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The two-body problem with spin in relativistic quantum mechanics: the case of positronium

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Abstract

Use of the Dirac equation for a single particle in an electromagnetic field has led to many successful predictions. For more than one particle, the approach is usually through quantum field theory. In this contribution, we follow the original Dirac approach, but for a two-body problem, starting with a discussion of positronium. The problem can be reduced to that of solving a set of radial equations, but unfortunately obtaining an exact solution of them by means of a recurrence procedure, as was done for the hydrogen atom by Dirac, does not seem feasible. However, an evaluation of the relativistic corrections to the order $(1/c^2)$ is made for parapositronium and orthopositronium. These results are discussed and their relevance to other problems of this type—such as that of the quark–antiquark system—are mentioned, as solving these will be the eventual objective of future work.

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1. Introduction

The Dirac equation for a single charged particle in an electromagnetic field has been used extremely successfully in explaining many aspects of relativistic phenomena in quantum mechanics. For more than one charged particle, the interactions are best treated in relativistic quantum field theory. However, a description along the lines followed by Dirac himself in the one-particle case was obtained in a Poincaré invariant fashion for the two-body problem by a method similar to the one used by Moshinsky and Smirnov (p 326 of [1]). The procedure even allowed the removal of the centre-of-mass motion. The simplest case is that of two particles with spins $s = \frac{1}{2}$ interacting through some type of potential. An example would be the case of positronium or that of a quark and an antiquark interacting through a potential which, for simplicity, we shall assume is central.

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The Hamiltonian that we have to deal with has the form

$$H' = (c\boldsymbol{\alpha}_1 \cdot \boldsymbol{p}'_1 + m_1c^2\beta_1) + (c\boldsymbol{\alpha}_2 \cdot \boldsymbol{p}'_2 + m_2c^2\beta_2) + V(r') \tag{1}$$

where: $r' = |\boldsymbol{r}'_1 - \boldsymbol{r}'_2|$; m_1, m_2 and $\boldsymbol{p}'_1, \boldsymbol{p}'_2$ are respectively the masses and momenta of the two particles; and $V(r')$ the central potential. We denote here the Hamiltonian, momenta and coordinates in cgs units with a prime, as we want to reserve unprimed letters for use with a more convenient set of units.

We shall start our discussion with the case of positronium, using an approach that differs from those in most of the hundreds of papers written on the subject. Rather than give references to all of these, we just mention a very recent book [2] in which they can be found.

2. The Hamiltonian for positronium

In the case of positronium, it is convenient to use atomic units with a slight modification, i.e.

$$\hbar = \mu = e = 1 \tag{2}$$

where e is the charge of the electron or positron and μ is the reduced mass which, as the masses m of the electron and positron are equal, is

$$\mu = (m/2). \tag{3}$$

We also go, following [1], to the centre-of-mass frame by introducing the total and relative momenta

$$\boldsymbol{p}'_1 = \boldsymbol{P} + \boldsymbol{p}, \qquad \boldsymbol{p}'_2 = \boldsymbol{P} - \boldsymbol{p} \tag{4}$$

or, equivalently,

$$\boldsymbol{P} = \boldsymbol{p}'_1 + \boldsymbol{p}'_2, \qquad \boldsymbol{p} = \tfrac{1}{2}(\boldsymbol{p}'_1 - \boldsymbol{p}'_2). \tag{5}$$

As we are not interested in the motion of the system as a whole, we can take $\boldsymbol{P} = 0$, and thus in our units the equation of motion corresponding to equation (1) becomes

$$\left\{[c(\boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2) \cdot \boldsymbol{p} + 2(\beta_1 + \beta_2)c^2] - \frac{1}{r}\right\}\Psi = E\Psi. \tag{6}$$

Note that the velocity of light c remains in the equation, though it is a dimensionless parameter. From the fine-structure constant

$$\frac{e^2}{\hbar c} \simeq \frac{1}{137} \tag{7}$$

we see that the velocity of light in atomic units is given approximately by the number 137 given above.

What now are the forms of $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \beta_1, \beta_2$? As this is a two-body problem, they are given by the direct products

$$\begin{aligned}
\boldsymbol{\alpha}_1 &= \begin{pmatrix} 0 & \boldsymbol{\sigma}_1 \\ \boldsymbol{\sigma}_1 & 0 \end{pmatrix} \otimes \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \\
\boldsymbol{\alpha}_2 &= \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \otimes \begin{pmatrix} 0 & \boldsymbol{\sigma}_2 \\ \boldsymbol{\sigma}_2 & 0 \end{pmatrix} \\
\beta_1 &= \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \otimes \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \qquad \beta_2 = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \otimes \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.
\end{aligned} \tag{8}$$

