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Autor(en): **Reuse, F.**

Objektyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **53 (1980)**

Heft 4

PDF erstellt am: **13.09.2024**

Persistenter Link: <https://doi.org/10.5169/seals-115138>

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A relativistic two-body model for hydrogen-like and positronium-like systems II

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(20. VIII. 1980; rev. 12. XII. 1980)

Abstract. This paper is devoted to a generalization of a relativistic two-body model previously formulated in the spin-free approximation. New terms have been introduced for the description of the spin interactions. Except for fixed physical constants like masses, charges and gyromagnetic factors for both particles, our interaction terms contain two dimensionless parameters $h_{(1)}$ and $h_{(2)}$, one for each particle.

The resulting fine and hyperfine structures are evaluated up to contributions of order α^4 , for arbitrary mass ratio. In the particular case of the hydrogen atom, for $h_{e-} = 1.048$, the model predicts the correct fine and hyperfine structures of the hydrogen spectrum, (including the Lamb shifts). On the other hand, the fine and hyperfine structures of the positronium are obtained, taking for $h_{e-} = h_{e+}$ the values 1.048, as in the hydrogen atom.

1. A two body model for interacting spin $-\frac{1}{2}$ particles

The two body model of hydrogen-like systems described in part one [1], did not account the interactions due to the spins. We now generalize the above model to a more realistic situation where the spins interact with the electromagnetic field, giving rise to the so-called fine and hyperfine structure of the spectra.

Essentially this generalization is incorporated into the same scheme as in [1]. According to [1] we again postulate the equality $n_{(1)}^\mu = n_{(2)}^\mu \equiv n^\mu$ for the bound states of the system. We then write a self adjoint operator K_n (on the Hilbert space $H_n \otimes H_n$) which differs from the one given in (I17)³⁾ by some new covariant terms including spin operators. The construction of the new evolution operator K_n that we propose is based upon the following assumption. First, each particle interacts with the field produced by the other. Second this interaction is described by terms of the same form as the one given in (I12) for a particle interacting with an external field.

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³⁾ This notation means formula (17) of [I].

More precisely we propose the following evolution operator (with q^μ standing for $q_{(2)}^\mu - q_{(1)}^\mu$)

$$\begin{aligned}
 K_n = & \frac{1}{2M_{(1)}} g^{\mu\nu} (p_{(1)\mu} - \mathcal{A}_{(1)\mu}(-q))(p_{(1)\nu} - \mathcal{A}_{(1)\nu}(-q)) \\
 & - \frac{g_{(1)}\mu_{(1)}}{2M_{(1)}c^2} (p_{(1)\mu} - \mathcal{A}_{(1)\mu}(-q))\tilde{F}_{(1)\nu}^\mu(-q)W_{(1)}^\nu \\
 & + \frac{h_{(1)}^2\mu_{(1)}^2}{8M_{(1)}c^4} F_{(1)\mu\nu}(-q)n^\nu F_{(1)\rho}^\mu(-q)n^\rho \\
 & + \frac{1}{2M_{(2)}} g^{\mu\nu} (p_{(2)\mu} - \mathcal{A}_{(2)\mu}(q))(p_{(2)\nu} - \mathcal{A}_{(2)\nu}(q)) \\
 & - \frac{g_{(2)}\mu_{(2)}}{2M_{(2)}c^2} (p_{(2)\mu} - \mathcal{A}_{(2)\mu}(q))\tilde{F}_{(2)\nu}^\mu(q)W_{(2)}^\nu \\
 & + \frac{h_{(2)}^2\mu_{(2)}^2}{8M_{(2)}c^4} F_{(2)\mu\nu}(q)n^\nu F_{(2)\rho}^\mu(q)n^\rho
 \end{aligned} \tag{1}$$

Where e , $M_{(1)}$, $\mu_{(1)} = e\hbar/2M_{(1)}$ and $(-e)$, $M_{(2)}$, $\mu_{(2)} = (-e)\hbar/2M_{(2)}$ respectively denote the charges, the masses and the Bohr magnetons of the particles (1) and (2). Moreover $g_{(1)}$ and $g_{(2)}$ denote their gyromagnetic factors and $h_{(1)}$, $h_{(2)}$ are dimensionless phenomenological constants.

In this expression $\mathcal{A}_{(1)\mu}(-x) \equiv \mathcal{A}_{(1)\mu}(x_{(1)} - x_{(2)})$ (resp. $\mathcal{A}_{(2)\mu}(x) \equiv \mathcal{A}_{(2)\mu}(x_{(2)} - x_{(1)})$) denotes the effective 4-potential as seen by particle (1) (respectively (2)), associated with the 4-vector potential $A_{(1)\mu}(-x) \equiv A_{(1)\mu}(x_{(1)} - x_{(2)})$ (resp. $A_{(2)\mu}(x) \equiv A_{(2)\mu}(x_{(2)} - x_{(1)})$) created by particle (2) (resp. (1)). Similarly $F_{(1)\mu\nu}(-x)$ (resp. $F_{(2)\mu\nu}(x)$) are the corresponding electromagnetic field tensors:

$$F_{(i)\mu\nu}(x_{(i)} - x_{(j)}) = \frac{\partial A_{(i)\nu}(x_{(i)} - x_{(j)})}{\partial x_{(i)}^\mu} - \frac{\partial A_{(i)\mu}(x_{(i)} - x_{(j)})}{\partial x_{(i)}^\nu}, \quad (i, j) = (1, 2), (2, 1) \tag{2}$$

Finally the dual field tensors are given by

$$\tilde{F}_{(i)\mu\nu} = -\frac{c^2}{2} \epsilon_{\mu\nu}{}^{\rho\lambda} F_{(i)\rho\lambda}, \quad i = 1, 2 \tag{3}$$

