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Two fermion relativistic bound states

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Abstract

We consider the relativistic quantum mechanics of a two interacting fermions system. We first present a covariant formulation of the kinematics of the problem and give a short outline of the classical results. We then quantize the system with a general interaction potential and deduce the explicit equations in a spherical basis. The case of the Coulomb interaction is studied in detail by numerical methods, solving the eigenvalue problem for $j = 0$, $j = 1$, $j = 2$ and determining the spectral curves for a varying ratio of the mass of the interacting particles. Details of the computations, together with a perturbative approach in the mass ratio and an extended description of the ground states of para- and orthopositronium, are given in the appendices.

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1. Introduction

The relativistic two-body problem and the properties of bound states in relativistic quantum mechanics have a very long history, and a really large number of solutions has been devised. Some of these proposals stress the properties of covariance of the model, others assume as a starting point the constraint dynamics or arise directly from a classical symplectic context, others determine effective interactions from field theory in order to get results to be compared with phenomenological data. The bound state spectra are considered with particular interest, being rather difficult to treat in a pure quantum field theory framework. A historical overview of the subject can be found in [1]. The research, however, has actively continued up to the present day and several papers have been published on both the mathematical and the phenomenological aspects of the problem (see e.g. [2–13] and references therein).

Some years ago the present authors also made a contribution to this discussion, proposing a Lorentz invariant classical model for the two-body Coulomb and gravitational interactions where the relativistic covariance is nonlinearly realized [14]. The paper was written in plain coordinate language but it was rather strongly influenced by geometrical and symplectic ideas. These were developed elsewhere from a mathematical viewpoint and in a more general context, using group theoretical ideas for the treatment of classical spinning particles [15],

or studying rigorously the mathematics of skew-commutative phase spaces [16]. We could however observe that a peculiar property of the coordinate system determined in [14]—and briefly recalled in section 2 for the sake of completeness—is that the relative time coordinate disappears from the dynamics, and a symplectic reduction of the phase space is made possible [17]: the relative time plays the role of a gauge and therefore it can be given an arbitrary form. The procedure then permits, if needed, the reconstruction of two separate world-lines in the Minkowski space, whose structure and correlation are obviously dependent upon the chosen form of the relative time gauge function.

The present paper revisits our previous model and deals with its canonical quantization, assuming that the interacting particles are fermions with arbitrary masses. We therefore develop our arguments and find the wave equation for the two-fermion system in a framework of pure relativistic quantum mechanics, without any reference to second quantization techniques: this is, probably, the simplest way to transfer the classical results to the quantum context and to obtain complete control of the symmetry and covariance properties of the theory. The wave equation is determined in the presence of a general scalar potential, but the explicit results are focused on the Coulomb interaction, with the purpose of calculating the spectrum of the lowest bound states and in particular of determining the dependence of the levels upon the mass ratio of the interacting particles for any value of the total angular momentum. It proves that the equations and the results are continuous in the mass ratio, so that they provide a unified scheme ranging from positronium (two equal masses), to the hydrogen atom and finally to the Dirac limit (one of the masses becomes infinite). Although written in a rather compact form, the equations we find are not easy to study analytically. This means that no simple formula for the energy levels is available as in the case of the Dirac equation and numerical procedures are therefore necessary if we want to determine the spectroscopy of the system. Appropriate plots will illustrate the results obtained: from these it will be possible to establish regular and simple behaviour of the energy levels versus an appropriate mass ratio parameter. We find, for instance, that for two finite masses the degeneracy of the Dirac levels $2s_{1/2}-2p_{1/2}$ is removed and for the hydrogen atom we reproduce a small fraction of the entire Lamb shift: it is interesting to observe that the correct kinematics gives a non-negligible fraction of the splitting. The continuous dependence of the spectrum upon the ratio of the component masses suggests also in a natural way a perturbative treatment in the neighbourhood of the Dirac limit. Except for positronium, the main systems of physical interest—such as the hydrogen atom and, to a lesser degree, muonium and the mesic atom—have a very small mass ratio and can be treated accordingly. We have shown how to develop this framework and we have applied it to the ground state of the hydrogen atom.

A comparison with the results of [8–10] is in order. Indeed, the equations found in our quantum mechanical framework agree with those deduced by different methods in the quoted references, although a bit of work is usually required to reduce the latter. Concerning the results, we may observe that all those papers develop a perturbative approach in the fine structure constant up to α^4 ; complete numerical results are given for equal masses [9], and for different masses with a vanishing total angular momentum [10]. In [8] we find a perturbative formula, corrected up to α^4 , expressing the Lamb shift due to the Coulomb interaction. The results of that formula are practically coincident with our numerical results for the hydrogen atom, but appear to be less accurate when the masses of the two fermions become closer and closer: the comparison suggests that, to a high degree of accuracy, the perturbation expansions must be treated with some caution and numerical computations appear to be necessary and more reliable. Complete numerical results for equal masses and values zero and one of the angular momentum are found in [9]. The computations are carried out by finite element methods

and they are in complete agreement with our results obtained by the numerical solution of a singular boundary value problem. The authors observe that positronium presents an inversion in the energy of the two levels indicated as $2s_{1/2}$ and $2p_{3/2}$ in the Dirac spectroscopy, the first being higher than the second. As a matter of fact we have drawn a complete plot of these terms for any mass ratio, showing their actual crossing. Finally, in the two papers of [10], quantum field theoretical methods are used to determine the equations for fermion systems under the Coulomb and the complete electromagnetic interactions respectively. The equations are derived by defining an appropriate non-conventional vacuum and by studying the conditions to be imposed on the coefficient functions of the states with a fixed number of particles in order to be eigenstates of the particle–electromagnetic field Hamiltonian. Interest is especially addressed to the properties of the system related to the variation of the coupling constant α and the perturbative aspects in terms of α are widely developed. Complete numerical results are given for a vanishing value of the angular momentum and perturbative results up to α^4 for non-vanishing angular momentum. The wave equation we derive for the two fermions agrees with the results of [10], upon restriction to the static Coulomb interaction.

The two fermion relativistic bound states are relevant not only for electrodynamical purposes and atomic physics, but also in the framework of phenomenological meson spectroscopy. The limited progress of the QCD lattice programme for the mesons has stimulated interest in new treatments of two-body quantum systems that could replace the non-relativistic quark model [11] and predict the masses of the mesons, from the lighter to the heavier ones, assuming from the experimental data the least number of values for physical quark parameters. Numerical approaches have devised new methods of solving the Bethe–Salpeter equation with interactions derived from QCD effective potentials, see e.g. [12]. New wave equations from the quantization of constraint theories have been proposed in a long series of papers (see [5, 6] and references therein). The authors start from two coupled Dirac equations; using the Poincaré symmetry and some supersymmetric ideas, they are able to determine the general structure of the interactions compatible with the constraint scheme. The application to the phenomenology of mesons gives very good agreement with the experimental data.

We have written this paper trying to make it self-consistent. Some details of the computations have been explained in the appendices. A brief summary is as follows. In section 2 we recall the basic definitions and establish the kinematics and the dynamics of the system together with their invariance properties and their validity in any reference frame. In section 3 the quantization procedure is explained and applied to the relativistic two-fermion problem. In section 4 we deduce the equations for an arbitrary scalar potential. Given the general form of the state vector with definite energy, angular momentum and parity—whose explicit expression involves eight unknown functions and is reported in appendix A—we give a short, transparent and comprehensive deduction of the equations for the unknown functions and specify them to the particular case of the Coulomb interaction. The computations leading to the final result are sketched in appendix B. The Dirac limit is treated in section 5: here we present a procedure that permits us to recover continuously the Dirac equation for the finite mass constituent when the mass of the other goes to infinity. Finally, in section 6 we discuss the numerical results with $j = 0$, $j = 1$ and $j = 2$ for the whole range of masses: the results for $j = 0$ should be compared with a first-order perturbative approach in the ratio of the constituent masses, described in appendix C. A few details of the numerical procedure are given in appendix D. In appendix E we report on some details of the ground state of positronium. In particular we calculate the wavefunctions of parapositronium and orthopositronium, we show that the non-relativistic limit correctly reproduces the Schrödinger

equation for the Coulomb problem and we make some comments on the hyperfine splitting. In this paper we shall use a unit system with $\hbar = c = 1$, and for the presentation of the results we also assume the electron mass equal to unity.

2. The classical problem and the dynamical variables

We first outline the procedure for two classical scalar particles with given masses m_i , $i = 1, 2$, whose individual Minkowski coordinates are denoted by $x_{(i)}^\mu$ and whose canonical conjugate momenta are $p_{(i)}^\mu$. Starting from the collective coordinates

$$\begin{aligned} P^\mu &= p_{(1)}^\mu + p_{(2)}^\mu, & X^\mu &= \frac{1}{2}(x_{(1)}^\mu + x_{(2)}^\mu), \\ q^\mu &= \frac{1}{2}(p_{(1)}^\mu - p_{(2)}^\mu), & r^\mu &= x_{(1)}^\mu - x_{(2)}^\mu, \end{aligned} \quad (2.1)$$

it has been shown in [14] that a good set of canonical conjugate variables is provided by the following definitions:

$$P^\mu, \quad Z^\mu = X^\mu + \frac{\varepsilon_{abc} P_a \eta_b^\mu L_c}{\sqrt{P^2} [P_0 + \sqrt{P^2}]} + \frac{\varepsilon_a^\mu}{\sqrt{P^2}} (q_a \check{r} - r_a \check{q}) + \frac{P^\mu}{P^2} \check{q} \check{r} \quad (2.2)$$

$$\check{q} = \varepsilon_0^\mu q_\mu, \quad \check{r} = \varepsilon_0^\mu r_\mu, \quad q_a = \varepsilon_a^\mu q_\mu, \quad r_a = \varepsilon_a^\mu r_\mu$$

where $\eta^{\mu\nu}$ is the Lorentz metric tensor, ε_{abc} is the three-dimensional skew-symmetric tensor and where the sum over repeated indices must be assumed. In equation (2.2) the tensor ε_α^μ ($\mu, \alpha = 0, 3$) given by

$$\varepsilon_a^\mu(P) = \eta_a^\mu - \frac{P_a [P^\mu + \eta_0^\mu \sqrt{P^2}]}{\sqrt{P^2} [P_0 + \sqrt{P^2}]}, \quad \varepsilon_0^\mu(P) = P^\mu / \sqrt{P^2} \quad (2.3)$$

realizes the Lorentz transformation to the $P_a = 0$ reference frame and therefore it satisfies the identities

$$\eta_{\mu\nu} \varepsilon_\alpha^\mu(P) \varepsilon_\beta^\nu(P) = \eta_{\alpha\beta}, \quad \eta_{\alpha\beta} \varepsilon_\alpha^\mu(P) \varepsilon_\beta^\nu(P) = \eta^{\mu\nu}. \quad (2.4)$$

Indeed it can be observed that both r_a and q_a are Wigner vectors of spin one, as well as that Z_a has the structure of a position vector of the Newton–Wigner type for a particle with angular momentum L_a , where

$$L_a = \varepsilon_{abc} r_b q_c. \quad (2.5)$$

We can remark that the variables (2.2) arise quite naturally as global and relative coordinates in a two-body Poincaré invariant dynamics constructed by using the algebraic and coalgebraic properties of the Weyl homogeneous spaces. Indeed a four-component position operator for each constituent is built in terms of the generators of the corresponding Weyl algebra, whose non-trivial cohomology permits us to deduce global and relative operators. The breaking of the scale invariance leaves the resulting dynamical system Poincaré symmetric [15]. This procedure, although different in the algebraic assumptions and in the results, presents clear analogies with the classic paper [18], (see also subsequent literature, e.g. [13]), where the two-body theory was for the first time coherently based on the algebra of the Poincaré generators corresponding to each particle.