Introducing these direct products explicitly into equation (6), we can write it in the form

$$\mathcal{O}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix} \equiv \left\{2c\begin{bmatrix}0 & \boldsymbol{s}_1\cdot\boldsymbol{p} & -\boldsymbol{s}_2\cdot\boldsymbol{p} & 0\\ \boldsymbol{s}_1\cdot\boldsymbol{p} & 0 & 0 & -\boldsymbol{s}_2\cdot\boldsymbol{p}\\ -\boldsymbol{s}_2\cdot\boldsymbol{p} & 0 & 0 & \boldsymbol{s}_1\cdot\boldsymbol{p}\\ 0 & -\boldsymbol{s}_2\cdot\boldsymbol{p} & \boldsymbol{s}_1\cdot\boldsymbol{p} & 0\end{bmatrix} + 4c^2\begin{bmatrix}I & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -I\end{bmatrix} - \left(E+\frac{1}{r}\right)\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}\right\}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix} = 0 \tag{9}$$

where we have replaced Pauli matrices $\boldsymbol{\sigma}_t$, $t = 1$ or 2, by spin matrices:

$$\boldsymbol{s}_1 = \tfrac{1}{2}\boldsymbol{\sigma}_1, \qquad \boldsymbol{s}_2 = \tfrac{1}{2}\boldsymbol{\sigma}_2. \tag{10}$$

Note that actually the matrices in (9) are 16×16, because $\boldsymbol{s}_t \to \boldsymbol{s}_t \otimes I$, $I \to I \otimes I$ and each of the ψ_λ, $\lambda = 1, 2, 3, 4$, actually have four components, as we shall show later.

The question that comes immediately to mind is that of whether equation (9) can be reduced to one depending on the single radial variable r and whether, if it can be put into that form, an exact solution of this equation could be obtained.

3. The radial form of the two-body problem

The relativistic two-body problem with spin is given by equation (9) and to transform it to a set of equations involving only the radial variable r we need the angular and spinorial part of the ket, which is obviously

$$|(l,s)jm\rangle = \sum_{\mu,\sigma}\langle l\mu, s\sigma|jm\rangle Y_{l\mu}(\theta,\varphi)\chi_{s\sigma} \tag{11}$$

where, with the addition of two spins $s = \frac{1}{2}$, the total spin s can take only the values $s = 0$ or $s = 1$ with projections which are respectively $\sigma = 0$ or $\sigma = 1, 0, -1$. The total angular momentum j and its projection are integrals of motion, as the full problem is invariant under rotations, and the orbital angular momentum is restricted to $l = j$ if $s = 0$ and to $l = j+1, j, j-1$ if $s = 1$. Note that states with $l = j \pm 1$ and j have opposite parity. $\chi_{s\sigma}$ represents the spin wavefunction $\chi_{s\sigma} = |\frac{1}{2}\frac{1}{2}s\sigma\rangle$.

The wavefunction ψ_λ, $\lambda = 1, 2, 3, 4$ of equation (9) can now be written as

$$\psi_\lambda = \sum_{l,s} f_{ls}^{\lambda j}(r)|(l,s)jm\rangle. \tag{12}$$

To get the radial equations involving the $f_{ls}^{\lambda j}(r)$ we need only to have the matrix representation of the operator $\mathcal{O}$ of equation (9) with respect to the angular and spinorial ket of equation (11). As $\mathcal{O}$ can be written in the matrix form $\mathcal{O} = \|\mathcal{O}_{\lambda'\lambda}\|$, we have from equation (9) that

$$\begin{aligned}\mathcal{O}_{\lambda'\lambda} = {} & 2c\{(\boldsymbol{s}_1\cdot\boldsymbol{p})[\delta_{\lambda'=1,\lambda=2} + \delta_{\lambda'=2,\lambda=1} + \delta_{\lambda'=3,\lambda=4} + \delta_{\lambda'=4,\lambda=3}]\\ & - (\boldsymbol{s}_2\cdot\boldsymbol{p})[\delta_{\lambda'=1,\lambda=3} + \delta_{\lambda'=3,\lambda=1} + \delta_{\lambda'=4,\lambda=2} + \delta_{\lambda'=2,\lambda=4}]\}\\ & + 4c^2(\delta_{\lambda'=1,\lambda=1} - \delta_{\lambda'=4,\lambda=4}) - \left(E+\frac{1}{r}\right)\delta_{\lambda'\lambda}\end{aligned} \tag{13}$$

and, ignoring the trivial entries in the matrix $\langle(l',s')jm|\mathcal{O}_{\lambda'\lambda}|(l,s)jm\rangle$, the only one that merits attention is $(\boldsymbol{s}_t\cdot\boldsymbol{p})$, $t = 1, 2$ [3]:

$$\begin{aligned}\langle(l's')jm|\boldsymbol{s}_t\cdot\boldsymbol{p}|(l,s)jm\rangle = {} & (-1)^{l'+s-j}\\ & \times[(2l'+1)(2s'+1)]^{1/2}W(ll'ss';1j)\langle l'\|p\|l\rangle\langle\tfrac{1}{2}\tfrac{1}{2}s'\|s_t\|\tfrac{1}{2}\tfrac{1}{2}s\rangle.\end{aligned} \tag{14}$$