The expression for $A_{(1)\mu}(x_{(1)} - x_{(2)})$ and $A_{(2)\mu}(x_{(2)} - x_{(1)})$ are suggested by the following classical considerations. The 4-vector potential $A_\mu(x)$ corresponding to a classical particle of charge e and magnetic moment M^μ whose motion is uniform and in the direction n^μ (suppose $q^\mu(\tau) = n^\mu\tau$), is given by

$$A_\mu(x) = \frac{e}{4\pi\epsilon_0 c^2} \frac{n_\mu}{d(n, x)} + \frac{1}{4\pi\epsilon_0 c^2} \tilde{f}_{\mu\nu}(n, x) M^\nu$$

where $d(n, x)$ is defined in (I18) and where $\tilde{f}_{\mu\nu}(n, x)$ stands for

$$\frac{\epsilon_{\mu\nu\rho\lambda} x^\rho n^\lambda}{d^3(n, x)}$$

This expression $A_\mu(x)$ can be found by considering the case $n = n_0 = (0, 0, 0, 1)$. We then have

$$A_\mu(x) \equiv (\mathbf{A}(x), -V(x)) = \left(\frac{1}{4\pi\epsilon_0 c^2} \frac{\mathbf{M} \wedge \mathbf{x}}{|\mathbf{x}|^3}, -\frac{e}{4\pi\epsilon_0} \frac{1}{|\mathbf{x}|} \right)$$

which is a well known result. The above 4-vector field verifies the Lorentz gauge condition $\partial_\mu A^\mu(x) \equiv 0$ because

$$\partial^\mu d(n, x) = \frac{x^\mu + n^\mu (n_\nu x^\nu)/c^2}{d(n, x)}$$

and thus

$$\partial^\mu \tilde{f}_{\mu\nu}(n, x) \equiv 0$$

In view of the previous results where n^μ plays the role of a 4-velocity and as regards to the evolution properties of n in our model, we propose the following expression for $A_{(2)\mu}(q_{(2)} - q_{(1)}) \equiv A_{(2)\mu}(q)$, the 4-vector field as seen by the particle (2) and created by the particle (1) of charge e and magnetic moment $g_{(1)}\mu_{(1)} W_{(1)}^\mu$:

$$A_{(2)\mu}(q) = \frac{e}{4\pi\epsilon_0 c^2} \frac{n_\nu}{d(n, q)} + \frac{g_{(1)}\mu_{(1)}}{4\pi\epsilon_0 c^2} \tilde{f}_{\mu\nu}(n, q) W_{(1)}^\nu \quad (4)$$

Analogously for $A_{(1)\mu}(q_{(1)} - q_{(2)}) \equiv A_{(1)\mu}(-q)$, the 4-vector field as seen by the particle (1) and created by the particle (2) of charge $-e$ and magnetic moment $g_{(2)}\mu_{(2)} W_{(2)}^\mu$, we find

$$A_{(1)\mu}(-q) = \frac{-e}{4\pi\epsilon_0 c^2} \frac{n_\mu}{d(n, q)} - \frac{g_{(2)}\mu_{(2)}}{4\pi\epsilon_0 c^2} \tilde{f}_{\mu\nu}(n, q) W_{(2)}^\nu \quad (5)$$

In other words, in this model, the usual dependence of the field on the particle velocity is replaced by a dependence on the corresponding mean value which is precisely given by n^μ .

Finally, in view of the expressions (5) and (4) for $A_{(1)\mu}(-q)$ and $A_{(2)\mu}(q)$ and according to (I17), we propose the following expressions for the effective 4-potentials $\mathcal{A}_{(1)\mu}(-q)$ and $\mathcal{A}_{(2)\mu}(q)$

$$\mathcal{A}_{(1)\mu}(-q) = e \left\{ \lambda_{(1)} \frac{-e}{4\pi\epsilon_0 c^2} \frac{n_\mu}{d(n, q)} - \frac{g_{(2)}\mu_{(2)}}{4\pi\epsilon_0 c^2} \tilde{f}_{\mu\nu}(n, q) W_{(2)}^\nu \right\} \quad (6)$$

and similarly

$$\mathcal{A}_{(2)\mu}(q) = -e \left\{ \lambda_{(2)} \frac{e}{4\pi\epsilon_0 c^2} \frac{n_\mu}{d(n, q)} + \frac{g_{(1)}\mu_{(1)}}{4\pi\epsilon_0 c^2} \tilde{f}_{\mu\nu}(n, q) W_{(1)}^\nu \right\} \quad (7)$$

where the values of $\lambda_{(1)}$ and $\lambda_{(2)}$ are given by (I60).

At this point, the general expression (1) of K_n and the definitions (4), (5), (6) and (7) completely define the model (via (2) and (3)).

The energy spectrum associated to the bound states of the system has to be calculated in a perfectly similar way as in [1]. Let us recall that in [1] we had been led, as a first step, to an eigenvalue problem (see (I38)) which, in a formal way, looked like a non-relativistic bound state problem for a particle in an external

potential. (Actually, in (I38) we had directly written the corresponding radial equation).

Presently we also will be led, in a first step of the evaluation of the spectrum, to a non-relativistic bound state problem as above, i.e. to an eigenvalue problem, relatively to a "fictitious hamiltonian" (depending on the energy W). The expression of this "hamiltonian" is given by (23) and by (21) and (22). To determine the expressions (21) and (22) we first have to develop the explicit expression of K_n obtained from (1), taking into account the explicit forms of $A_{(i)\mu}$, $\mathcal{A}_{(i)\mu\nu}$, $F_{(i)\mu\nu}$ and $\tilde{F}_{(i)\mu\nu}$ obtained from (4), (5), (6) and (7) via (2) and (3).

This is a straightforward calculation where (as in [1]) it is convenient to replace $p_{(1)\mu}$ and $p_{(2)\mu}$ by their expression in terms of the total and relative energy momentum P_μ and p_μ as defined in (I20) and (I22).