Using (2.2), the mass shell conditions for each of the two particles read

$$p_{(i)}^2 = \frac{1}{4} P^2 + (-)^{i+1} \sqrt{P^2} \check{q} + \check{q}^2 - q_a q_a = m_i^2, \quad (2.6)$$

from which

$$\sqrt{P^2} \check{q} = \frac{1}{2} (m_1^2 - m_2^2), \quad \frac{1}{2} P^2 + 2\check{q}^2 - 2q_a q_a = m_1^2 + m_2^2. \quad (2.7)$$

Therefore the total mass $\lambda = \sqrt{P^2}$ results in

$$(q_a q_a + m_1^2)^{1/2} + (q_a q_a + m_2^2)^{1/2} = \lambda, \quad (2.8)$$

while the variable \check{q} can be fixed, generating a symplectic reduction of the phase space. Its conjugate coordinate \check{r} —the relative time coordinate—is cyclic and assumes the character of a gauge function that is chosen *a posteriori* in order to recover the complete Minkowski description for the two particles. In particular cases it could be useful to fix $\check{r} = 0$, but in principle there is no necessity requiring such a condition.

It is finally straightforward to construct a Lorentz covariant dynamics by introducing non-trivial interaction terms depending only upon q_a and r_a . One of the simplest choices is to add scalar potentials that are functions of the Lorentz scalar $r = (r_a r_a)^{1/2}$. Hence, a relativistic two-body system interacting by means of a potential $V(r)$ is described by

$$(q_a q_a + m_1^2)^{1/2} + (q_a q_a + m_2^2)^{1/2} = h(r), \quad (2.9)$$

with

$$h(r) = \lambda - V(r). \quad (2.10)$$

The equation of the orbits for the Coulomb interaction, $V(r) = -\alpha/r$, is obtained from the canonical equations deduced from (2.9). Introducing the variables u and θ defined by

$$u = \lambda - \frac{\alpha}{r}, \quad \cos \theta = \frac{r_3}{r} \quad (2.11)$$

and denoting by L the value of the conserved angular momentum, the equation reads

$$\frac{d\theta}{du} = u \left[u^4 - (4L^2/\alpha^2)u^2(\lambda - u)^2 - 2(m_1^2 + m_2^2)u^2 + (m_1^2 - m_2^2)^2 \right]^{-1/2} (4L^2/\alpha^2)^{1/2}, \quad (2.12)$$

and it can be integrated in terms of elliptic functions (see [14] for details). In the case of equal masses, $m_1 = m_2 = m$, the solution for the orbits can be given in terms of elementary functions. For instance, for $\alpha^2 < 4L^2$ —the most relevant case from our point of view as it gives bounded orbits—the solution is

$$\frac{4L^2 - \alpha^2}{(r_a r_a)^{1/2}} = (4L^2 \lambda^2 + 4(\alpha^2 - 4L^2)m^2)^{1/2} \cos(\theta[1 - \alpha^2/4L^2]^{1/2}) \quad (2.13)$$

and corresponds to the motion of a particle in an external Coulomb field (see e.g. [19]).

3. The quantization of the free two-fermion system

The next step is the quantization of equation (2.9) with $V(r) = 0$. The scalar quantization of the double square root Hamiltonian has received much attention and has also been discussed recently in terms of functional inequalities [21]. However, since most of the physically interesting situations involve fermionic components, we assume particles of that nature and quantize the system accordingly.

The Dirac operators corresponding to each single particle are

$$D_1 = \left(\frac{1}{2}P_\mu + q_\mu\right)\gamma_{(1)}^\mu - m_1, \quad D_2 = \left(\frac{1}{2}P_\mu - q_\mu\right)\gamma_{(2)}^\mu - m_2 \quad (3.1)$$

where we have introduced the following tensor products of gamma matrices:

$$\gamma_{(1)}^\mu = \gamma^\mu \otimes \mathbf{I}_4, \quad \gamma_{(2)}^\mu = \mathbf{I}_4 \otimes \gamma^\mu, \quad (3.2)$$

where \mathbf{I}_4 is the unity matrix in four dimensions.

The operators D_1 and D_2 can be rewritten in terms of the canonical set (2.2). At the same time the constant γ_μ matrices will be recast in terms of the new set of matrices $\{\check{\gamma}(P), (\gamma_a(P))_{a=1,3}\}$, where

$$\check{\gamma}(P) = \varepsilon_0^\mu(P)\gamma_\mu, \quad \gamma_a(P) = \varepsilon_a^\mu(P)\gamma_\mu. \quad (3.3)$$

The two Dirac equations (3.1) become then

$$\frac{1}{2}\lambda\check{\gamma}_{(1)} + \check{q}\check{\gamma}_{(1)} - q_a\gamma_{(1)a} = m_1, \quad \frac{1}{2}\lambda\check{\gamma}_{(2)} - \check{q}\check{\gamma}_{(2)} + q_a\gamma_{(2)a} = m_2. \quad (3.4)$$

We observe that the square of $\check{\gamma}_{(i)}$ gives the unity matrix. We next multiply equations (3.4) on the left by $\check{\gamma}_{(1)}$ and $\check{\gamma}_{(2)}$ respectively, and we obtain

$$\frac{1}{2}\lambda + \check{q} - q_a\check{\gamma}_{(1)}\gamma_{(1)a} = \check{\gamma}_{(1)}m_1, \quad \frac{1}{2}\lambda - \check{q} + q_a\check{\gamma}_{(2)}\gamma_{(2)a} = \check{\gamma}_{(2)}m_2. \quad (3.5)$$

By summing and subtracting, we finally get

$$\lambda = q_a(\check{\gamma}_{(1)}\gamma_{(1)a} - \check{\gamma}_{(2)}\gamma_{(2)a}) + \check{\gamma}_{(1)}m_1 + \check{\gamma}_{(2)}m_2 \quad (3.6a)$$

$$\check{q} = \frac{1}{2}q_a(\check{\gamma}_{(1)}\gamma_{(1)a} + \check{\gamma}_{(2)}\gamma_{(2)a}) + \check{\gamma}_{(1)}m_1 - \check{\gamma}_{(2)}m_2. \quad (3.6b)$$

The right-hand sides of the two equations (3.6) are commuting. Multiplying those equations term by term, we get

$$\lambda\check{q} = m_1^2 - m_2^2, \quad (3.7)$$

and we see that the variable \check{q} remains fixed, in complete agreement with the classical symplectic reduction. In fact the canonical conjugate relative time coordinate \check{r} is cyclic again: this is signified, in particular, by the Lorentz scalar identity for the phase of plane waves

$$p_{(1)}^\mu x_{(1)\mu} + p_{(2)}^\mu x_{(2)\mu} = P^\mu Z_\mu - q_a r_a. \quad (3.8)$$

We finally observe that definition (3.3) is actually a Lorentz transformation on the γ^μ four-vector determining a unitary transformation. Therefore, as long as P is conserved, the matrices (3.3) will be represented by the usual γ matrices. The different behaviour under Lorentz transformations is however signified by the use of notation (3.3). In conclusion, equation (3.6a) is the Lorentz-invariant equation for the two-fermion system. It is also straightforward to calculate the explicit expressions for the 16 eigenvalues λ and the result is rather obvious. In fact we have four singular values

$$\begin{aligned} \lambda = & \pm(q_a q_a + m_1^2)^{1/2} \pm (q_a q_a + m_2^2)^{1/2}, \\ & \pm(q_a q_a + m_1^2)^{1/2} \mp (q_a q_a + m_2^2)^{1/2}, \end{aligned} \quad (3.9)$$

each one with multiplicity four. Defining

$$M = m_1 + m_2, \quad \mu = m_1 - m_2, \quad \rho = \mu/M, \quad (3.10)$$

we make a linear transformation on the tensor product of the two spinor spaces that diagonalizes the system at rest, in such a way that the four singular values (3.9) appear in the order M , $-M$, $-\mu$ and μ . We also find it convenient to perform a further linear transformation that, in each four-dimensional eigenspace, diagonalizes the square and the third component of the total spin

$$S = \mathbf{I}_4 \otimes \sigma + \sigma \otimes \mathbf{I}_4 \quad (3.11)$$

σ being the Dirac spin. For each singular value of the mass, the diagonalized spin will then be ordered with the triplet always following the singlet.

The wave equation will now be obtained by applying the canonical quantization rules to equation (3.6a). In view of the bases we have chosen, the natural coordinates to be used are the spherical ones, in terms of which the free Hamiltonian operator reads

$$H_0 = \begin{pmatrix} \mathcal{J}_M & \mathcal{H}_0 \\ \mathcal{H}_0 & \mathcal{J}_\mu \end{pmatrix}, \quad (3.12)$$

where each matrix element is actually an 8×8 block. Explicitly

$$\mathcal{J}_M = M \begin{pmatrix} \mathbf{I}_4 & 0 \\ 0 & -\mathbf{I}_4 \end{pmatrix}, \quad \mathcal{J}_\mu = \mu \begin{pmatrix} \mathbf{I}_4 & 0 \\ 0 & -\mathbf{I}_4 \end{pmatrix} \quad (3.13)$$

and

$$\mathcal{H}_0 = \begin{pmatrix} 0 & X_+ & X_0 & X_- & 0 & X_+ & X_0 & X_- \\ -X_- & X_0 & X_- & 0 & -X_- & -X_0 & -X_- & 0 \\ X_0 & -X_+ & 0 & X_- & X_0 & X_+ & 0 & -X_- \\ -X_+ & 0 & -X_+ & -X_0 & -X_+ & 0 & X_+ & X_0 \\ 0 & X_+ & X_0 & X_- & 0 & X_+ & X_0 & X_- \\ -X_- & -X_0 & -X_- & 0 & -X_- & X_0 & X_- & 0 \\ X_0 & X_+ & 0 & -X_- & X_0 & -X_+ & 0 & X_- \\ -X_+ & 0 & X_+ & X_0 & -X_+ & 0 & -X_+ & -X_0 \end{pmatrix}. \quad (3.14)$$

The matrix elements in (3.14) are the spherical operators

$$X_\pm = -2^{-1/2}(\pm q_x + iq_y), \quad X_0 = q_z, \quad (3.15)$$

where $q_a \rightarrow -i\partial/\partial x_a$.

We finally recall that the global parity transformation is given by the product of orbital and internal parity transformations. In our picture the internal parity is given by

$$\check{\gamma} \otimes \check{\gamma} = \begin{pmatrix} \mathbf{I}_8 & 0 \\ 0 & -\mathbf{I}_8 \end{pmatrix}. \quad (3.16)$$

It is straightforward to verify that the global angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$ and the parity are conserved. Together with λ they provide a classification of the states of the global symmetry. Concerning the problem of canonical realization, Poincaré representations and invariant scalar products we refer to the paper [20]. It is also straightforward to observe that the conservation properties continue to hold in the presence of interactions depending upon the Lorentz scalars $r_a r_a$, $q_a q_a$ and $q_a r_a$: this fact will be used in the next section to determine a reduced set of differential equations and to state the boundary value problem in the space of the square-integrable functions on the relative \mathbf{R}^3 .

4. The spectral problem for an interacting system

The construction of the states with assigned angular momentum (j, m) and given parity $(-)^j$ or $(-)^{j+1}$ is done as usual, by multiplying the contributions coming from the composition of orbital and intrinsic angular momenta by functions of r . The expressions of the states Ψ_+ and Ψ_- are reported in equations (A.1) and (A.3) given in appendix A.