In equation (14), W is a Racah coefficient and the reduced matrix elements are given by [4]

$$\langle l'\|p\|l\rangle = \mathrm{i}\delta^{l'}_{l-1}\sqrt{\frac{l}{2l-1}}\left(\frac{\partial}{\partial r}+\frac{l+1}{r}\right) - \mathrm{i}\delta^{l'}_{l+1}\sqrt{\frac{l+1}{2l+3}}\left(\frac{\partial}{\partial r}-\frac{l}{r}\right) \tag{15}$$

and by [3]

$$\langle \tfrac{1}{2}\tfrac{1}{2}s'\|s_t\|\tfrac{1}{2}\tfrac{1}{2}s\rangle = (-1)^{1-s}W\left(\tfrac{1}{2}\tfrac{1}{2}1s';s\tfrac{1}{2}\right)\sqrt{\tfrac{3}{4}} \tag{16}$$

where the latter clearly shows that when $s'=1$, $s=0$, it will not vanish.

Thus the orbital spin states $|(j,0)jm\rangle$ and $|(j,1)jm\rangle$ that have the same parity and, because of (16), have no spin selection rule will be connected and, because of parity, will also be connected with the states $|(j\pm 1,1)jm\rangle$ by the matrix element of equation (14), as $\boldsymbol{p}$ is a polar vector.

We can then write out explicitly the set of first-order radial equations for $f^{\lambda j}_{ls}(r)$, but we shall not do this because, despite several people having attempted it, it did not prove possible to find a recursion relation that allowed the exact solution of the problem, unlike in the Dirac discussion [5] of the hydrogen atom. Thus what we actually do is to go to the second-order equation obtained from the operator $\mathcal{O}$ and carry out an expansion in powers of $1/c^2$.

4. The second-order equation for the two-body problem

The matrix wave equation (9) can be written in terms of the submatrices:

$$2c\begin{pmatrix} \boldsymbol{s}_1\cdot\boldsymbol{p} & -\boldsymbol{s}_2\cdot\boldsymbol{p} \\ -\boldsymbol{s}_2\cdot\boldsymbol{p} & \boldsymbol{s}_1\cdot\boldsymbol{p}\end{pmatrix}\begin{pmatrix}\psi_2\\ \psi_3\end{pmatrix} = \begin{pmatrix} E+1/r-4c^2 & 0\\ 0 & E+1/r+4c^2\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix} \tag{17}$$

$$2c\begin{pmatrix} \boldsymbol{s}_1\cdot\boldsymbol{p} & -\boldsymbol{s}_2\cdot\boldsymbol{p} \\ -\boldsymbol{s}_2\cdot\boldsymbol{p} & \boldsymbol{s}_1\cdot\boldsymbol{p}\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix} = \left(E+\frac{1}{r}\right)\begin{pmatrix}\psi_2\\ \psi_3\end{pmatrix}. \tag{18}$$

Dividing equation (18) by $(E+1/r)$ and substituting in equation (17), we obtain

$$4c^2\begin{pmatrix} \boldsymbol{s}_1\cdot\boldsymbol{p} & -\boldsymbol{s}_2\cdot\boldsymbol{p} \\ -\boldsymbol{s}_2\cdot\boldsymbol{p} & \boldsymbol{s}_1\cdot\boldsymbol{p}\end{pmatrix}\frac{1}{(E+1/r)}\begin{pmatrix} \boldsymbol{s}_1\cdot\boldsymbol{p} & -\boldsymbol{s}_2\cdot\boldsymbol{p} \\ -\boldsymbol{s}_2\cdot\boldsymbol{p} & \boldsymbol{s}_1\cdot\boldsymbol{p}\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix}$$
$$= \begin{pmatrix} E+1/r-4c^2 & 0\\ 0 & E+1/r+4c^2\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix}. \tag{19}$$