Such a calculation leads to K_n expressed as a sum of terms. In this sum we have to distinguish four kinds of terms. Grouping together the terms of the same kind, K_n may be written in the following way

$$K_n = K_n^{(0)} + K_n^{(1)} + K_n^{(2)} + K_n^{(3)} \tag{8}$$

where $K_n^{(0)}$ denotes the spin free evolution operator which has been considered in [1]. This operator reads

$$K_n^{(0)} = \frac{g^{\mu\nu}}{2M} \left(P_\mu + \alpha^2 m \frac{a_0 n_\mu}{d(n, q)} \right) \left(P_\nu + \alpha^2 m \frac{a_0 n_\nu}{d(n, q)} \right) + \frac{g^{\mu\nu}}{2m} \left(p_\mu + \lambda \alpha^2 m \frac{a_0 n_\mu}{d(n, q)} \right) \left(p_\nu + \lambda \alpha^2 m \frac{a_0 n_\nu}{d(n, q)} \right) \tag{9}$$

For convenience we have introduced the fine-structure constant $\alpha = e^2/4\pi\epsilon_0\hbar c$ and the Bohr radius $a_0 = 4\pi\epsilon_0\hbar^2/me^2$. On the other hand let us remember that $M = M_{(1)} + M_{(2)}$ denotes the total mass and $m = M_{(1)}M_{(2)}/M$ the reduced mass. Moreover, from (I60) $\lambda = \sqrt{1 - m/M}$, when $M_{(2)} \leq M_{(1)}$.

The operator $K_n^{(1)}$ denotes the terms of K_n which are of the type of a spin-orbit coupling. This operator reads

$$K_n^{(1)} = \frac{\alpha^4 mc^2}{2\hbar} a_0^3 \{ P^\mu \tilde{f}_{\mu\nu}(n, q) [G_{(1)}^{SO} W_{(1)}^\nu + G_{(2)}^{SO} W_{(2)}^\nu] + p^\mu \tilde{f}_{\mu\nu}(n, q) [g_{(1)}^{SO} W_{(1)}^\nu + g_{(2)}^{SO} W_{(2)}^\nu] \} \tag{10}$$

where

$$\left. \begin{aligned} G_{(1)}^{SO} &= \frac{g_{(1)}}{2} \frac{mM_{(2)}}{M^2}, & G_{(2)}^{SO} &= -\frac{g_{(2)}}{2} \frac{mM_{(1)}}{M^2} \\ \text{and} \\ g_{(1)}^{SO} &= \frac{g_{(1)}}{2} \frac{M_{(2)}(M + M_{(1)})}{M^2}, & g_{(2)}^{SO} &= \frac{g_{(2)}}{2} \frac{M_{(1)}(M + M_{(2)})}{M^2} \end{aligned} \right\} \tag{11}$$

(Note that for formal symmetry reasons we have factorized \hbar^{-1} in (11). Let us remember that $\hbar = \alpha m c a_0$.)

The operator $K_n^{(2)}$ groups the hyperfine structure like-term of K_n . We have:

$$K_n^{(2)} = \alpha^4 mc^2 \frac{m}{4M} \left\{ g_{(1)} g_{(2)} \frac{n_\mu P^\mu}{Mc^2} + g^{HS} \frac{n_\mu p^\mu}{mc^2} \right\} \frac{a_0^3}{d^3(n, q)} T(n, q) \quad (12)$$

where

$$g^{HS} = g_{(1)} g_{(2)} \frac{M_{(1)} - M_{(2)}}{2M} \quad (13)$$

In the above expression, $T(n, q)$ denotes the so-called tensor coupling operator between $W_{(1)}^\mu$ and $W_{(2)}^\mu$

$$T(n, q) = W_{(1)\mu} W_{(2)}^\mu - 3 \frac{q_\mu W_{(1)}^\mu q_\nu W_{(2)}^\nu}{d(n, q)^2} \quad (14)$$

Finally, $K_n^{(3)}$ denotes all remaining terms of K_n .

$$K_n^{(3)} = \alpha^6 mc^2 \left\{ g^D + g^{DT} T(n, q) + \frac{2}{3} g^{DS} W_{(1)}^\mu W_{(2)\mu} \right\} \frac{a_0^4}{d^4(n, q)} \quad (15)$$

where the dimensionless constants g^D , g^{DT} and g^{DS} are given by

$$\left. \begin{aligned} g^D &= \frac{1}{32M^3} \left\{ M_{(2)}^3 h_{(1)}^2 + M_{(1)}^3 h_{(2)}^2 + 2M_{(1)} M_{(2)}^2 g_{(1)}^2 \right. \\ &\quad \left. + 2M_{(1)}^2 M_{(2)} g_{(2)}^2 \right\} \\ g^{DT} &= \frac{m}{8M} \left(\frac{1}{3} - 2 \frac{m}{M} - \lambda \frac{M_{(1)} - M_{(2)}}{M} \right) g_{(1)} g_{(2)} \\ g^{DS} &= \frac{m}{8M} g_{(1)} g_{(2)} \end{aligned} \right\} \quad (16)$$

in view of (I29), and

$$g^{DS} = \frac{m}{8M} g_{(1)} g_{(2)}$$

As we shall see, these terms will contribute to the spectrum in a similar way as the so-called Darwin terms in the usual Breit model. For this reason we call those terms Darwin-like-terms.

As in [1], we now denote that the commutation relations

$$[K_n, P_\mu] = 0$$

hold since K_n does not depend on Q^μ . Hence, as expected, the total energy-momentum of the system is a constant of the motion. Consequently we have to consider solutions $\psi(X, x)$ of the equation

$$K_n \psi(X, x) = -\frac{Mc^2}{2} \psi(X, x) \quad (17)$$

of the form (I32) which satisfy the additional condition (I33)

$$\psi(X, x) = \exp(iP_\mu X^\mu / \hbar) \phi(x), \quad P_\mu = W n_\mu / c^2$$

On the other hand, for convenience and without loss of generality, we choose n^μ to be equal to n_0^μ . This choice simply corresponds to a description of the system relatively to its rest-frame.