The eigenvalue problem comes out when we try to determine the eight unknown functions

$$a_i(r), \quad b_i(r), \quad c_i(r), \quad d_i(r), \quad (i = 0, 1) \quad (4.1)$$

in the state Ψ by solving the homogeneous equation

$$(H_0 - h(r))\Psi = 0, \quad (4.2)$$

with $h(r)$ as in (2.10). Since the parity and the angular momentum are conserved, equation (4.2) produces two different spectral problems to be discussed separately.

4.1. The spectral problem for the state Ψ_+

When substituting $\Psi = \Psi_+$ in (4.2), we obtain a system of equations given by the vanishing of the coefficients of the different spherical harmonics in each component of the resulting vector. This system is composed of 34 first-order differential equations, but, as one should expect, only eight of them are independent. The detailed expressions for the eight equations are written in appendix B.

It turns out that appropriate changes of the initial variables can help to give the system a much simpler and readable form. To this purpose, we first define the sums and differences

$$s_{\pm}(r) = s_0(r) \pm s_1(r) \quad (s = a, b, c, d) \quad (4.3)$$

and we consider the following linear combinations of the $c_{\pm}(r)$ and $d_{\pm}(r)$:

$$\begin{aligned} u_+(r) &= -\frac{\sqrt{j}c_+(r) - \sqrt{j+1}d_+(r)}{\sqrt{1+2j}}, & u_-(r) &= -\frac{\sqrt{j}c_-(r) - \sqrt{j+1}d_-(r)}{\sqrt{1+2j}}, \\ v_+(r) &= -\frac{\sqrt{j+1}c_+(r) + \sqrt{j}d_+(r)}{\sqrt{1+2j}}, & v_-(r) &= -\frac{\sqrt{j+1}c_-(r) + \sqrt{j}d_-(r)}{\sqrt{1+2j}}. \end{aligned} \quad (4.4)$$

A rather simple formulation for the system can then be given in terms of $a_{\pm}(r)$, $b_{\pm}(r)$, $u_{\pm}(r)$ and $v_{\pm}(r)$. Indeed, from a straightforward computation, we find that the eight independent equations split into four algebraic relations and four first-order differential equations. The former read

$$\begin{aligned} \sqrt{j(j+1)}a_+(r) - \frac{r}{2}(h(r)v_+(r) + \mu v_-(r)) &= 0, \\ \sqrt{j(j+1)}b_-(r) + \frac{r}{2}(\mu u_+(r) + h(r)u_-(r)) &= 0, \\ Ma_+(r) - h(r)a_-(r) = 0, & \quad h(r)b_+(r) - Mb_-(r) = 0 \end{aligned} \quad (4.5)$$

while the differential equations are

$$\begin{aligned} \frac{da_+(r)}{dr} + \frac{\sqrt{j(j+1)}\mu}{rh(r)}b_-(r) + \frac{(-h(r)^2 + \mu^2)}{2h(r)}u_+(r) &= 0 \\ \sqrt{j} \left(\frac{db_-(r)}{dr} - \frac{jb_-(r)}{r} \right) - \frac{\sqrt{j+1}}{2}(\mu u_+(r) + h(r)u_-(r)) + \frac{\sqrt{j}}{2}(\mu v_+(r) + h(r)v_-(r)) &= 0 \\ \frac{du_+(r)}{dr} - \frac{M-h(r)}{2}(a_+(r) + a_-(r)) + \frac{2}{r}u_+(r) - \frac{j\sqrt{j+1}}{r}v_+(r) &= 0 \\ \frac{dv_-(r)}{dr} + \frac{M-h(r)}{2}(b_+(r) + b_-(r)) - \frac{\sqrt{j(j+1)}}{r}u_-(r) + \frac{1}{r}v_-(r) &= 0. \end{aligned} \quad (4.6)$$

By means of (4.5) we eliminate the four variables that are not differentiated, obtaining a system of four first-order differential equations in the four unknown functions $a_+(r)$, $b_-(r)$, $u_+(r)$ and $v_-(r)$. If we arrange the latter respectively as the four components of a vector $Y(r) \equiv {}^t(y_1(r), y_2(r), y_3(r), y_4(r))$, the system is given the compact form

$$\frac{dY(r)}{dr} + \mathcal{M}Y(r) = 0, \quad (4.7)$$

where \mathcal{M} is a matrix with general structure

$$\mathcal{M} = \begin{bmatrix} 0 & E(r) & F(r) & 0 \\ E(r) & \frac{1}{r} & 0 & -F(r) \\ G(r) & 0 & \frac{2}{r} & E(r) \\ 0 & -G(r) & E(r) & \frac{1}{r} \end{bmatrix}. \quad (4.8)$$

The explicit expressions of $E(r)$, $F(r)$ and $G(r)$ for the even case are the following ones:

$$E_e(r) = \frac{\sqrt{j(j+1)}\mu}{rh(r)} \quad (4.9a)$$

$$F_e(r) = -\frac{h(r)}{2} \left(1 - \frac{\mu^2}{h^2(r)} \right) \quad (4.9b)$$

$$G_e(r) = \frac{h(r)}{2} \left(1 - \frac{r^2 M^2 + 4j(j+1)}{r^2 h^2(r)} \right). \quad (4.9c)$$

Specifying the matrix elements (4.9) to the case of the Coulomb interaction, where

$$h(r) = \lambda + \alpha/r, \quad (4.10)$$

and where α is the fine structure constant, we have

$$E_{e,\text{Coul}}(r) = \frac{\sqrt{j(j+1)}\mu}{\lambda r + \alpha} \quad (4.11a)$$

$$F_{e,\text{Coul}}(r) = -\frac{(\lambda r + \alpha)^2 - \mu^2 r^2}{2r(\lambda r + \alpha)} \quad (4.11b)$$

$$G_{e,\text{Coul}}(r) = \frac{(\lambda r + \alpha)^2 - M^2 r^2 - 4j(j+1)}{2r(\lambda r + \alpha)}. \quad (4.11c)$$

Some remarks are in order. First of all, from (4.8) and (4.9) we see that the transformation

$$\mu \rightarrow -\mu, \quad y_1(r) \rightarrow -y_1(r), \quad y_3(r) \rightarrow -y_3(r) \quad (4.12)$$

is a symmetry of the system, corresponding to the fact that the ordering of the two particles is irrelevant.

In the second place, from (4.9a), we see that $E_e(r) = 0$ either for $j = 0$ or $\mu = 0$. In these cases the fourth-order system splits into separate second-order subsystems, one for the functions $y_1(r)$ and $y_3(r)$, the other for $y_2(r)$ and $y_4(r)$. The subsystems, in turn, can be presented as the following two independent second-order differential equations:

$$\frac{d^2}{dr^2} y_1(r) + \left(\frac{2}{r} - \frac{\frac{d}{dr} F(r)}{F(r)} \right) \frac{d}{dr} y_1(r) - F(r)G(r)y_1(r) = 0 \quad (4.13a)$$

$$\frac{d^2}{dx^2} y_2(x) + \left(\frac{2}{r} - \frac{\frac{d}{dr} F(r)}{F(r)} \right) \frac{d}{dr} y_2(r) - \left(\frac{\frac{d}{dr} F(r)}{rF(r)} + F(r)G(r) \right) y_2(r) = 0. \quad (4.13b)$$

As discussed in section 5, the Dirac limit shows that for $j = 0$ only (4.13a) makes sense.

Although the linear system (4.7) and, in particular, equation (4.13a) do not look extremely complicated, they are still difficult enough to prevent the possibility of an easy analytical solution. For instance, according to a somewhat old fashioned—but actually still the most up to date—classification of differential equations according to the number of their elementary singularities (for definitions and detail we refer to the classical text [22]), equations (4.13) with the Coulomb coefficients (4.11) present eight elementary singularities, while analytical properties of the solutions have been studied and classified for differential equations having at most six elementary singularities. Numerical techniques are therefore necessary if we want to determine the spectral properties, both for equal and different masses.

4.2. The spectral problem for the state Ψ_-

The differential equations generated by the action of the Hamiltonian on the odd state are easily derived by observing that the transformation (A.3) amounts to changing m_1 into $-m_1$, which means $\mu \rightarrow -M$ and $M \rightarrow -\mu$. The general structure for the matrix of the odd linear system, therefore, remains the one given in (4.8). The matrix elements, on the other hand, are as follows:

$$E_o(r) = -\frac{\sqrt{j(j+1)}M}{rh(r)} \quad (4.14a)$$

$$F_o(r) = -\frac{h(r)}{2} \left(1 - \frac{M^2}{h^2(r)} \right) \quad (4.14b)$$

$$G_o(r) = \frac{h(r)}{2} \left(1 - \frac{r^2\mu^2 + 4j(j+1)}{r^2h^2(r)} \right). \quad (4.14c)$$

and also the Coulomb explicit expressions are obtained from (4.11) by the exchanges $(M, \mu) \rightarrow (-\mu, -M)$. The system decouples for $j = 0$, but, in contrast to what occurs in the even case, this circumstance is not realized when the particles have equal masses.

5. The Dirac limit

In this section we prove that (4.7) and (4.8) have the correct Dirac limit. This means that when the mass of one of the two interacting particles, say m_1 , tends to infinity, the system reduces to the Dirac equation for a charged fermion in an external potential.

The limit is defined by assuming that the mass $m_2 \equiv m_e$ remains finite and gives the mass scale. The rescaling of the mass parameters of the system is then

$$\mu = \frac{2\rho m_e}{1-\rho}, \quad M = \frac{2m_e}{1-\rho}. \quad (5.1)$$

We also take a dimensionless independent variable

$$x = m_e r, \quad (5.2)$$

and define a coefficient η by means of the relation

$$h(x) = \left(\eta - v(x) + \frac{1+\rho}{1-\rho} \right) m_e \quad (5.3)$$

where $v(x)$ is the potential expressed in terms of x and divided by m_e . It proves convenient to define the shorthand

$$\eta(x) = \eta - v(x). \quad (5.4)$$

We now take the limit $\rho \rightarrow 1$ on the matrix elements. For the even system in the dimensionless variable x , we find

$$E_e(x) \rightarrow \sqrt{j(j+1)}/x, \quad F_e(x) \rightarrow -(1 + \eta(x)), \quad G_e(x) \rightarrow \eta(x) - 1. \quad (5.5)$$

For the odd system:

$$E_o(r) \rightarrow -\sqrt{j(j+1)}/x, \quad F_o(r) \rightarrow (1 - \eta(x)), \quad G_o(r) \rightarrow (1 + \eta(x)). \quad (5.6)$$

Let us prove that the equations obtained by the use of (5.5) and (5.6) are actually equivalent to pairs of Dirac equations [23], that we write in our rescaled variables as

$$\frac{d}{dx} \begin{pmatrix} xf(x) \\ xg(x) \end{pmatrix} + \begin{pmatrix} \frac{\kappa}{x} & -(1 + \eta - v(x)) \\ (-1 + \eta - v(x)) & -\frac{\kappa}{x} \end{pmatrix} \begin{pmatrix} xf(x) \\ xg(x) \end{pmatrix}. \quad (5.7)$$

It is not difficult to realize that a mixing is necessary in order to decouple the fourth-order system in two second-order subsystems to be compared to the Dirac equation. This is physically clear, since from a description focusing on the angular momentum properties of the bosonic global system, we want to determine the equation for a fermionic object that constitutes only a part of the compound. The required linear transformation is generated by the orthogonal constant matrix

$$U = \frac{1}{\sqrt{2j+1}} \begin{pmatrix} 0 & 0 & \sqrt{j} & \sqrt{j+1} \\ 0 & 0 & \sqrt{j+1} & -\sqrt{j} \\ \sqrt{j+1} & -\sqrt{j} & 0 & 0 \\ \sqrt{j} & \sqrt{j+1} & 0 & 0 \end{pmatrix}. \quad (5.8)$$

By defining

$$z_i(x) = \sum_{j=1}^4 (U^{-1})_{ij} x y_j(x) \quad (5.9)$$

it is straightforward to see that both in the even and the odd cases the equations for the variables $z_1(x)$ and $z_4(x)$ decouple from the equations for $z_2(x)$ and $z_3(x)$. The comparison with (5.7) shows that the subsystems obtained in the even case are respectively the Dirac equations with $\kappa = -(j+1)$ and $\kappa = j$ (here we must change $z_3(x)$ into $-z_3(x)$): these are the two allowed values of κ for the states whose orbital momentum is j in the Dirac spectroscopy [23]. In the odd case the decoupled systems agree respectively with the Dirac equations with $\kappa = j+1$ (here changing $z_4(x)$ into $-z_4(x)$) and $\kappa = -j$: these values correspond to orbital angular momenta equal to $j+1$ and $j-1$.