We note now that the commutator

$$\left[(\boldsymbol{s}_t\cdot\boldsymbol{p}),\ \left(E+\frac{1}{r}\right)^{-1}\right] = \frac{1}{\mathrm{i}}\left(E+\frac{1}{r}\right)^{-2}(\boldsymbol{s}_t\cdot\boldsymbol{r})r^{-3} \tag{20}$$

and so we can write equation (19) as

$$\frac{4c^2}{\mathrm{i}}\left(E+\frac{1}{r}\right)^{-2}r^{-3}\begin{pmatrix} \boldsymbol{s}_1\cdot\boldsymbol{r} & -\boldsymbol{s}_2\cdot\boldsymbol{r} \\ -\boldsymbol{s}_2\cdot\boldsymbol{r} & \boldsymbol{s}_1\cdot\boldsymbol{r}\end{pmatrix}\begin{pmatrix} \boldsymbol{s}_1\cdot\boldsymbol{p} & -\boldsymbol{s}_2\cdot\boldsymbol{p} \\ -\boldsymbol{s}_2\cdot\boldsymbol{p} & \boldsymbol{s}_1\cdot\boldsymbol{p}\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix}$$
$$+\frac{4c^2}{(E+1/r)}\begin{pmatrix} \boldsymbol{s}_1\cdot\boldsymbol{p} & -\boldsymbol{s}_2\cdot\boldsymbol{p} \\ -\boldsymbol{s}_2\cdot\boldsymbol{p} & \boldsymbol{s}_1\cdot\boldsymbol{p}\end{pmatrix}\begin{pmatrix} \boldsymbol{s}_1\cdot\boldsymbol{p} & -\boldsymbol{s}_2\cdot\boldsymbol{p} \\ -\boldsymbol{s}_2\cdot\boldsymbol{p} & \boldsymbol{s}_1\cdot\boldsymbol{p}\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix}$$
$$= \begin{pmatrix} E+1/r-4c^2 & 0\\ 0 & E+1/r+4c^2\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix}. \tag{21}$$

This last equation still involves the spins of the two particles $\boldsymbol{s}_1$, $\boldsymbol{s}_2$, but it can be transformed so as to involve only the total spin.

Using the relation between the Pauli spin matrices

$$\sigma_i\,\sigma_j = \delta_{ij} + \mathrm{i}\epsilon_{ijk}\sigma_k \tag{22}$$

we obtain straightforwardly that equation (21) can be written as

$$\left[\frac{1}{\mathrm{i}}4c^2\left(E+\frac{1}{r}\right)^{-2}r^{-3}\right]$$
$$\times\begin{bmatrix}\frac{1}{2}(\boldsymbol{r}\cdot\boldsymbol{p})+\frac{\mathrm{i}}{2}(\boldsymbol{S}\cdot\boldsymbol{L}) & \frac{1}{2}(\boldsymbol{r}\cdot\boldsymbol{p})+\frac{\mathrm{i}}{2}(\boldsymbol{S}\cdot\boldsymbol{L})-(\boldsymbol{S}\cdot\boldsymbol{r})(\boldsymbol{S}\cdot\boldsymbol{p})\\ \frac{1}{2}(\boldsymbol{r}\cdot\boldsymbol{p})+\frac{\mathrm{i}}{2}(\boldsymbol{S}\cdot\boldsymbol{L})-(\boldsymbol{S}\cdot\boldsymbol{r})(\boldsymbol{S}\cdot\boldsymbol{p}) & \frac{1}{2}(\boldsymbol{r}\cdot\boldsymbol{p})+\frac{\mathrm{i}}{2}(\boldsymbol{S}\cdot\boldsymbol{L})\end{bmatrix}$$
$$\times\begin{bmatrix}\psi_1\\ \psi_4\end{bmatrix}+\frac{4c^2}{(E+1/r)}\begin{bmatrix}\frac{1}{2}p^2 & \frac{1}{2}p^2-(\boldsymbol{S}\cdot\boldsymbol{p})^2\\ \frac{1}{2}p^2-(\boldsymbol{S}\cdot\boldsymbol{p})^2 & \frac{1}{2}p^2\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_4\end{bmatrix}$$
$$=\begin{bmatrix}E+r^{-1}-4c^2 & 0\\ 0 & E+r^{-1}+4c^2\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_4\end{bmatrix} \tag{23}$$

where $\boldsymbol{S}$ is the total spin and $\boldsymbol{L}$ the orbital angular momentum when they denote operators, while we use lower case letters s, l for the eigenvalues, i.e.

$$\boldsymbol{S}=\boldsymbol{s}_1+\boldsymbol{s}_2, \qquad \boldsymbol{L}=\boldsymbol{r}\times\boldsymbol{p}. \tag{24}$$

We note now that in equation (23) only the components of the total spin vector $\boldsymbol{S}$ appear and they will commute with the square S^2 of this operator. Thus S^2 is an integral of motion whose eigenvalue $s(s+1)$ is either 0 or 2. We can then separate equation (23) into two parts, one in which $s=0$, relating to parapositronium, and the other with $s=1$, relating to orthopositronium.

Furthermore, for orthopositronium we note that parity is a good quantum number and so we can distinguish the cases in which $l=j$ from those in which $l=j\pm 1$.

We shall discuss separately the cases of parapositronium and orthopositronium.