In such a situation

$$d(n_0, \mathbf{x}) = |\mathbf{x}| \equiv r$$

$$\tilde{f}_{i4}(n_0, \mathbf{x}) \equiv 0, \quad \tilde{f}_{ij}(n_0, \mathbf{x}) = \varepsilon_{ijk4} \frac{x^k}{r^3}, \quad i, j, k = 1, 2, 3$$

and

$$W_{(i)}^\mu = (\mathbf{S}_{(i)}, 0), \quad i = 1, 2$$

Then

$$T(n_0, \mathbf{x}) = \mathbf{S}_{(1)}\mathbf{S}_{(2)} - 3 \frac{(\mathbf{x}\mathbf{S}_{(1)})(\mathbf{x}\mathbf{S}_{(2)})}{r^2} \equiv T(\mathbf{x}) \tag{18}$$

abbreviated below by $T(\mathbf{x})$.

In view of the above expressions, obviously no term $K_{n_0}^{(i)}$ depends explicitly on q^4 . As a consequence $n_0^\mu p_\mu \equiv -i\hbar\partial/\partial x^4$ commutes with K_{n_0} (and with P_μ too). More generally this means

$$[n_\mu p^\mu, K_n] = 0$$

Moreover (in the case where $n^\mu = n_0^\mu$) the total relative momentum operators

$$\mathbf{J} = \mathbf{L} + \hbar\mathbf{S}$$

where $\mathbf{L} = \mathbf{q} \wedge \mathbf{p}$ and $\mathbf{S} = \mathbf{S}_{(1)} + \mathbf{S}_{(2)}$, which obviously commute with P_μ and $n_0^\mu p_\mu$, also commute with K_{n_0} because of the rotational invariance of the system.

Consequently, for the same reasons as in [1], we have to determine solutions of (17) for $n^\mu = n_0^\mu$, of the particular form

$$\psi(X, \mathbf{x}) = \exp(iP_\mu X^\mu/\hbar) \exp(-iwx^4/\hbar) \phi_J^M(\mathbf{x}) \tag{19}$$

where $P_\mu = Wn_\mu/c^2$ and where $\phi_J^M(\mathbf{x})$ is a four-component, spatial relative wave function verifying

$$\mathbf{J}^2 \phi_J^M(\mathbf{x}) = J(J+1)\hbar^2 \phi_J^M(\mathbf{x}), \quad J = 0, 1, \dots$$

and

$$J_3 \phi_J^M(\mathbf{x}) = M\hbar \phi_J^M(\mathbf{x}), \quad M = -J, \dots, J-1, J.$$

The functions (19) are then solution of (17) if the spatial relative wave function $\phi_J^M(\mathbf{x})$ obeys the following equation

$$K_{n_0}^{Pw} \phi_J^M(\mathbf{x}) = -\frac{Mc^2}{2} \phi_J^M(\mathbf{x}) \tag{20}$$

obtained by considering the restriction of (17) to the spectral subspace which is associated to the eigenvalues $P_\mu = Wn_\mu/c^2$ and w . Hence

$$K_{n_0}^{Pw} = \mathcal{H} + \mathcal{V}^{(1)} + \mathcal{V}^{(2)} + \mathcal{V}^{(3)}$$

where \mathcal{H} , $\mathcal{V}^{(1)}$, $\mathcal{V}^{(2)}$ and $\mathcal{V}^{(3)}$ denote the corresponding spectral restrictions of $K_{n_0}^{(0)}$, $K_{n_0}^{(1)}$, $K_{n_0}^{(2)}$ and $K_{n_0}^{(3)}$ respectively. Clearly, from (9), (10), (12) and (15):

$$\mathcal{H} = \left. \begin{aligned} & -\frac{1}{2Mc^2} \left(W + \Lambda \alpha^2 mc^2 \frac{a_0}{r} \right)^2 \\ & -\frac{1}{2mc^2} \left(w + \lambda \alpha^2 mc^2 \frac{a_0}{r} \right)^2 + \frac{\mathbf{p}^2}{2m} \end{aligned} \right\} \quad (21)$$

$$\left. \begin{aligned} \mathcal{V}^{(1)} &= \frac{\alpha^4 mc^2}{2\hbar} \frac{a_0^3}{r^3} \mathbf{L}(g_{(1)}^{SO} \mathbf{S}_{(1)} + g_{(2)}^{SO} \mathbf{S}_{(2)}) \\ \mathcal{V}^{(2)} &= -\alpha^4 mc^2 \frac{m}{4M} \left\{ g_{(1)} g_{(2)} \frac{W}{Mc^2} + g^{HS} \frac{w}{mc^2} \right\} \frac{a_0^3}{r^3} T(\mathbf{x}) \end{aligned} \right\} \quad (22)$$

and

$$\mathcal{V}^{(3)} = \alpha^6 mc^2 \left\{ g^D + g^{DT} T(\mathbf{x}) + \frac{2}{3} g^{DS} \mathbf{S}_{(1)} \mathbf{S}_{(2)} \right\} \frac{a_0^4}{r^4}$$

Finally the eigenvalue equation (20) for $\phi_J^M(\mathbf{x})$ reads

$$\left\{ \frac{\mathbf{p}^2}{2m} - \chi \alpha^2 mc^2 \frac{a_0}{r} - \frac{\alpha^4 mc^2}{2} \frac{a_0^2}{r^2} + \mathcal{V}^{(1)} + \mathcal{V}^{(2)} + \mathcal{V}^{(3)} \right\} \phi_J^M(\mathbf{x}) = \varepsilon \phi_J^M(\mathbf{x}) \quad (23)$$

where (as in (I38)) with $\Lambda = 1$ and $K = -Mc^2/2$)

$$\chi = \Lambda \frac{W}{Mc^2} + \lambda \frac{w}{mc^2} \quad (24)$$

and

$$\varepsilon = \frac{1}{2} \left(\frac{W^2}{Mc^2} + \frac{w^2}{mc^2} - Mc^2 \right) \quad (25)$$

Following the same argument as in [1], the bound states of the system are supposed to correspond to the solutions of (23) that belong to $C^4 \otimes L^2(\mathbb{R}^3, d^3x)$. The corresponding values of ε together with the condition $\langle \dot{q}^\mu \rangle_\Phi = 0$ lead to the values of W belonging to the energy spectrum. For symmetry reasons, the ‘‘mean value’’ $\langle \dot{\mathbf{q}} \rangle_\Phi$ can be expected to vanish. On the other hand, the relation

$$\dot{q}^4 \equiv \frac{i}{\hbar} [K_{n_0}, q^4] = \frac{p^4}{m} + \lambda \alpha^2 \frac{a_0}{r} + g^{HS} \alpha^4 \frac{m}{4M} \frac{a_0^3}{r^3} T(\mathbf{x})$$

and the condition $\langle \dot{q}^4 \rangle_\Phi = 0$ imply the equality

$$\frac{\bar{w}}{mc^2} = -\lambda \alpha^2 \left\langle \frac{a_0}{r} \right\rangle_\Phi - g^{HS} \alpha^4 \frac{m}{4M} \left\langle \frac{a_0^3}{r^3} T(\mathbf{x}) \right\rangle_\Phi \quad (26)$$

in the same way as in (I42), (I43) and (I44).