The previous discussion clearly shows that the complete treatment is continuous in the parameter $1 - \rho$: indeed, when this parameter is small, it can be effectively used to compute perturbative corrections to the Dirac equation. Thus, although the general features of the spectrum—e.g. its boundedness from below—are clearly dependent upon the potential function $v(x)$ and can be studied in each particular case by well-established criteria [24], the continuity in $1 - \rho$ of the differential operator implies the continuity in $1 - \rho$ of its spectrum that therefore shares the qualitative properties of the limiting case. We report in appendix C the calculation of the first-order correction to the hydrogen ground state and we find excellent agreement with the numerical results.

6. Discussion of the results

In this section we present the results obtained. We display the tables containing the values of the variable ρ and the corresponding level with ten meaningful figures; the corresponding plots are then drawn. The energy parameter w that appears both in the tables and in the plots is related to the parameter η defined in (5.4) by the relation

$$\eta = 1 + \frac{1}{2}(1 + \rho)\alpha^2 w. \quad (6.1)$$

In terms of the eigenvalue λ , this equation is equivalent to $\lambda = M + m_R \alpha^2 w$, where m_R is the classical reduced mass $m_R = m_1 m_2 / (m_1 + m_2)$. This means that the correction of energy levels due to the classical reduction to the centre-of-mass frame is already accounted for by the scale. Hence, the dependence upon ρ shown below is a genuine relativistic effect.

The results will be given in atomic units, i.e. $m_e = 1$ in addition to $\hbar = 1$ and $c = 1$. The values of ρ with greater physical relevance are $\rho = \rho_e$, corresponding to the hydrogen atom, $\rho = \rho_\mu$, that refers to the mesic atom and $\rho = 0$, for positronium. The value of w for $\rho = 1$ has been taken from the analytical formula for the Dirac spectrum. It is natural to begin from the ground state. We find that for any value of the two fermion masses the lowest energy level is degenerate with multiplicity two and the corresponding states are the first (i.e. with lowest eigenvalue) even state with $j = 0$ and the first odd state with $j = 1$. We specify the results in the table here below and we shall comment on the degeneracy later on.

ρ	$w_{+,j=0,I}$	$w_{-,j=1,I}$
0.0	-0.499 995 0109	-0.499 995 0109
0.2	-0.499 995 4766	-0.499 995 4766
0.4	-0.499 996 8737	-0.499 996 8737
0.6	-0.499 999 2025	-0.499 999 2025
ρ_μ	-0.500 002 4182	-0.500 002 4182
ρ_e	-0.500 006 6312	-0.500 006 6312
1.0	-0.500 006 6566	-0.500 006 6566

Here $\rho_e = 0.998\,911$ corresponds to the hydrogen atom data and $\rho_\mu = 0.797\,576$ refers to the mesic atom. The plot of the ground state versus ρ is shown in figure 1. The difference $w_{+,j=0,I}(\rho_e) - w_{+,j=0,I}(1) = 0.254 \times 10^{-7}$ should be compared with the value 0.253×10^{-7} obtained in appendix C by a perturbative calculation.

The triplet given by the first even excited state with $j = 0$ —corresponding to the state $2s_{1/2}$ in the Dirac limit—together with the even states that in the Dirac limit reduce to $2p_{1/2}$ and $2p_{3/2}$ is presented in the first plot of figure 2. Their numerical values are respectively reported in the table that follows:

ρ	$w_{+,j=0,II}$	$w_{+,j=1,I}$	$w_{+,j=1,II}$
0.0	-0.124 999 6884	-0.125 000 5200	-0.125 000 2427
0.2	-0.124 999 7840	-0.125 000 6292	-0.125 000 2030
0.4	-0.125 000 0710	-0.125 000 8727	-0.125 000 1675
0.6	-0.125 000 5493	-0.125 001 2005	-0.125 000 1864
ρ_μ	-0.125 001 2098	-0.125 001 5984	-0.125 000 2673
ρ_e	-0.125 002 0750	-0.125 002 0774	-0.125 000 4151
1.0	-0.125 002 0802	-0.125 002 0802	-0.125 000 4160

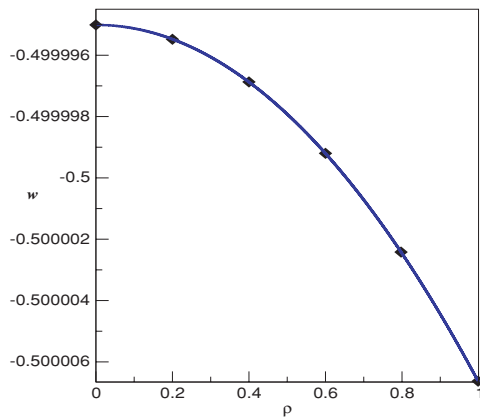


Figure 1. The dependence of the degenerate ground state on ρ : the levels $w_{+,j=0,1}$ and $w_{-,j=1,1}$.

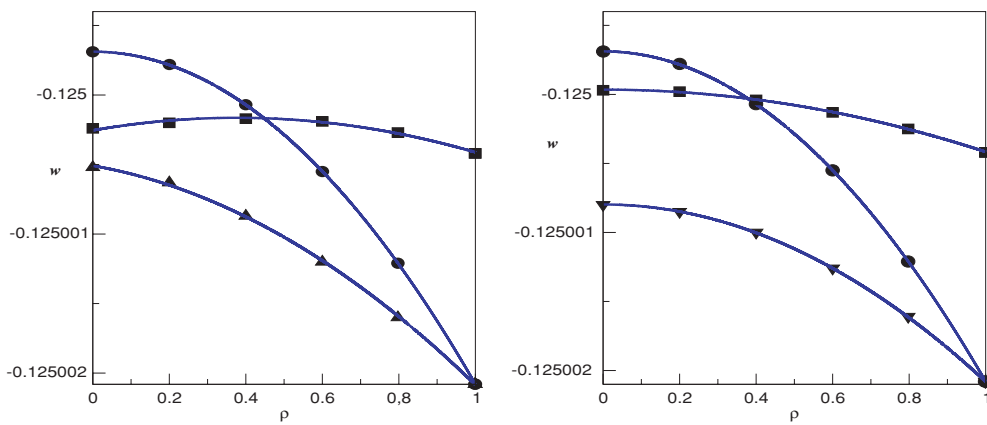


Figure 2. The spectral curves for varying masses from the even and odd states. In the left plot (even states), circles represent the curve $w_{+,j=0,II}$ that reduces to the state $2s_{1/2}$ in the Dirac limit, triangles the curve $w_{+,j=1,I}$ reducing to the state $2p_{1/2}$ and squares the curve $w_{+,j=1,II}$ reducing to $2p_{3/2}$. In the right plot (odd states), circles to refer to $w_{-,j=1,I}$, triangles to $w_{-,j=0,I}$, squares to $w_{-,j=2,I}$.

In the final table we give the values for the three states that constitute the odd counterpart of the even triplet and that are shown in the second plot of figure 2. They arise from the three different values $j = 0, 1, 2$ of the angular momentum.

ρ	$w_{-,j=0,I}$	$w_{-,j=1,II}$	$w_{-,j=2,I}$
0.0	-0.125 000 7974	-0.124 999 6884	-0.124 999 9654
0.2	-0.125 000 8487	-0.124 999 7840	-0.124 999 9834
0.4	-0.125 001 0026	-0.125 000 0710	-0.125 000 0375
0.6	-0.125 001 2592	-0.125 000 5493	-0.125 000 1276
ρ_μ	-0.125 001 6134	-0.125 001 2098	-0.125 000 2520
ρ_e	-0.125 002 0774	-0.125 002 0750	-0.125 000 4150
1.0	-0.125 002 0802	-0.125 002 0802	-0.125 000 4160

From the data we discover one more degeneracy: indeed the even state $w_{+,j=0,II}$ and the odd state $w_{-,j=1,II}$, obviously equal in the Dirac limit, remain degenerate for any value of ρ .

This occurrence, in the present case and for the fundamental state as well, is certainly not evident from a mathematical or computational point of view: indeed the equations that have been solved to find the even spectral curves and the systems that give the the odd ones are completely unrelated. We can however understand this apparently peculiar behaviour by thinking of the non-relativistic limit. Here, unless the spin-orbit coupling is explicitly included, the total spin and the orbital angular momentum are separately conserved. Moreover, if no spin-spin interaction is present, the relative orientations of the two spins between themselves and with respect to the orbital angular momentum are effective in determining the parity, but have no influence on the energy of the state. The result is that the even and the odd states are degenerate with respect to parity. This degeneracy survives in the Dirac limit: although the spin-orbit interaction is now directly accounted for, one of the two constituent particles is infinitely heavy and thus at rest, so that only the spin of the light particle matters. The situation is different in our relativistic equation, when both constituents have finite mass and each of them gives its own contribution to the spin-orbit coupling: in fact we obtain different shifts for the even and odd terms, but for those states that in the non-relativistic limit have a vanishing orbital angular momentum. In the particular case of positronium, we see that the two states $w_{+,j=0,1}$ and $w_{-,j=1,1}$ correspond to para- and orthopositronium respectively. Their degeneracy could be removed by introducing the spin-spin interaction, responsible for the hyperfine splitting. We shall comment on this subject in appendix E.

Coming back to the figures, we observe that the solid curves are the parabolas obtained by the best fit of the data and they are in excellent agreement with the data themselves. The perturbative formula given in [8] for the Coulomb Lamb shift, $\delta w = (\alpha^4/12)(1-\rho)/(1+\rho)^2$, can reproduce parabolic behaviour only for ρ in the neighbourhood of zero or unity. Only the second of these possibilities is actually realized: this shows the necessity of a more detailed numerical analysis when the masses become closer and closer. It is nevertheless interesting to observe the increasing impact of the relativistic effects with decreasing mass difference. In particular it has to be noted that the crossing of the levels $w_{+,j=0,\text{II}}$ and $w_{+,j=1,\text{II}}$ as well as $w_{-,j=1,\text{II}}$ and $w_{-,j=2,\text{I}}$: this, for instance, reflects the necessity of the different method in use to classify the positronium states with respect to the Dirac scheme.