5. The relativistic energy correction for parapositronium to order $(1/c^2)$

Before embarking on our discussion, we first note that in cgs units the rest energy of positronium is $2mc^2=4\mu c^2$ where μ is the reduced mass.

In the units of equation (2), the rest energy is $4c^2$. Thus we can denote our total energy E as

$$E=4c^2+\epsilon \tag{25}$$

where ϵ is actually the binding energy of positronium that we want to determine.

For parapositronium, as $s=0$, the terms containing the vector $\boldsymbol{S}$ in equation (23) vanish and thus using equation (25) our equation becomes

$$-\mathrm{i}\,2c^2(4c^2+\epsilon+r^{-1})^{-2}r^{-3}(\boldsymbol{r}\cdot\boldsymbol{p})\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix}$$
$$+2c^2(4c^2+\epsilon+r^{-1})^{-1}p^2\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix}$$
$$=\begin{bmatrix}\epsilon+r^{-1} & 0\\ 0 & \epsilon+r^{-1}+8c^2\end{bmatrix}\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix}. \tag{26}$$

The left-hand side of equation (26) can be diagonalized with the help of the matrix

$$U=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix} \tag{27}$$

as

$$U^{-1}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}U=\begin{pmatrix}2 & 0\\ 0 & 0\end{pmatrix}. \tag{28}$$

Writing then

$$\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix} = U\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix} \tag{29}$$

and multiplying equation (26) by U^{-1} on the left-hand side, we get

$$-4ic^2(4c^2+\epsilon+r^{-1})^{-2}r^{-3}(\boldsymbol{r}\cdot\boldsymbol{p})\psi_+ + 4c^2(4c^2+\epsilon+r^{-1})^{-1}p^2\psi_+ = \left[4c^2+\epsilon+\frac{1}{r}\right]\psi_+ - 4c^2\psi_-, \tag{30}$$

$$0 = [4c^2+\epsilon+r^{-1}]\psi_- - 4c^2\psi_+. \tag{31}$$

Using equation (31) to express ψ_- in terms of ψ_+ and substituting in equation (30), we obtain

$$-4ic^2(4c^2+\epsilon+r^{-1})^{-2}r^{-3}(\boldsymbol{r}\cdot\boldsymbol{p})\psi_+ + 4c^2(4c^2+\epsilon+r^{-1})^{-1}p^2\psi_+ = 4c^2[(\epsilon+r^{-1})(4c^2)^{-1}+1]\psi_+ - 4c^2[1+(\epsilon+r^{-1})(4c^2)^{-1}]^{-1}\psi_+. \tag{32}$$

We now wish to express equation (32) in terms of inverse powers of c^2 using the well known expansion

$$(1+x)^{-n} = \sum_{m=0}^{\infty}(-1)^m\frac{(n+m-1)!}{(n-1)!m!}x^m, \qquad |x|<1. \tag{33}$$

Now defining w:

$$w \equiv (4c^2+\epsilon+r^{-1}) = 4c^2\left[1+\frac{(\epsilon+r^{-1})}{4c^2}\right], \tag{34}$$

we have from equation (33) the expansions

$$4c^2w^{-1} = 1+\sum_{m=1}^{\infty}(-1)^m\left(\frac{\epsilon+r^{-1}}{4c^2}\right)^m \tag{35}$$

$$4c^2w^{-2} = -\sum_{m=1}^{\infty}(-1)^m\frac{m(\epsilon+r^{-1})^{m-1}}{(4c^2)^m} \tag{36}$$

and so substituting in equation (32) we get

$$\mathrm{i}\sum_{m=1}^{\infty}(-1)^m\frac{m(\epsilon+r^{-1})^{m-1}}{(4c^2)^m}r^{-3}(\boldsymbol{r}\cdot\boldsymbol{p})\psi_+ + \left\{1+\sum_{m=1}^{\infty}(-1)^m\frac{(\epsilon+r^{-1})^m}{(4c^2)^m}\right\}p^2\psi_+ = 2(\epsilon+r^{-1})\psi_+ - \sum_{m=2}^{\infty}(-1)^m\frac{(\epsilon+r^{-1})^m}{(4c^2)^{m-1}}\psi_+. \tag{37}$$

If we disregard in equation (37) all the terms containing $(1/c^2)$ (or equivalently consider $c\to\infty$), and divide what is left by the factor 2, we get the equation

$$\left(\frac{1}{2}p^2-\frac{1}{r}\right)\psi_+ = \epsilon\psi_+ \tag{38}$$

which is precisely the non-relativistic equation for positronium in the units of equation (2) and the binding energy ϵ becomes of course [6]

$$\epsilon_\nu = -\frac{1}{2\nu^2}, \qquad \nu = n+l+1 \tag{39}$$

with ν, n being respectively the total and radial quantum number and l the orbital angular momentum.