2. Evaluation of the energy spectrum

This section is devoted to the evaluation of the energy-spectrum of the previous two-body model of hydrogen-like systems, up to terms in α^4 .

As regards to (23) we have to consider a problem whose formal analogy with a non-relativistic two-body problem is obvious. At first, our aim is to calculate the

values of ε corresponding to the solutions of (23) in $C^4 \otimes L^2(\mathbb{R}^3, d^3x)$, by a perturbative procedure treating the sum

$$\mathcal{V} = -\frac{\alpha^4 mc^2 a_0^2}{2r^2} + \mathcal{V}^{(1)} + \mathcal{V}^{(2)} + \mathcal{V}^{(3)} \tag{27}$$

as a perturbation in (23). The solutions of the unperturbed problem, where:

$$\mathcal{H}_0 = \frac{\mathbf{p}^2}{2m} - \chi\alpha^2 mc^2 \frac{a_0}{r} \equiv \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{\mathbf{L}^2}{2mr^2} - \chi\alpha^2 mc^2 \frac{a_0}{r} \tag{28}$$

are well known. There are wave functions associated to given angular momentum quantum numbers l whose normalized radial part $R_{nl}(r) \in L^2(\mathbb{R}_+, r^2 dr)$ correspond to the eigenvalues of \mathcal{H}_0

$$\varepsilon_n^{(0)} = -\alpha^2 mc^2 \frac{\chi^2}{2n^2}, \quad n = 1, 2, \dots \tag{29}$$

For a given principal quantum number n , the degeneracy relatively to l corresponds to the values $l = 0, 1, \dots, n - 1$. Because of (24) and (25) the above result yields a relation between W and w . By replacing w in this relation by its unperturbed mean value $\bar{w}_n^{(0)}$ we finally obtain the unperturbed energy spectrum $W_n^{(0)}$. The mean value $\bar{w}_n^{(0)}$ is given by

$$\frac{\bar{w}_n^{(0)}}{mc^2} = -\lambda\alpha^2 \left\langle \frac{a_0}{r} \right\rangle_{\Phi_{nl}^{(0)}} = -\frac{\lambda\alpha^2}{n^2} \left(\Lambda \frac{W}{Mc^2} + \lambda \frac{\bar{w}_n^{(0)}}{mc^2} \right)$$

We refer to (26), without the perturbation term $g^{HS} \alpha^4 m/4M(a_0^3/r^3)T(\mathbf{x})$, and to the analogy of the present calculations with those performed in [1] from (I43) to (I49). (Actually the only difference is that here $\gamma = l$.)

We then get

$$\bar{w}_n^{(0)} = -\frac{\lambda\Lambda\alpha^2 mc^2}{n^2 + \lambda^2\alpha^2} \frac{W}{Mc^2}$$

and finally

$$W_n^{(0)} = Mc^2 \left[1 + \frac{m}{M} \frac{\alpha^2}{n^2 + \alpha^2(1 - m/M)} \right]^{-1/2} \tag{30}$$

using the value of λ proposed in [1]. Expanding this result we have

$$W_n^{(0)} = Mc^2 - mc^2 \left\{ \frac{\alpha^2}{2n^2} - (1 - m/4M) \frac{\alpha^4}{2n^4} + O(\alpha^6) \right\} \tag{31}$$

A corresponding set of normalized eigenfunctions is given by

$$R_{nl}(r) Y_{jl}^M(\theta, \phi) \tag{32}$$

where $Y_{jl}^M(\theta, \phi) \in C^4$ denote the angular eigenfunctions of $\mathbf{J}^2, J_3, \mathbf{L}^2$ and \mathbf{j}^2, \mathbf{j} being given by

$$\mathbf{j} = \mathbf{L} + \hbar\mathbf{S}_{(2)}, \tag{33}$$

for the eigenvalues $J(J+1)\hbar^2$, $M\hbar$, $l(l+1)\hbar^2$ and $j(j+1)\hbar^2$ respectively. This choice is done, assuming a non-symmetric situation where $M_{(1)} > M_{(2)}$. The particle-antiparticle system where $M_{(1)} = M_{(2)}$ will be discussed in Section 4.

Obviously the total momentum quantum numbers J and M are “good” quantum numbers for the perturbed system. On the other hand, concerning l and j , we first notice that the operators

$$\mathbf{LS}_{(1)}, \quad \mathbf{LS}_{(2)}, \quad T(\mathbf{x}) \quad \text{and} \quad \mathbf{S}_{(1)}\mathbf{S}_{(2)}$$

appearing in the expression of \mathcal{V} do not change the parity. Then for given J and M , the eigenfunctions $\phi_J^M(\mathbf{x})$ of $\mathcal{H}_0 + \mathcal{V}$, i.e. satisfying (23), are then necessarily of one of the following forms ($J \neq 0$)

$$R_+(r)Y_{JJ+\frac{1}{2}}^M(\theta, \phi) + R_-(r)Y_{JJ-\frac{1}{2}}^M(\theta, \phi) \tag{34}$$

(i.e. a superposition of wave functions for $l = J$ and $j = J \pm \frac{1}{2}$) or

$$R_+(r)Y_{JJ+1J+\frac{1}{2}}^M(\theta, \phi) + R_-(r)Y_{JJ-1J-\frac{1}{2}}^M(\theta, \phi) \tag{35}$$