We conclude this discussion of the results with some observations on a possible formulation of a more realistic model involving a minimal coupling that accounts for the complete electro-dynamical interaction. In fact this type of coupling can be arranged quite easily in our quantum mechanical framework and, if we study the case of a closed two-body system and we do want to keep a pure relativistic quantum mechanical description, we can try to express the vector potential itself in terms of the dynamical variables of the two particles. The Liénard-Wiechert potentials provide the most natural answer to the raised question. Unfortunately they introduce a delay in the propagation of the interaction that induces a considerable amount of difficulty in the solution of the corresponding wave equation and indeed the necessity of rendering its solution less tough is a major source of approximations, that, in most cases, produce not very satisfactory results (see [8] and references therein for a discussion on the subject). Indeed if one stops at the lowest order of approximation in the Liénard-Wiechert potentials, neglecting the propagation delay, one finds an interaction energy

$$V_{\text{em}}(r) = \frac{\alpha}{r} + \frac{\alpha}{2r} (v_{(1)a} v_{(2)a} + (n_a v_{(1)a})(n_a v_{(2)a})) \quad (6.2)$$

that has to be substituted for $V(r)$ in (2.10). According to the Dirac prescription, when switching to quantum mechanics, the particle velocities $v_{(i)a}$ will be substituted by the $\alpha_{(i)a} = -\check{\gamma}_{(i)} \gamma_{(i)a}$ matrices, so as to obtain an invariant formulation of the Breit approximation

for the electromagnetic interaction. The final wave equation reads

$$\lambda = q_a (\check{\gamma}_{(1)} \gamma_{(1)a} - \check{\gamma}_{(2)} \gamma_{(2)a}) + (\check{\gamma}_{(1)} m_1 + \check{\gamma}_{(2)} m_2) + \frac{\alpha}{r} + \frac{\alpha}{2r} \check{\gamma}_{(1)} \check{\gamma}_{(2)} (\gamma_{(1)a} \gamma_{(2)a} + (n_a \gamma_{(1)a})(n_a \gamma_{(2)a})). \quad (6.3)$$

The difficulties of a direct solution of equation (6.3) have been known for a long time (see [25, 26]): a perturbative interpretation of the term involving the vector potential, averaged over the pure Coulomb wavefunction—very often at the non-relativistic Schrödinger level of approximation—is therefore what is usually computed. The calculation can be found in [8] and produces a perfect cancellation of the α^4 -perturbative Coulomb splitting. From the previous discussion it is clear that the result should be tested numerically using the relativistic Coulomb wavefunctions for any value of the mass ratio. This numerical test is however beyond the purpose of the present paper. In any case—and as was certainly to be expected—it appears that the acceleration and delay effects of the Liénard–Wiechert potentials—and therefore the radiative corrections—are essential for obtaining physical results.

Appendix A. The state vectors

We give here the explicit form of the 16 component state vectors of definite energy, angular momentum (j, m) and even and odd parity with respect to the angular momentum, namely $(-)^j$ and $(-)^{j+1}$. We call them Ψ_+ and Ψ_- respectively. The even state is then given by

$$\Psi_+ = {}^t(\Psi_+^{(M)}, \Psi_+^{(-M)}, \Psi_+^{(-\mu)}, \Psi_+^{(\mu)}). \quad (A.1)$$

The four components are actually multiplets composed of a singlet and a triplet and will be indicated as

$$\Psi_+^{(\Lambda)} = {}^t(\psi_{+0}^{(\Lambda)}, \psi_{+1+}^{(\Lambda)}, \psi_{+1_0}^{(\Lambda)}, \psi_{+1-}^{(\Lambda)}), \quad (A.2)$$

where $\Lambda = \pm M, \mp \mu$. According to a common practice and in order to deduce real differential equations in appendix B, we shall introduce an imaginary unity in front of the coefficient functions $c_i(r)$ and $d_i(r)$. The explicit expressions of the state vector components are the following:

$$\begin{aligned} \psi_{+0}^{(M)} &= Y_m^j(\theta, \phi) a_0(r), & \psi_{+1+}^{(M)} &= -\frac{\sqrt{j-m+1}\sqrt{j+m}}{\sqrt{2j}\sqrt{j+1}} Y_{m-1}^j(\theta, \phi) b_0(r) \\ \psi_{+1_0}^{(M)} &= \frac{m}{\sqrt{j}\sqrt{1+j}} Y_m^j(\theta, \phi) b_0(r), & \psi_{+1-}^{(M)} &= \frac{\sqrt{j-m}\sqrt{j+m+1}}{\sqrt{2j}\sqrt{j+1}} Y_{m+1}^j(\theta, \phi) b_0(r) \\ \psi_{+0}^{(-M)} &= Y_m^j(\theta, \phi) a_1(r), & \psi_{+1+}^{(-M)} &= -\frac{\sqrt{j-m+1}\sqrt{j+m}}{\sqrt{2j}\sqrt{j+1}} Y_{m-1}^j(\theta, \phi) b_1(r) \\ \psi_{+1_0}^{(-M)} &= \frac{m}{\sqrt{j}\sqrt{1+j}} Y_m^j(\theta, \phi) b_1(r), & \psi_{+1-}^{(-M)} &= \frac{\sqrt{j-m}\sqrt{j+m+1}}{\sqrt{2j}\sqrt{j+1}} Y_{m+1}^j(\theta, \phi) b_1(r) \\ \psi_{+0}^{(-\mu)} &= 0 \\ \psi_{+1+}^{(-\mu)} &= \frac{\sqrt{j+m-1}\sqrt{j+m}}{\sqrt{2j}\sqrt{2j-1}} Y_{m-1}^{j-1}(\theta, \phi) ic_0(r) + \frac{\sqrt{j-m+1}\sqrt{j-m+2}}{\sqrt{2j+2}\sqrt{2j+3}} Y_{m-1}^{j+1}(\theta, \phi) id_0(r) \\ \psi_{+1_0}^{(-\mu)} &= \frac{\sqrt{j-m}\sqrt{j+m}}{\sqrt{j}\sqrt{2j-1}} Y_m^{j-1}(\theta, \phi) ic_0(r) - \frac{\sqrt{j-m+1}\sqrt{j+m+1}}{\sqrt{1+j}\sqrt{2j+3}} Y_m^{j+1}(\theta, \phi) id_0(r) \\ \psi_{+1-}^{(-\mu)} &= \frac{\sqrt{j-m-1}\sqrt{j-m}}{\sqrt{2j}\sqrt{2j-1}} Y_{m+1}^{j-1}(\theta, \phi) ic_0(r) + \frac{\sqrt{j+m+1}\sqrt{j+m+2}}{\sqrt{2j+2}\sqrt{2j+3}} Y_{m+1}^{j+1}(\theta, \phi) id_0(r) \end{aligned}$$

$$\begin{aligned}
\psi_{+0}^{(\mu)} &= 0 \\
\psi_{+1+}^{(\mu)} &= \frac{\sqrt{j+m-1}\sqrt{j+m}}{\sqrt{2j}\sqrt{2j-1}} Y_{m-1}^{j-1}(\theta, \phi) ic_1(r) + \frac{\sqrt{j-m+1}\sqrt{j-m+2}}{\sqrt{2j+2}\sqrt{2j+3}} Y_{m-1}^{j+1}(\theta, \phi) id_1(r) \\
\psi_{+1_0}^{(\mu)} &= \frac{\sqrt{j-m}\sqrt{j+m}}{\sqrt{j}\sqrt{2j-1}} Y_m^{j-1}(\theta, \phi) ic_1(r) - \frac{\sqrt{j-m+1}\sqrt{j+m+1}}{\sqrt{j+1}\sqrt{2j+3}} Y_m^{j+1}(\theta, \phi) id_1(r) \\
\psi_{+1-}^{(\mu)} &= \frac{\sqrt{j-m-1}\sqrt{j-m}}{\sqrt{2j}\sqrt{2j-1}} Y_{m+1}^{j-1}(\theta, \phi) ic_1(r) + \frac{\sqrt{j+m+1}\sqrt{j+m+2}}{\sqrt{2j+2}\sqrt{2j+3}} Y_{m+1}^{j+1}(\theta, \phi) id_1(r)
\end{aligned}$$

where $Y_q^k(\theta, \phi)$ are the spherical harmonic functions. Concerning the state with opposite parity, it can be seen that the action of the parity transformation is simply the exchange of the first eight components with the second eight ones. Therefore, in order to determine the differential equations describing the odd states of the system, we shall use the state Ψ_- given by

$$\Psi_- = \begin{pmatrix} 0 & \mathbf{I}_8 \\ \mathbf{I}_8 & 0 \end{pmatrix} \Psi_+. \quad (\text{A.3})$$

As observed in section 4.2 this amounts to changing the sign of the mass m_1 .

Appendix B. The original system

As we said in section (4.2), in order to determine the system of differential equations describing the two body problem, we shall apply the Hamiltonian operator H_0 , given in (3.12), to the state vector (A.1). In each component we require the vanishing of the coefficient of each different spherical harmonic. This leads to a system of 34 differential equations in the unknown functions $a_i(r)$, $b_i(r)$, $c_i(r)$ and $d_i(r)$ ($i = 0, 1$), that appear in the state vector. However, as expected, only eight of these differential equations are independent. They read

$$\begin{aligned}
\sqrt{j} \left(\frac{d}{dr} + \frac{j+1}{r} \right) (a_0(r) + a_1(r)) - \sqrt{j+1} \left(\frac{d}{dr} + \frac{j+1}{r} \right) (b_0(r) - b_1(r)) \\
+ \sqrt{2j+1} c_0(r) (\mu + h(r)) = 0
\end{aligned} \quad (\text{B.1a})$$

$$\begin{aligned}
\sqrt{j} \left(\frac{d}{dr} + \frac{j+1}{r} \right) (a_0(r) + a_1(r)) + \sqrt{j+1} \left(\frac{d}{dr} + \frac{j+1}{r} \right) (b_0(r) - b_1(r)) \\
- \sqrt{2j+1} c_1(r) (\mu - h(r)) = 0
\end{aligned} \quad (\text{B.1b})$$

$$\begin{aligned}
\sqrt{j+1} \left(\frac{d}{dr} - \frac{j}{r} \right) (a_0(r) + a_1(r)) + \sqrt{j} \left(\frac{d}{dr} - \frac{j}{r} \right) (b_0(r) - b_1(r)) \\
- \sqrt{2j+1} d_0(r) (\mu + h(r)) = 0
\end{aligned} \quad (\text{B.1c})$$

$$\begin{aligned}
\sqrt{j+1} \left(\frac{d}{dr} - \frac{j}{r} \right) (a_0(r) + a_1(r)) - \sqrt{j} \left(\frac{d}{dr} - \frac{j}{r} \right) (b_0(r) - b_1(r)) \\
+ \sqrt{2j+1} d_1(r) (\mu - h(r)) = 0
\end{aligned} \quad (\text{B.1d})$$

$$\begin{aligned}
\sqrt{j} \left(\frac{d}{dr} - \frac{j-1}{r} \right) (c_0(r) + c_1(r)) - \sqrt{j+1} \left(\frac{d}{dr} + \frac{j+2}{r} \right) (d_0(r) + d_1(r)) \\
+ \sqrt{2j+1} a_0(r) (M - h(r)) = 0
\end{aligned} \quad (\text{B.1e})$$

$$\begin{aligned} \sqrt{j} \left(\frac{d}{dr} - \frac{j-1}{r} \right) (c_0(r) + c_1(r)) - \sqrt{j+1} \left(\frac{d}{dr} + \frac{j+2}{r} \right) (d_0(r) + d_1(r)) \\ - \sqrt{2j+1} a_1(r) (M + h(r)) = 0 \end{aligned} \quad (\text{B.1f})$$

$$\begin{aligned} \sqrt{j+1} \left(\frac{d}{dr} - \frac{j-1}{r} \right) (c_0(r) - c_1(r)) + \sqrt{j} \left(\frac{d}{dr} + \frac{j+2}{r} \right) (d_0(r) - d_1(r)) \\ - \sqrt{2j+1} b_0(r) (M - h(r)) = 0 \end{aligned} \quad (\text{B.1g})$$

$$\begin{aligned} \sqrt{j+1} \left(\frac{d}{dr} - \frac{j-1}{r} \right) (c_0(r) - c_1(r)) + \sqrt{j} \left(\frac{d}{dr} + \frac{j+2}{r} \right) (d_0(r) - d_1(r)) \\ - \sqrt{2j+1} b_1(r) (M + h(r)) = 0. \end{aligned} \quad (\text{B.1h})$$

Once definitions (4.3) and (4.4) are used, a straightforward, although somewhat lengthy computation, leads directly to (4.5) and (4.6).

