Dirac–Coulomb Hamiltonian, originally written in a 16-component spinor representation. The case of a hydrogen-like atom was again discussed as an example, and the results obtained by various authors [1] were retained, including the effects of the recoil through the reduced mass and the spectral fine structure induced by the joint spin–orbit coupling of the two fermions constituting the binary. The resulting fine-structure splitting remains the same for the binary as for the single Dirac electron, and it is independent of the mass ratio. However, this fine structure is only revealed by the *ortho*-fermionium and not the *para*-fermionium, a result which should experimentally be tested with hydrogen.

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