(i.e. a superposition of wave functions for $l = J + 1, j = J + \frac{1}{2}$ and $l = J - 1, j = J - \frac{1}{2}$). In particular for $J = 0$, the form is

$$R(r)Y_{00\frac{1}{2}}^0(\theta, \phi) \quad \text{or} \quad R(r)Y_{01\frac{1}{2}}^0(\theta, \phi)$$

Let us now denote by $E_{n,J,M}$ the two-dimensional (one-dimensional if $J = 0$) subspace of $\mathbb{C}^4 \otimes L^2(\mathbb{R}^3, d^3x)$ generated, for $n > J$ and M fixed, by

$$R_{nl}(r)Y_{Jl}^M(\theta, \phi), \quad l = J, \quad j = J \pm \frac{1}{2} \tag{36}$$

Correspondingly, we denote by $F_{n,J,M}$ the two-dimensional (one-dimensional if $J = 0$ or if $n = J + 1, J$) subspaces generated, for $n \leq J$ and M fixed, by

$$R_{nl}(r)Y_{Jl}^M(\theta, \phi), \quad l = J \pm 1, \quad j = J \pm \frac{1}{2} \tag{37}$$

Because of the Darwin-like-term $\mathcal{V}^{(3)}$ in (41), which introduces a singular potential with a r^{-4} behaviour, our perturbative treatment depends on whether we consider an eigenvalue associated to an eigenfunction with a $l = 0$ -component or without such a component. In other words we have to discuss separately the perturbations of an unperturbed solution in $E_{n,J,M}$ with $J \neq 0$, respectively in $F_{n,J,M}$ with $J \neq 1$ or in $E_{n,0,0}$, respectively in $F_{n,1,M}$.

Let us consider the first case where a $l = 0$ -component does not appear in the solution. Then the contribution of order α^4 from (27) to the spectrum can be obtained by a standard first order perturbation.

More precisely, suppose W and w to be fixed parameters in (23). Then the perturbative term (27) contributes to ε with terms of order α^4 and higher. Actually the contribution to ε is given by the eigenvalues of the restriction of \mathcal{V} to the subspaces $E_{n,J,M}$, $J \neq 0$ and $F_{n,J,M}$, $J \neq 1$, as is usual in a first order perturbation calculation. Since the Darwin-like-term $\mathcal{V}^{(3)}$ obviously gives rise to a contribution of order α^6 we can neglect it in the present calculation. Let us denote by $\alpha^4 mc^2 \varepsilon_{n,J}^{(1)}(w, W)$ the contribution of order α^4 from \mathcal{V} to ε , i.e. to one of the eigenvalues of $\mathcal{V}|_{E_{n,J,M}}$ or $\mathcal{V}|_{F_{n,J,M}}$ (when $\mathcal{V}^{(3)}$ is neglected).

The resulting relation between w, W which comes from (25) reads

$$\begin{aligned} \frac{1}{2} \left(\frac{W^2}{Mc^2} + \frac{w^2}{mc^2} - Mc^2 \right) &= \varepsilon_n^{(0)} + \alpha^4 mc^2 \varepsilon_{nJ}^{(1)}(w, W) + O(\alpha^6) \\ &= -\alpha^2 mc^2 \frac{\chi(w, W)^2}{2n^2} + \alpha^4 mc^2 \varepsilon_{nJ}^{(1)}(w, W) + O(\alpha^6) \end{aligned} \quad (38)$$

where we recall that χ , given by (24), depends on w and W . In the same way as previously, in order to obtain an equation determining the energy spectrum, we have to replace w by its corresponding mean value $\bar{w}_{n,J}$ for states $\Phi_{n,J,M}$ built up from solutions of (23) (we refer to (I43)) and verifying the condition (26). Presently, solutions of (23) differ from the unperturbed one by α^4 and higher terms. Under this condition the right hand side of (26) differs from the one in the unperturbed case by terms of order α^4 and higher. Thus

$$\bar{w}_{nJ} = \bar{w}_n^{(0)} + \Delta \bar{w}_{nJ}$$

where $\Delta \bar{w}_{nJ} = O(\alpha^4)$. For what follows, it is important to remember that $\bar{w}_n^{(0)} = O(\alpha^2)$.

Consequently, putting

$$W = W_n^{(0)} + \Delta W_{nJ} \quad (39)$$

in (38), where w was been replaced by $\bar{w}_n^{(0)} + \Delta \bar{w}_{nJ}$, we easily conclude that ΔW_{nJ} necessarily contains α^4 and higher order contributions. More precisely we conclude that

$$\Delta W_{nJ} = \alpha^4 mc^2 \varepsilon_{nJ}^{(1)}(w = 0, W = Mc^2) + O(\alpha^6) \quad (40)$$

In other words, the contributions of order α^4 from \mathcal{V} to the energy spectrum are obtained from the restriction to $E_{n,J \neq 0, M}$ and $F_{n,J \neq 1, M}$ of

$$\begin{aligned} \mathcal{V}' &= -\frac{\alpha^4 mc^2 a_0^2}{2 r^2} + \frac{\alpha^4 mc^2 a_0^3}{2\hbar r^3} \mathbf{L}(g_{(1)}^{SO} \mathbf{S}_{(1)} + g_{(2)}^{SO} \mathbf{S}_{(2)}) \\ &\quad - \alpha^4 mc^2 \frac{m}{4M} g_{(1)} g_{(2)} \frac{a_0^3}{r^3} T(\mathbf{x}) \end{aligned} \quad (41)$$

as follows from (27) (where $\mathcal{V}^{(3)}$ has been neglected) and (22) where we set $w = 0$ and $W = Mc^2$. Moreover the restriction has to be considered for subspaces $E_{n,J,M}$ and $F_{n,J,M}$ associated to the radial wave functions $R_{nl}(r)$ for $w = 0$ and $W = Mc^2$ i.e. to the radial wave function of (28) with $\chi = 1$, (see (24)).