If we include in equation (32) all the terms up to those of order $(1/c^2)$, and again divide by 2, we get the expression

$$H_p\psi_+ = \left\{[(p^2/2) - r^{-1}] - \frac{1}{8c^2}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\right) - \frac{1}{32c^2}p^4\right\}\psi_+ = \epsilon\psi_+ \tag{40}$$

where in the terms of order $(1/c^2)$ we replace, as usual [6], $(\epsilon + r^{-1})$ by $(p^2/2)$ and use the fact that

$$r^{-3}(\boldsymbol{r}\cdot\boldsymbol{p}) = -\frac{\mathrm{i}}{r^2}\frac{\partial}{\partial r}. \tag{41}$$

An equivalent result was obtained using another procedure by Królikowski [7].

The corresponding formula for the hydrogen atom [6] in atomic units $\hbar = m = c = 1$ is

$$H_h\Psi \equiv \left\{\left[\frac{1}{2}p^2 - \frac{1}{r}\right] + \frac{1}{c^2}\left(-\frac{p^4}{8} - \frac{1}{4r^2}\frac{\partial}{\partial r} + \frac{1}{2r^3}(\boldsymbol{L}\cdot\boldsymbol{S})\right)\right\}\psi = \epsilon\psi. \tag{42}$$

We note that in parapositronium there are no spin–orbit coupling terms, as we should expect from the fact that the total spin $s = 0$. Furthermore, the coefficients of the other terms in equations (40) and (42) are different.

6. The relativistic correction of orthopositronium to order $(1/c^2)$

We now consider the full equation (23) but with the spin having the value 1, which implies that the total spin vector $\boldsymbol{S}$ appears and its components S_i, $i = 1, 2, 3$, commute with S^2. This indicates that the latter is an integral of motion, whose eigenvalue is $s(s+1) = 2$. We decompose the right-hand side of equation (23) into the form

$$(E + r^{-1})\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - 4c^2\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{43}$$

We now write

$$\begin{pmatrix}\psi_1\\ \psi_4\end{pmatrix} = U\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix}, \tag{44}$$

where U is given in equation (27), and we multiply equation (23) by U^{-1} on the left.

Before writing down the resulting expressions, we note that

$$\begin{aligned} &U^{-1}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}U = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}; \qquad U^{-1}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}U = -\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix};\\ &U^{-1}\begin{pmatrix}a & b\\ b & a\end{pmatrix}U = \begin{pmatrix}a+b & 0\\ 0 & a-b\end{pmatrix}. \end{aligned} \tag{45}$$

Furthermore, for compactness in the equation, we write

$$a \equiv \frac{1}{2}(\boldsymbol{r}\cdot\boldsymbol{p}) + \frac{\mathrm{i}}{2}(\boldsymbol{S}\cdot\boldsymbol{L}), \qquad b \equiv \frac{1}{2}(\boldsymbol{r}\cdot\boldsymbol{p}) + \frac{\mathrm{i}}{2}(\boldsymbol{S}\cdot\boldsymbol{L}) - (\boldsymbol{S}\cdot\boldsymbol{r})(\boldsymbol{S}\cdot\boldsymbol{p}) \tag{46}$$

$$u \equiv \tfrac{1}{2}p^2, \qquad v \equiv \tfrac{1}{2}p^2 - (\boldsymbol{S}\cdot\boldsymbol{p})^2 \tag{47}$$

$$w \equiv (E + r^{-1}) \tag{48}$$

where again we use the expression (25) for E, so w is the same as in equation (34).

Substituting the results (43)–(48) in equation (23) as modified by (45), we get for ψ_+, ψ_- the equations

$$\{-4\mathrm{i}c^2w^{-2}r^{-3}(a+b) + 4c^2w^{-1}(u+v) - w\}\psi_+ = 4c^2\psi_- \tag{49}$$

$$\{-4\mathrm{i}c^2w^{-2}r^{-3}(a-b) + 4c^2w^{-1}(u-v) - w\}\psi_- = 4c^2\psi_+. \tag{50}$$

Using equation (49) to express ψ_- in terms of ψ_+ and substituting in equation (50), we obtain

$$\{[-4ic^2w^{-2}r^{-3}(a-b)+4c^2w^{-1}(u-v)-w] \times[-4ic^2w^{-2}r^{-3}(a+b)+4c^2w^{-1}(u+v)-w]\}\psi_+ = 16c^4\psi_+. \tag{51}$$