Appendix C. A perturbative calculation in the mass ratio

We now present a perturbative approach to the ground level of the hydrogen atom, taking as perturbation parameter the quantity

$$\epsilon = 1 - \rho_H = 1 - \frac{m_P - m_e}{m_P + m_e} = 0.001\,088\,6411. \quad (\text{C.1})$$

As we have said in section 4, for $j = 0$ the system splits into two subsystems obtained by (4.7) and (4.8), or, equivalently, by the second-order equation (4.13a). For later convenience in the development of the perturbative calculations we introduce the modified unknown functions $\phi(r)$, $\theta(r)$ defined by

$$y_1(r) = \frac{\sqrt{F(r)}}{r} \phi(r), \quad y_2(r) = \frac{\sqrt{F(r)}}{r} \theta(r). \quad (\text{C.2})$$

In particular we see that second-order equation (4.13a) written in terms of $\phi(r)$ does not present the first derivative term:

$$\frac{d^2}{dr^2} \phi(r) + \left(\frac{1}{2} \frac{d}{dr} \left(\frac{r^2 \frac{d}{dr} F(r)}{r^2 F(r)} \right) - G(r) F(r) - \frac{3}{4} \left(\frac{d}{dr} F(r) \right)^2 \right) \phi(r) = 0. \quad (\text{C.3})$$

For $F(r)$ and $G(r)$ we shall then assume their Coulomb explicit form (4.9). Finally, the parameters are rescaled according to (5.1) and (5.3) and, correspondingly, we write the series expansions of the eigenvalue and the eigenfunction components in terms of ϵ :

$$\lambda = \sum_n \epsilon^n \lambda_n, \quad y_j(x) = \sum_n \epsilon^n y_j^{(n)}(x) \quad (j = 1, 3). \quad (\text{C.4})$$

At the lowest order in ϵ we have the system

$$\begin{aligned} \frac{d}{dx} y_1^{(0)}(x) - \left(1 + \lambda_0 + \frac{\alpha}{x} \right) y_3^{(0)}(x) = 0 \\ \frac{d}{dx} y_3^{(0)}(x) + \frac{2}{x} y_3^{(0)}(x) + \left(\lambda_0 - 1 + \frac{\alpha}{x} \right) y_1^{(0)}(x) = 0 \end{aligned} \quad (\text{C.5})$$

in which we obviously recognize the Dirac equation for $j = 0$. The solution of the system has therefore the well-known expressions [19],

$$\begin{aligned} y_1^{(0)}(x) = N_0 \sqrt{1 + \lambda_0} e^{-\frac{\xi}{2}} \xi^{\sqrt{1 - \alpha^2} - 1} ({}_1F_1(a, b, \xi) + A {}_1F_1(a + 1, b, \xi)) \\ y_3^{(0)}(x) = -N_0 \sqrt{-\lambda_0 + 1} e^{-\frac{\xi}{2}} \xi^{\sqrt{1 - \alpha^2} - 1} ({}_1F_1(a, b, \xi) - A {}_1F_1(a + 1, b, \xi)) \end{aligned} \quad (\text{C.6})$$

where

$$\xi = 2\sqrt{1 - \lambda_0^2}x, \quad A = \frac{\sqrt{1 - \alpha^2}\sqrt{1 - \lambda_0^2} - \lambda_0\alpha}{\alpha + \sqrt{1 - \lambda_0^2}} \quad (\text{C.7})$$

while the parameters of the confluent hypergeometric functions are

$$a = \sqrt{1 - \alpha^2} - \frac{\lambda_0\alpha}{\sqrt{1 - \lambda_0^2}}, \quad b = 1 + 2\sqrt{1 - \alpha^2}. \quad (\text{C.8})$$

Finally N_0 is the normalizing constant that obviously makes sense only when assuming the spectral condition

$$\lambda_0 = \left(1 + \frac{\alpha^2}{(n + \sqrt{1 - \alpha^2})^2}\right)^{-\frac{1}{2}} \quad (\text{C.9})$$

with integer n . Letting

$$\lambda_0 = 1 + \alpha^2 w_0, \quad (\text{C.10})$$

the value for the ground state of the Dirac equation is $w_0 = -0.500\,006\,6566$.

We now switch the perturbative machine on. In the first place we observe that, according to (C.2), the functions $\phi^{(0)}(x)$ and $\theta^{(0)}(x)$ are just obtained by the product with the limiting value of the rescaled multiplicative factor, i.e. $x^{-1}(1 + \lambda_0 + \alpha/x)^{1/2}$. In particular, $\phi^{(0)}(x)$ solves the second-order equation

$$\frac{d^2}{dx^2}\phi^{(0)}(x) - \left(\frac{x^2 - (x\lambda_0 + \alpha)^2}{x^2} + \frac{3}{4}\frac{\alpha^2}{(x + x\lambda_0 + \alpha)^2x^2}\right)\phi^{(0)}(x) = 0. \quad (\text{C.11})$$

We then go to the linear terms in the expansion parameter ϵ and, after some simple calculations, we find a second-order equation in $\phi_1(x)$ involving λ_1 and the zeroth-order quantities. As it should be, according to the standard scheme of perturbation theory, the second-order self-adjoint operator acting on $\phi_1(x)$ is the same as the one acting on $\phi_0(x)$ in the zeroth-order equation (C.11). Indeed:

$$\begin{aligned} &\frac{d^2}{dx^2}\phi^{(1)}(x) - \left(\frac{x^2 - (x\lambda_0 + \alpha)^2}{x^2} + \frac{3}{4}\frac{\alpha^2}{(x + x\lambda_0 + \alpha)^2x^2}\right)\phi^{(1)}(x) \\ &\quad - \left[\frac{1}{x^3}\left(\frac{(3x + x\lambda_0 + \alpha)^2}{4} - 2x(x + x\lambda_0 + \alpha) - x^2\lambda_1\right)(x + x\lambda_0 + \alpha)\phi^{(0)}(x) \right. \\ &\quad + \left(\lambda_1 - \frac{(x + x\lambda_0 + \alpha)^2}{4x^2}\right)\frac{d}{dx}\theta^{(0)}(x) + \left(\lambda_1\left(\frac{\alpha}{2x(x + x\lambda_0 + \alpha)} + \frac{1}{x}\right) \right. \\ &\quad \left. \left. - \frac{1}{8x^3}(x + x\lambda_0 + \alpha)(-\alpha + 2x + 2x\lambda_0)\right)\theta^{(0)}(x)\right] = 0. \quad (\text{C.12}) \end{aligned}$$

Therefore the correction λ_1 can be calculated from equation (C.12) in the standard way: we take for $\phi_0(x)$ and $\theta_0(x)$ the solution obtained by (C.6) and the spectral condition, we multiply (C.12) by $\phi_0(x)$ and integrate the result from zero to infinity. Letting then $\lambda_1 = \alpha^2 w_1$ and carrying over the numerical calculations we have indicated, we obtain the value $w_1 = 0.232\,995 \times 10^{-4}$, so that the correction to the ground state of hydrogen results in $(1 - \rho_H)w_1 = 0.253\,509 \times 10^{-7}$. This result is in excellent agreement with what is found from the numerical integration, as presented in section 6. When applied to muonium [2], where we have $(1 - \rho_{\text{muonium}}) = 0.009\,6261$, the correction would amount to $0.224\,28 \times 10^{-6}$.

Appendix D. The numerical scheme

We outline the numerical methods used to integrate the even and odd fourth-order differential systems and to find the spectrum. For the numerical treatment we have rewritten the mass parameters in the systems according to the definitions (5.1) and (5.3) and we have adopted the independent variable $x = m_e r$.

As a first remark, we see that both systems are singular at zero and infinity. Therefore, in order to start the numerical integration, the appropriate asymptotic solutions at the two singular points must be determined by the appropriate developments. We report here and elsewhere on some further details of these solutions. As a general feature, however, it turns out that among the four independent solutions that can be determined at each singular point, two of them are divergent and would produce not square-integrable wavefunctions, i.e. outside the Hilbert space where we want to solve the spectral problem. These solutions will therefore be rejected.

Once the two acceptable solutions in zero and infinity have been determined, the eigenvalue will be obtained by adapting to our problem the well-known ‘double shooting method’. More precisely, for each of the acceptable solutions both at zero and at infinity we start the numerical integration up to a chosen crossing point x_c . In x_c we impose the matching conditions for each component of the wavefunction. These give rise to the following linear system:

$$K_1 y_j^{(0,1)}(x_c) + K_2 y_j^{(0,2)}(x_c) = K_3 y_j^{(\infty,1)}(x_c) + K_4 y_j^{(\infty,2)}(x_c) \quad (\text{D.1})$$

where $j = 1, 4$. The first superscripts ‘0’ and ‘∞’ evidently refer to the singular point where the integration started, while the second subscripts ‘1’ and ‘2’ denote the solution chosen at each boundary. Being linear and homogeneous, the system (D.1) has non-trivial solutions in K_1, K_2, K_3 and K_4 provided its determinant is vanishing. The condition

$$\det \begin{pmatrix} y_1^{(0,1)}(x_c) & y_1^{(0,2)}(x_c) & y_1^{(\infty,1)}(x_c) & y_1^{(\infty,2)}(x_c) \\ y_2^{(0,1)}(x_c) & y_2^{(0,2)}(x_c) & y_2^{(\infty,1)}(x_c) & y_2^{(\infty,2)}(x_c) \\ y_3^{(0,1)}(x_c) & y_3^{(0,2)}(x_c) & y_3^{(\infty,1)}(x_c) & y_3^{(\infty,2)}(x_c) \\ y_4^{(0,1)}(x_c) & y_4^{(0,2)}(x_c) & y_4^{(\infty,1)}(x_c) & y_4^{(\infty,2)}(x_c) \end{pmatrix} = 0 \quad (\text{D.2})$$

gives therefore the equation that has to be solved in order to find the spectral values λ . Needless to say that when the system decouples into two separate second-order differential equations, no additional modification to the usual double shooting method is necessary and each equation has been solved independently.

We now describe the behaviour at the singular points of the two systems.