These calculations are in all respects similar to the ones of the usual evaluation of fine and hyperfine structure in the non-relativistic case. For this reason we only give the results of these calculations and refer to [2] for more details.

We first consider the matrix elements

$$\mathcal{V}'_{ij' nJM} = \int_0^\infty r^2 dr \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi R_{nJ}^*(r) Y_{JJ'}^M(\theta, \phi) + \mathcal{V}' R_{nJ}(r) Y_{JJ'}^M(\theta, \phi)$$

i.e. the restriction of \mathcal{V}' to $E_{n,J,M}$ relative to the basis (36).

For $j = j' = J + \frac{1}{2}$ ($J \neq 0, J = l < n$), we obtain

$$\mathcal{V}_{j j'}^{mJM} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J+1} \left\{ 2 + \frac{g_{(1)}^{SO}(2J+3) - g_{(2)}^{SO}(2J+1)}{(J+1)(2J+1)} - \frac{m}{2M} \frac{g_{(1)}g_{(2)}}{(J+1)(2J+1)} \right\}$$

and for $j = j' = J - \frac{1}{2}$ ($J \neq 0, J = l < n$),

$$\mathcal{V}_{j j'}^{mJM} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J+1} \left\{ 2 - \frac{g_{(1)}^{SO}(2J-1) - g_{(2)}^{SO}(2J+1)}{J(2J+1)} - \frac{m}{2M} \frac{g_{(1)}g_{(2)}}{J(2J+1)} \right\} \quad (42)$$

The non-diagonal elements (where $j = J - \frac{1}{2}$ and $j' = J + \frac{1}{2}$) are given by

$$\mathcal{V}_{j j'}^{mJM} = (\mathcal{V}_{j' j}^{mJM})^* = \frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J+1} \frac{2g_{(1)}^{SO} - m/2M \cdot g_{(1)}g_{(2)}}{\sqrt{J(J+1)(2J+1)}}$$

The eigenvalues of this 2×2 hermitian matrix correspond to the contribution of order α^4 , from \mathcal{V} to the energy spectrum when $J \neq 0$.

We now consider the matrix elements

$$\mathcal{V}_{j j'}^{mJM} = \int_0^\infty r^2 dr \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi R_{nl}^*(r) Y_{Jl}^M(\theta, \phi)^+ \mathcal{V}' R_{nl}(r) Y_{Jl'}^M(\theta, \phi)$$

i.e. the restriction of \mathcal{V}' to $F_{n,J,M}$ relative to the basis (37).

For $j = j' = J + \frac{1}{2}$ ($l = l' = J + 1$) ($J \neq 1, J + 1 < n$)

$$\mathcal{V}_{j j'}^{nJM} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J+3} \left\{ 2 + \frac{g_{(1)}^{SO} + g_{(2)}^{SO}}{J+1} + \frac{m}{2M} \frac{g_{(1)}g_{(2)}}{(J+1)(2J+1)} \right\}$$

For $j = j' = J - \frac{1}{2}$ ($l = l' = J - 1$) ($J \neq 1, J \leq n$)

$$\mathcal{V}_{j j'}^{nJM} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J-1} \left\{ 2 - \frac{g_{(1)}^{SO} + g_{(2)}^{SO}}{J} + \frac{m}{2M} \frac{g_{(1)}g_{(2)}}{J(2J+1)} \right\} \quad (43)$$

In this case the non-diagonal elements vanish.⁴⁾

Thus, the above diagonal elements (43) are simply the contribution of order α^4 of \mathcal{V} to the order spectrum when $J \neq 1$.

Next, we have to consider the particular situations where a $l = 0$ -component appears, and for which the above perturbative procedure does not apply. This corresponds to the subspaces $E_{n,0,0}$ and $F_{n,1,M}$.

In the first case ($J = l = 0, j = \frac{1}{2}$) the solution of (23) has the following form

$$\phi_0^0(\mathbf{x}) = R(r) Y_{00\frac{1}{2}}^0(\theta, \phi)$$

⁴⁾ It can be shown that: $\int_0^\infty R_{n+2}(r)^* \frac{a_0^3}{r^3} R_{nl}(r) r^2 dr = 0$ for $n \geq 3$.

Since

$$\mathbf{L}\mathbf{S}_{(1)}Y_{00\frac{1}{2}}^0 = \mathbf{L}\mathbf{S}_{(2)}Y_{00\frac{1}{2}}^0 = 0, \quad T(\mathbf{x})Y_{00\frac{1}{2}}^0 = 0$$

and

$$\mathbf{S}_{(1)}\mathbf{S}_{(2)}Y_{00\frac{1}{2}}^0 = -\frac{3}{4}Y_{00\frac{1}{2}}^0$$

the eigenvalue equation (23) implies the following radial equation for $R(r)$, obtained by taking (22) into account

$$\left\{ \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \chi\alpha^2 mc^2 \frac{a_0}{r} - \frac{\alpha^4 mc^2 a_0^2}{2 r^2} + \alpha^6 mc^2 (g^D - \frac{1}{2}g^{DS}) \frac{a_0^4}{r^4} \right\} R(r) = \varepsilon R(r) \quad (44)$$

In fact we have to find values of ε corresponding to solutions of (44) belonging to $L^2(\mathbb{R}_+, r^2 dr)$.

It can be shown [5] that such solutions behave as follows, near the origin:

$$R(r) = \exp(-\alpha^2 \sqrt{2g^D - g^{DS}} a_0/r) \cdot O(1) \quad \text{for } r \rightarrow 0 \quad (45)$$

when one, of course, assumes that $2g^D - g^{DS} > 0$.