Using now the expansions of equations (35) and (36) for $(4c^2w^{-1})$ and $(4c^2w^{-2})$, we see that equation (51) becomes

$$\left[\left\{i\sum_{m=1}^{\infty}(-1)^m\frac{m(\epsilon+r^{-1})^{m-1}}{(4c^2)^m}r^{-3}(a-b) + \left[1+\sum_{m=1}^{\infty}(-1)^m\left(\frac{\epsilon+r^{-1}}{4c^2}\right)^m\right](u-v)-(4c^2+\epsilon+r^{-1})\right\} \times\left\{i\sum_{m=1}^{\infty}(-1)^m\frac{m(\epsilon+r^{-1})^{m-1}}{(4c^2)^m}r^{-3}(a+b) + \left[1+\sum_{m=1}^{\infty}(-1)^m\left(\frac{\epsilon+r^{-1}}{4c^2}\right)^m\right](u+v)-(4c^2+\epsilon+r^{-1})\right\}\right]\psi_+ = 16c^4\psi_+. \tag{52}$$

We now keep only terms up to order $(1/c^2)$ in equation (52) and replace a, b, u, v in (46), (47) by their values, and note that there is a term $16c^4$ on the left-hand side that cancels with the $16c^4$ on the right-hand side. Furthermore, we divide the equation that remains by $(-8c^2)$ and after simplifications we obtain for orthopositronium, up to terms of the order $(1/c^2)$, the equation

$$H_o\psi_+ \equiv \left\{\left(\frac{p^2}{2}-\frac{1}{r}\right)-\frac{1}{8c^2}\left[\frac{1}{r^2}\frac{\partial}{\partial r}-r^{-3}(\boldsymbol{S}\cdot\boldsymbol{L}) + (\boldsymbol{S}\cdot\boldsymbol{p})^2[p^2-(\boldsymbol{S}\cdot\boldsymbol{p})^2]\right]-\frac{p^4}{32c^2}\right\}\psi_+ = \epsilon\psi_+. \tag{53}$$

Again, as in the case of parapositronium, we replace $(\epsilon + r^{-1})$ by $(p^2/2)$ in the terms of order $(1/c^2)$, and $-ir^{-3}(\boldsymbol{r}\cdot\boldsymbol{p})$ by $-r^{-2}\,\partial/\partial r$.

We have then, to order $(1/c^2)$, the Hamiltonian for parapositronium in equation (40) and orthopositronium in equation (53), and they differ from each other as well as from the corresponding formula (42) for the hydrogen atom. Clearly the value of the spin $s = \frac{1}{2}$ for the hydrogen atom and $s = 0$ or $s = 1$ for parapositronium and orthopositronium influence the parts of order $(1/c^2)$ in their respective Hamiltonians.

7. Evaluation of the relativistic energy corrections in positronium up to order $(1/c^2)$

We note first that, compared with the non-relativistic energy $-(1/2\nu^2)$ of equation (39), the relativistic correction to order $(1/c^2)$ is very small as, from equation (7), we have

$$\frac{1}{c^2} \simeq \frac{1}{(137)^2} = 5.328\times10^{-5} \tag{54}$$

and thus we can limit our consideration to first-order perturbation theory using the eigenstates of equation (41.32) on p 197 of reference [1] for the Coulomb problem with a spin part, of the form

$$|n(l,s)jm\rangle \equiv R_{nl}(r)|(l,s)jm\rangle \tag{55}$$

where the ket representing the orbital spin part is given in equation (11), the radial part $R_{nl}(r)$ has the form of equation (41.32) on p 197 of reference [1]:

$$R_{nl}(r) = \frac{2}{\nu^2}\, R_{nl}(\rho); \qquad \nu = n + l + 1 \tag{56}$$

and the right-hand function is the eigenfunction of the Sturm–Coulomb problem of the form of equation (41.17) on p 195 of reference [1], i.e.

$$R_{nl}(\rho) = \sqrt{\frac{n!}{(n+2l+1)!}}\rho^l L_n^{2l+1}(\rho)\mathrm{e}^{-\rho/2}, \qquad \rho \equiv (2r/\nu). \tag{57}$$

The Hamiltonians of the parapositronium and orthopositronium are given by the terms inside the curly brackets of equations (40) and (53), and will be designated respectively as

$$H_p \qquad \text{and} \qquad H_o. \tag{58}$$

The eigenvalues of these Hamiltonians (which are written out only up to terms $(1/c^2)$) will be given by the matrix elements of their expectation values:

$$\langle n(l,s)jm|H_q|n(l,s)jm\rangle \qquad \text{where } q = p, o. \tag{59}$$

The evaluation of these matrix elements is straightforward using the results of p 346 of reference [1] and the table 2^5 on p 117 of reference [6], and we just give their values, denoting the energies by ϵ_{pnl} or ϵ_{onl} depending on whether they correspond to the parapositronium or orthopositronium. For the latter, the kets of equation (55) reduce to

$$|n(j,1)jm\rangle \qquad \text{and} \qquad |n(j\pm 1,1)jm\rangle \tag{60}$$

which have opposite parities and thus give independent results. For conciseness, we shall only discuss here the first case, i.e. $l = j$.