D.1. The behaviour at zero

We shall first consider the behaviour of the systems at the origin by expanding the equations of each system in a neighbourhood of $x = 0$. Accordingly, the solutions will be assumed of the form

$$y_i(x) = x^\nu \sum_{j=0}^N y_i^{(j)} x^j, \quad (i = 1, 4). \quad (\text{D.3})$$

The procedure is the standard one. We substitute (D.3) into the system (4.7) and take the different orders in x . The lowest order gives the indicial equations that produce four different values for the exponent ν , only two of which are acceptable. In correspondence to the indices,

some relations for the $y_i^{(0)}$ are established. It also turns out that the indices are equal both for the even and the odd systems. We have a first index

$$\nu_1 = -1 + \sqrt{1 - \frac{\alpha^2}{4} + j(1+j)} \quad (\text{D.4})$$

with corresponding relations

$$y_1^{(0)} = 1, \quad y_3^{(0)} = \frac{2}{\alpha}\nu_1, \quad y_2^{(0)} = y_4^{(0)} = 0 \quad (\text{D.5})$$

and a second index (only for $j > 0$)

$$\nu_2 = -1 + \sqrt{j(1+j) - \frac{\alpha^2}{4}} \quad (\text{D.6})$$

for which

$$y_1^{(0)} = y_3^{(0)} = 0, \quad y_2^{(0)} = 1, \quad y_4^{(0)} = -\frac{2}{\alpha}(1 + \nu_2). \quad (\text{D.7})$$

The corresponding (very cumbersome) series have been calculated formally up to the eighth order and have been tested by substitution in the differential equations with the help of a symbolic computer package. They have also been tested numerically, with physical values of the parameters and varying value of the coordinate x . In addition, this procedure has furnished an effective criterion for choosing the boundary point near zero: in fact we have assumed as acceptable a value of x where the ratio of the differential equation evaluated on the solution over the solution itself was at most of the order of 10^{-12} .

D.2. The behaviour at infinity

In order to determine the solutions in the neighbourhood of infinity, we consider the following asymptotic expansion for the components of the solution must be looked for in the form (see [27])

$$y_i(x) = e^{-\gamma x} x^\nu \sum_{j=0}^N y_i^{(j)} x^{-j} \quad (i = 1, 4). \quad (\text{D.8})$$

Contrary to what occurs at zero, also the indices of the asymptotic expansion depend upon the eigenvalue λ . At the lowest order, indeed, we find

$$\gamma^2 = \frac{1 + \rho^2}{(1 - \rho)^2} - \frac{\lambda^2}{4} - \frac{4\rho^2}{\lambda^2(1 - \rho)^4} \quad (\text{D.9})$$

and we shall take the positive square root to ensure the convergence. The next order determines the exponent ν , given by

$$\nu = -1 + \frac{1}{2\gamma} \left(\frac{\alpha\lambda}{2} - \frac{8\rho^2\alpha}{h^3(1 - \rho)^4} \right). \quad (\text{D.10})$$

The different choices of the two coefficients $y_1^{(0)}$ and $y_2^{(0)}$ then determine two different series and therefore two linearly independent asymptotic solutions of the system.

D.3. The wavefunction

Once the spectrum has been found, we can proceed to determine the wavefunction. If λ_* is one of the spectral values, then, in the system (D.1) we can fix one of the four parameters K_i

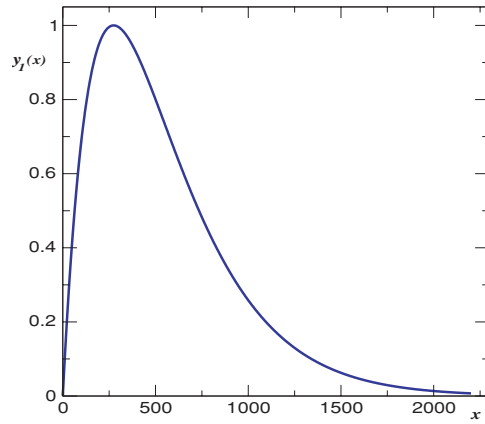


Figure 3. The first component of the wavefunction of the Coulomb hydrogen atom for the $w_{+,j=1,1}$ state.

to unity and solve for the remaining ones. For instance, for the hydrogen atom and the $2p_{1/2}$ state of the Dirac spectroscopy, for which $\lambda_* = -0.125\,002\,0774$, we find

$$K_1 = 40.266\,673\,71, \quad K_2 = 0.630\,449\,1167, \quad K_3 = 0.707\,106\,6401, \quad K_4 = 1. \quad (\text{D.11})$$

Therefore the complete wavefunction will result in

$$\begin{aligned} y_j(x) &= K_1 y_j^{(0,1)}(x) + K_2 y_j^{(0,2)}(x), & \text{for } x < x_c \\ &= K_3 y_j^{(\infty,1)}(x) + K_4 y_j^{(\infty,2)}(x), & \text{for } x > x_c. \end{aligned} \quad (\text{D.12})$$

The plot of $y_1(x)$ is given in figure 3.

Appendix E. The ground-state wavefunctions of parapositronium and orthopositronium

In this appendix we give some details on the two wavefunctions of the ground state of parapositronium and orthopositronium corresponding to the states $w_{+,j=0,1}$ and $w_{-,j=1,1}$, degenerate in energy. We finally comment on the calculation of the hyperfine splitting of the positronium ground level.

E.1. Parapositronium

The case of parapositronium, namely the state with even parity, is comparatively easy, since it can be solved by discussing the single second-order differential equation (4.13a) for the Coulomb potential, with $\rho = 0$ and $j = 0$. Its explicit form reads

$$\frac{d^2}{dx^2} y_1(x) + \left(\frac{2}{x} + \frac{2\alpha}{x((4+w\alpha^2)x+2\alpha)} \right) \frac{d}{dx} y_1(x) + \left(\frac{((4+w\alpha^2)x+2\alpha)^2}{16x^2} - 1 \right) y_1(x). \quad (\text{E.1})$$

Zero and infinity are the two singular points of this equation. At infinity there is a divergent solution and a convergent solution, so that the latter will be assumed. At zero both solutions are divergent, and only one of them, the solution we shall accept, is normalizable. The regular solution at zero has the following expansion:

$$y_1(x) \underset{x \rightarrow 0}{\simeq} A x^{(-1+\frac{\sqrt{4-\alpha^2}}{2})} \left(1 - \frac{(\alpha^2+2-\sqrt{4-\alpha^2})(4+w\alpha^2)}{\alpha(4\sqrt{4-\alpha^2}+4)} x \right), \quad (\text{E.2})$$

where A is an arbitrary integration constant.

The asymptotic behaviour of the solution by taking the dominant term of (E.1), at infinity. The solution of the corresponding asymptotic equation reads

$$y_1(x) \underset{x \rightarrow \infty}{\simeq} B \exp \left(-\frac{\alpha}{2} \sqrt{-w} \sqrt{2 + w \frac{\alpha^2}{4} x} \right) \quad (\text{E.3})$$

where B is an arbitrary integration constant. However, to calculate a better approximation to the asymptotic boundary conditions we can take the expansion of (E.1) up to terms of order x^{-2} . In fact the resulting equation can be exactly solved in terms of Whittaker M and W functions. Up to the usual integration constant we can fix equal to unity, the solution with regular behaviour at infinity is

$$y_1(x) \underset{x \rightarrow \infty}{\simeq} \frac{\sqrt{(4 + w\alpha^2)x + 2\alpha}}{x^{3/2}} W \left(\frac{4 + w\alpha^2}{2\sqrt{-w}\sqrt{w\alpha^2 + 8}}, \frac{\sqrt{1 - \alpha^2}}{2}, \frac{\alpha\sqrt{-w}\sqrt{w\alpha^2 + 8}}{2} x \right). \quad (\text{E.4})$$

Once the boundary behaviour is established, the wavefunction component $y_1(x)$ and its first derivative $y_1'(x)$ are computed by standard numerical integration. Finally, in order to determine the complete 16 component wavefunction, we only have to calculate the eight coefficient functions $a_i(x)$, $b_i(x)$, $c_i(x)$ and $d_i(x)$, $i = 0, 1$, in terms of $y_1(x)$ and its first derivative $y_1'(x)$. Recalling that $y_2(x) = 0$, and that from (4.7) and (4.8) we have

$$y_3(x) = \frac{2xy_1'(x)}{\alpha + x(4 + w\alpha^2)} \quad (\text{E.5})$$

simple substitutions lead to the following expressions:

$$\begin{aligned} a_0(x) &= \left(\frac{1}{2} + \frac{2x}{x(4 + w\alpha^2) + 2\alpha} \right) y_1(x), & a_1(x) &= \left(\frac{1}{2} - \frac{2x}{x(4 + w\alpha^2) + 2\alpha} \right) y_1(x), \\ b_0(x) &= b_1(x) = c_0(x) = c_1(x) = 0, & d_0(x) &= d_1(x) = \frac{1}{2} y_3(x). \end{aligned} \quad (\text{E.6})$$

The components $y_1(x)$ and $y_3(x)$ are respectively represented in the first plot of figure 4.

E.2. Orthopositronium

Let us then consider the wavefunction for the odd state. The system to be discussed is now given by (4.7), (4.8) and (4.11) with $\rho = 0$ and $j = 1$. Considering the series expansion at the origin, we see that we have two regular solutions with indices

$$\nu_1 = \sqrt{3 - \frac{\alpha^2}{4}} - 1, \quad \nu_2 = \sqrt{2 - \frac{\alpha^2}{4}} - 1. \quad (\text{E.7})$$

On the other hand, the asymptotic expansion then gives solutions presenting the exponential decrease

$$\exp \left(-\frac{\alpha}{2} \sqrt{-w} \sqrt{2 + w \frac{\alpha^2}{4} x} \right), \quad (\text{E.8})$$

exactly the same as for parapositronium.

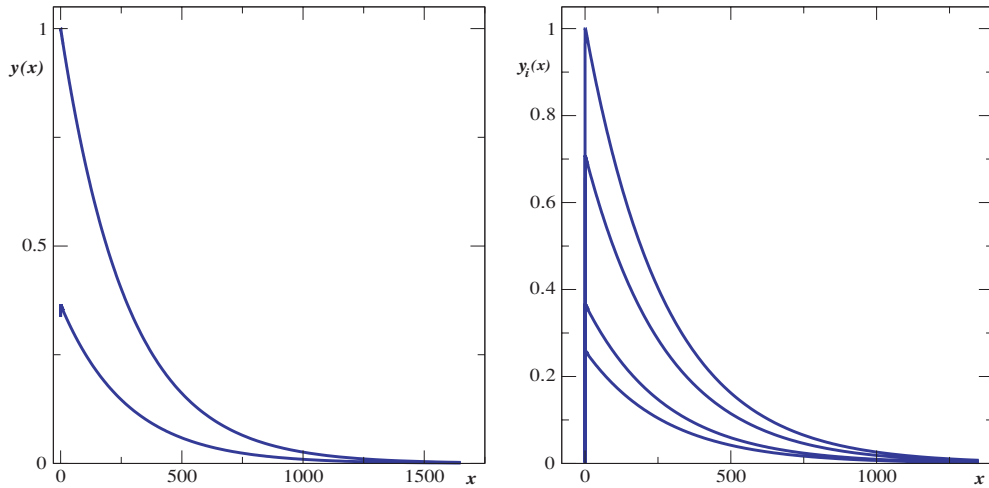


Figure 4. Left: the components of the ground state of parapositronium: $y_1(x)$ (upper) and $-200y_3(x)$ (lower). Right: the four components of the ground state wavefunction of orthopositronium: from top to bottom: $-y_4(x)$, $-y_3(x)$, $100y_2(x)$ and $-100y_1(x)$.

By applying the matching procedures described in appendix D.3 we find the four components $y_i(x)$. They are given in the second plot of figure 4.

Letting S be the matrix

$$S = \frac{2\sqrt{6}}{(4 + \alpha^2 w)x + 2\alpha} \begin{pmatrix} -\sqrt{2} & 1 & -\frac{(8 + \alpha^2 w)x + 2\alpha}{4\sqrt{2}} & -\frac{(8 + \alpha^2 w)x + 2\alpha}{4} \\ -\sqrt{2} & -1 & -\frac{\alpha}{4\sqrt{2}}(2 + \alpha w)x & \frac{\alpha}{4}(2 + \alpha w)x \\ -1 & -\sqrt{2} & \frac{(8 + \alpha^2 w)x + 2\alpha}{4} & \frac{(8 + \alpha^2 w)x + 2\alpha}{4\sqrt{2}} \\ -1 & \sqrt{2} & \frac{\alpha}{4}(2 + \alpha w)x & \frac{\alpha}{4\sqrt{2}}(2 + \alpha w)x \end{pmatrix} \quad (E.9)$$

the explicit relationships among the four components $y_k(x)$ and the eight coefficients of the complete state vector, $a_i(x)$, $b_i(x)$, $c_i(x)$, $d_i(x)$, $i = 0, 1$ are the following:

$$a_0(x) = a_1(x) = \frac{1}{2}y_1(x), \quad b_0(x) = -b_1(x) = \frac{1}{2}y_2(x) \quad (E.10)$$

and

$${}^t(c_0(x), c_1(x), d_0(x), d_1(x)) = S^t(y_1(x), y_2(x), y_3(x), y_4(x)). \quad (E.11)$$

E.3. The non-relativistic limit

In order to have a better insight into the solutions of the para- and orthopositronium ground states, we find it useful to look at the Schrödinger limit of the relativistic system and to show how the usual equations for the Coulomb problem are recovered.

In addition to the obvious substitutions $\mu = 0$ and $M = 2m_e$, the non-relativistic limit on the system (4.7) and (4.8) needs the use of the ‘atomic parameters’. This means that we have

to adopt the following rescaling for the independent variable and for the eigenvalue:

$$r = \frac{2z}{m_e \alpha}, \quad \lambda = 2m_e \left(1 + \frac{\alpha^2 w}{4} \right). \quad (\text{E.12})$$

As already noted in (4.1), when dealing with the even problem and assuming the coefficient functions (4.11), the system (4.7) and (4.8) decouples into two separate subsystems, the first one for $y_1(z)$ and $y_3(z)$, the second for $y_2(z)$ and $y_4(z)$. Thus, isolating $y_3(z)$,

$$y_3(z) = \frac{2\alpha z}{4z + z\alpha^2 w + \alpha^2} \frac{d}{dz} y_1(z), \quad (\text{E.13})$$

substituting it into the equation for $y_1(z)$ and taking the limit $\alpha \rightarrow 0$, we find

$$\frac{d^2}{dz^2} y_1(z) + \frac{2}{z} \frac{d}{dz} y_1(z) + \left(2w + \frac{2}{z} - \frac{j(j+1)}{z^2} \right) y_1(z) = 0, \quad (\text{E.14})$$

in which we recognize the usual $\ell = j$ radial Coulomb equation, that gives the well-known exponential solution $y_1(z) = \exp(-z)$, when $j = 0$ and $w = -1/2$. The analogous treatment for the second subsystem leads to exactly the same result.

For the odd case, assuming the coefficients (4.14), the system resulting from (4.7) and (4.8) does not decouple: as a consequence the treatment is just a little bit more technically complicated. In order to determine the non-relativistic limit we have to look for the equations satisfied by the ‘large’ components of the wavefunction. As shown in figure 4, they are $y_3(z)$ and $y_4(z)$. Therefore, after changing to the atomic variables, we isolate $y_1(z)$ and $y_2(z)$ from the last two equations of the system and we substitute the results in the first two. Taking the limit for $\alpha \rightarrow 0$, we get the following system of two coupled second-order differential equations:

$$\begin{aligned} \frac{d^2}{dz^2} y_3(z) + \frac{2}{z} \frac{d}{dz} y_3(z) + \left(2w + \frac{2}{z^2} - \frac{j(j+1)+2}{z^2} \right) y_3(z) + \frac{2}{z^2} \sqrt{j(j+1)} y_4(z) &= 0 \\ \frac{d^2}{dz^2} y_4(z) + \frac{2}{z} \frac{d}{dz} y_4(z) + \left(2w + \frac{2}{z^2} - \frac{j(j+1)}{z^2} \right) y_4(z) + \frac{2}{z^2} \sqrt{j(j+1)} y_3(z) &= 0. \end{aligned} \quad (\text{E.15})$$

The differential operators of both equations of (E.15) coincide. The matrix of the non-differentiated terms

$$\begin{bmatrix} 2w + \frac{2}{z} - \frac{j(j+1)+2}{z^2} & 2\sqrt{j(j+1)} \\ 2\sqrt{j(j+1)} & 2w + \frac{2}{z} - \frac{j(j+1)}{z^2} \end{bmatrix} \quad (\text{E.16})$$

is diagonalized by the constant matrix

$$T = \begin{bmatrix} \sqrt{j+1} & \sqrt{j} \\ -\sqrt{j} & \sqrt{j+1} \end{bmatrix}. \quad (\text{E.17})$$

Therefore, letting ${}^t(\varphi_1(z), \varphi_2(z)) = (T^{-1}){}^t(y_1(z), y_2(z))$ we obtain the two decoupled equations

$$\begin{aligned} \frac{d^2}{dz^2} \varphi_1(z) + \frac{2}{z} \frac{d}{dz} \varphi_1(z) + \left(2w + \frac{2}{z} - \frac{(j+1)(j+2)}{z^2} \right) \varphi_1(z) &= 0, \\ \frac{d^2}{dz^2} \varphi_2(z) + \frac{2}{z} \frac{d}{dz} \varphi_2(z) + \left(2w + \frac{2}{z} - \frac{j(j-1)}{z^2} \right) \varphi_2(z) &= 0, \end{aligned} \quad (\text{E.18})$$

corresponding to the radial Coulomb equations with $\ell = j+1$ and $\ell = j-1$.

E.4. Some considerations on the hyperfine shifts

Comparing the limiting classical wavefunctions with the results reported in figure 4, it appears that the relativistic corrections become weaker and weaker for large z , as expected by obvious physical reasons. Near zero the bare Coulomb potential is no longer sufficient for an accurate description of the system and, as observed also in case of the Lamb shift, the radiative corrections due to the self-energy and to the vacuum polarization should be accounted for. The length that, on a physical basis, can be assumed as a scale for the relevance of the mentioned relativistic effects is the Compton wavelength of the electron λ_e : it is interesting to remark that the sharp maximum of all the components of orthopositronium occurs approximately at $(\sqrt{2}/2)\lambda_e$.

These considerations can be brought to bear for a possible evaluation of the hyperfine shift of the ground states of para- and orthopositronium. Indeed the usual and very successful derivation of the shifts of the two ground levels is done by a perturbative method in a non-relativistic approximation. Of course, in view of the discussion of the previous subsection, we are able to obtain exactly the same results if we adopt the non-relativistic approximation and the same expressions for the spin–spin interaction and for the annihilation energy term. The latter are derived as effective potentials from a low momentum expansion of the one-photon exchange Feynman diagram [23], and the value of the hyperfine shifts of the ground levels are produced by the sum of two different contributions. The first one is the average of $4\pi\mu_0^2(7\mathbf{S}^2/3 - 2)\delta(\mathbf{r})$ and therefore implies the evaluation of the classical Coulomb wavefunction at zero, as in the original Fermi calculation [28]. This approach cannot be directly used with the wavefunction we have produced, since the relativistic effects naturally lead to a drastic modification of behaviour just at the origin. The averaging over the angles of the other term, $6\mu_0^2((\mathbf{S}\mathbf{r})(\mathbf{S}\mathbf{r})/r^5 - \mathbf{S}^2/3r^3)$, giving a rigorously vanishing value in the non-relativistic limit, is now negligible only for large values of r as expected, but it is divergent at the origin, even after the radial measure r^2 has been accounted for. One could try to determine a phenomenological value of the radial coordinate where to put a kind of cut-off both for the evaluation of the wavefunctions and for the integrations as well. However, in order to use the relativistic quantum mechanics for calculating the hyperfine splitting, we believe it would be much more appealing to deduce an effective interaction potential without assuming a low momentum approximation and including radiative corrections. These ideas will be developed elsewhere.

References

- [1] Kragh H 1984 *Am. J. Phys.* **52** 1024
- [2] Jungmann K P 1998 *Preprint physics/9809020*
- [3] Häckl R, Hund V and Pilkuhn H 1998 *Phys. Rev. A* **57** 3268
- [4] Mangin-Brinet M, Carbonell J and Karmanov V A 2003 *Phys. Rev. C* **68** 055203
- [5] Crater H and Liu B 2003 *Phys. Rev. C* **67** 024001
- [6] Crater H and Van Alstine P 2004 *Phys. Rev. D* **70** 034026
- [7] Shuryak E V and Zahed I 2004 *Preprint hep-ph/0403127*
- [8] Childers R W 1982 *Phys. Rev. D* **26** 2902
- [9] Scott T C, Shertzer J and Moore R A 1992 *Phys. Rev. A* **45** 4393
- [10] Darewych J W and Di Leo L 1996 *J. Phys. A: Math. Gen.* **29** 6817
Darewych J W and Duvirak A 2002 *Preprint nucl-th/0204006*
- [11] Goffrey S and Isgur N 1985 *Phys. Rev. D* **32** 189
- [12] Ricken R, Koll M, Metsch B Ch and Petry H R 2000 *Eur. Phys. J. A* **9** 221
- [13] Polyzou W N 2002 *J. Math. Phys.* **43** 6024
- [14] Giachetti R and Sorace E 1981 *Nuovo Cimento B* **63** 666
- [15] Sorace E and Tarlini M 1982 *Nuovo Cimento B* **71** 98

- Sorace E and Tarlini M 1982 *Lett. Nuovo Cimento* **35** 1
Sorace E 2002 *Ann. H Poincaré* **3** 659
- [16] Giachetti R, Ragionieri R and Ricci R 1981 *J. Diff. Geom.* **16** 297
Giachetti R and Ricci R 1986 *Adv. Math.* **62** 84
For quantization of anticommuting variables see references in Barducci A and Giachetti R 2003 *J. Phys. A: Math. Gen* **36** 8129
- [17] Giachetti R 1981 Hamiltonian systems with symmetry: an introduction *Riv. Nuovo Cimento* **4** 1
- [18] Bakamjian B and Thomas L H 1953 *Phys. Rev.* **92** 1300
- [19] Landau L and Lifschitz L 1970 *Théorie des Champs* (Moscow: MIR)
- [20] Longhi G and Lusanna L 1986 *Phys. Rev. D* **34** 3707
- [21] Vugalter S and Wiedl T 2003 *Ann. H Poincaré* **4** 301
- [22] Ince E L 1956 *Ordinary Differential Equations* (New York: Dover)
- [23] Landau L and Lifschitz L 1972 *Théorie Quantique Relativiste* (Moscow: MIR)
Thaller B 1992 *The Dirac Equation* (Berlin: Springer)
Yndurain F J 1996 *Relativistic Quantum Mechanics and Introduction to Field Theory* (Berlin: Springer)
- [24] Dunford N and Schwartz J 1963 *Linear Operators: Part II* (New York: Wiley)
- [25] Breit G 1930 *Phys. Rev.* **36** 383
- [26] Feldman G, Fulton T and Townsend J 1973 *Phys. Rev. A* **8** 1149
- [27] Cope F T 1934 *Am. J. Math.* **56** 411
Cope F T 1936 *Am. J. Math.* **58** 130
- [28] Fermi E 1930 *Z. Phys.* **60** 320