From equation (59) we obtain for parapositronium with $l = j$

$$\epsilon_{pnj} = -\frac{1}{2\nu^2} + \frac{\delta_{j0}}{4c^2\nu^3} - \frac{1}{32c^2}\frac{1}{\nu^4(j+1/2)}[4\nu - 3(j+1/2)] \tag{61}$$

where $\nu = (n + j + 1)$ and for the ground state $n = j = 0$ or $\nu = 1$ we get

$$\epsilon_{p00} = -\frac{1}{2} + \frac{3}{32c^2} \tag{62}$$

where $(1/c^2)$ is given by equation (54).

For orthopositronium with $l = j$ we obtain, again using equation (59),

$$\epsilon_{onj} = -\frac{1}{2\nu^2} + \frac{\delta_{j0}}{4c^2\nu^3} - \frac{1}{8c^2}\left[\frac{1}{\nu^3}\frac{1}{(j+\frac{1}{2})(j+1)j}\right] - \frac{1}{32c^2}\frac{1}{\nu^4(j+\frac{1}{2})}\left[4\nu - 3\left(j+\frac{1}{2}\right)\right]. \tag{63}$$

Note that our analysis is taken only up to order $(1/c^2)$ in the units of equation (2), which in cgs units becomes $(e^2/\hbar c)^2 \equiv \alpha^2$, the fine-structure constant. Thus our results give us terms only up to α^2. For higher-order terms we would have to continue the expansions in equation (37) or (52) to higher order in $(1/c^2)$, making the replacements for ϵ (the energy) from the previous order. We shall not do this, as the objective of our paper is to illustrate the two-body problem with spin in relativistic quantum mechanics, for which positronium is just an example—besides which, there has recently appeared an analysis of positronium, by Kniehl and Penin [8], in quantum electrodynamics (QED) that continues to a much higher order in $(e^2/\hbar c)$.

8. Conclusions

We have discussed the example of positronium in relativistic quantum mechanics and showed that the exact radial problem with spins 0 or 1 is similar to that of a particle in a Dirac equation with an r^{-1}-potential where the spin is $\frac{1}{2}$. In contrast to what was achieved in the one-body problem [5], these radial equations for positronium do not seem amenable to a solution by means of a recurrence relation. However, it was possible to obtain the relativistic corrections to order $(1/c^2)$ and they are quite different for the parapositronium and orthopositronium cases as well as for the hydrogen atom.

As we mentioned in the introduction, our interest in the problem is also related to the possible application to quark–antiquark systems, i.e., mesons. In equation (1) their masses were given respectively as m_1, m_2 and a simple form for the interaction $V(r')$ is

$$V(r') = d'r' - \frac{b'^2}{r'} \tag{64}$$

where d', b' are constants obtained from experimental data.

Since for the potential $V(r')$ of equation (64), even the non-relativistic limit has to be solved numerically, we preferred first to consider a problem in which the non-relativistic limit is well known, that of positronium. We plan to continue with the quark–antiquark problem, but using a variational approach with the help of harmonic oscillator functions. For this procedure it is convenient to make in equation (1) the change of variables

$$\boldsymbol{r}' = \sqrt{\hbar/\mu\omega}\,\boldsymbol{r}, \qquad \boldsymbol{p}' = \sqrt{\hbar\mu\omega}\,\boldsymbol{p}, \qquad H' = \mu c^2 H \tag{65}$$

with μ being the reduced mass $m_1 m_2 (m_1 + m_2)^{-1}$ and ω the frequency of the oscillator in our trial wavefunctions. In the centre-of-mass frame, our equation then has the form

$$H\psi = \left\{ a(\boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2)\cdot\boldsymbol{p} + \left(\frac{m_1}{\mu}\right)\beta_1 + \left(\frac{m_2}{\mu}\right)\beta_2 + \left(dr - \frac{b^2}{r}\right)\right\}\psi = E\psi \tag{66}$$

where

$$d = \frac{1}{a}\frac{d'(\hbar/\mu c)}{\mu c^2}, \qquad b^2 = \frac{b'^2(\mu c/\hbar)}{\mu c^2}a, \tag{67}$$

$$a = (\hbar\omega/\mu c^2)^{1/2}; \qquad E = (E'/\mu c^2). \tag{68}$$

Our objective is to make a variational determination of the eigenvalues and eigenstates of the non-relativistic problem stated as

$$H\psi \equiv \left[\frac{1}{2\mu}p^2 + \left(dr - \frac{b^2}{r}\right)\right]\psi = E\psi. \tag{69}$$

Once this is achieved, the relativistic corrections up to order $(1/c^2)$ can be carried out along the lines of the present paper.

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