For this reason it is convenient to set

$$R(r) = \exp(-\alpha^2 \sqrt{2g^D - g^{DS}} a_0/r) \tilde{R}(r) \quad (46)$$

By virtue of this definition an easy calculation shows that $\tilde{R}(r)$ obeys the following differential equation obtained from (44)

$$\left\{ \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \chi\alpha^2 mc^2 \frac{a_0}{r} - \frac{\alpha^4 mc^2 a_0^2}{2 r^2} - \alpha^4 mc^2 \sqrt{2g^D - g^{DS}} \frac{a_0^3}{r^2} \frac{d}{dr} \right\} \tilde{R}(r) = \varepsilon \tilde{R}(r) \quad (47)$$

A function $\tilde{R}(r)$ corresponding to a solution of (44) in $L^2(\mathbb{R}_+, r^2 dr)$ behaves near the origin as $\tilde{R}(r) = O(1)$ for $r \rightarrow 0$. On the other hand $R(r)$ as well as $\tilde{R}(r)$ are analytic functions of r in $]0, \infty]$, decreasing exponentially for $r \rightarrow \infty$. Consequently such functions $\tilde{R}(r)$ are in $L^2(\mathbb{R}_+, r^2 dr)$ and, conversely, solutions of (47) belonging to $L^2(\mathbb{R}_+, r^2 dr)$ give rise to a solution of (44) belonging to $L^2(\mathbb{R}_+, r^2 dr)$.

Hence, a first order standard perturbation calculation can be performed in (47). Treating the terms

$$-\frac{\alpha^4 mc^2 a_0^2}{2 r^2} - \alpha^4 mc^2 \sqrt{2g^D - g^{DS}} \frac{a_0^3}{r^2} \frac{d}{dr} \equiv \mathcal{V}' \quad (48)$$

in (47) as a (non self-adjoint) perturbation, we recognize the unperturbed solutions to be the usual Coulomb radial wave functions $R_{no}(r)$ associated to the eigenvalues

$$\varepsilon_n^{(0)} = -\alpha^2 mc^2 \frac{\chi^2}{2n^2}$$

Then, first order perturbation calculation leads to the following contribution of order α^4 to ε :

$$\alpha^4 mc^2 \varepsilon_{n0}^{(1)}(w, W) = \int_0^\infty R_{n0}^*(r) \mathcal{V}' R_{n0}(r) r^2 dr = -\frac{\alpha^4 mc^2}{2n^3} \{2\chi^2 - 4\sqrt{2g^D - g^{DS}} \chi^3\}$$

Finally, the corresponding contribution of order α^4 in the energy-spectrum is given by $\alpha^4 mc^2 \varepsilon_{n0}^{(1)}(0, Mc^2)$ (i.e. $\chi = 1$), as follows from a similar argument as the one that led to (40). Then, for $J = 0$ ($l = 0, j = \frac{1}{2}$) and for $n = 1, 2, \dots$ we have

$$\Delta W_{n0} = -\frac{\alpha^4 mc^2}{2n^3} \{2 - 4\sqrt{2g^D - g^{DS}}\} + O(\alpha^6) \quad (49)$$

This result completes (42) in the case $J = 0$.

Consider now the second particular case corresponding to solutions of (23) of the form (35) for $J = 1$. In this case

$$\phi_1^M(\mathbf{x}) = R_+(r) Y_{12\frac{3}{2}}^M(\theta, \phi) + R_-(r) Y_{10\frac{1}{2}}^M(\theta, \phi) \quad (50)$$

From (23) and (22), we obtain the following coupled radial equations for $R_+(r)$ and $R_-(r)$:

$$\begin{aligned} & \left\{ \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{\hbar^2}{2mr^2} \begin{bmatrix} 6 & 0 \\ 0 & 0 \end{bmatrix} - \chi \alpha^2 mc^2 \frac{a_0}{r} \right. \\ & - \frac{\alpha^4 mc^2}{2} \frac{a_0^2}{r^2} + \frac{\alpha^4 mc^2}{2} (g_{(1)}^{SO} + g_{(2)}^{SO}) \frac{a_0^3}{r^3} \begin{bmatrix} -\frac{3}{2} & 0 \\ 0 & 0 \end{bmatrix} \\ & - \alpha^4 mc^2 \frac{m}{4M} \left\{ g_{(1)} g_{(2)} \frac{W}{Mc^2} + g^{HS} \frac{w}{mc^2} \right\} \frac{a_0^3}{r^3} \begin{bmatrix} \frac{1}{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{bmatrix} \\ & \left. + \alpha^6 mc^2 \frac{a_0^4}{r^4} \left\{ g^D + \frac{1}{6} g^{DS} + g^{DT} \begin{bmatrix} \frac{1}{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{bmatrix} \right\} \right\} \begin{bmatrix} R_+(r) \\ R_-(r) \end{bmatrix} = \varepsilon \begin{bmatrix} R_+(r) \\ R_-(r) \end{bmatrix} \quad (51) \end{aligned}$$

since $Y_{12\frac{3}{2}}^M$ and $Y_{10\frac{1}{2}}^M$ are linearly independent angular functions. We have to determine the value of ε corresponding to solutions of (51) in $C^2 \otimes L^2(\mathbb{R}_+, r^2 dr)$.

As previously, it is convenient to set

$$\begin{bmatrix} R_+(r) \\ R_-(r) \end{bmatrix} = \exp(-\alpha^2 \sqrt{2g^D + \frac{1}{3}g^{DS}} a_0/r) \begin{bmatrix} \tilde{R}_+(r) \\ \tilde{R}_-(r) \end{bmatrix} \quad (52)$$

where we assume that $6g^D + g^{DS} > 0$. Substitution of (52) into (51) gives

$$\left\{ \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{\hbar^2}{2mr^2} \begin{bmatrix} 6 & 0 \\ 0 & 0 \end{bmatrix} - \chi \alpha^2 mc^2 \frac{a_0}{r} + \mathcal{V}' \right\} \begin{bmatrix} \tilde{R}_+(r) \\ \tilde{R}_-(r) \end{bmatrix} = \varepsilon \begin{bmatrix} \tilde{R}_+(r) \\ \tilde{R}_-(r) \end{bmatrix} \quad (53)$$

where \mathcal{V}' stands for

$$\begin{aligned} & -\alpha^4 mc^2 \frac{a_0^2}{r^2} + \frac{\alpha^4 mc^2}{2} (g_{(1)}^{SO} + g_{(2)}^{SO}) \frac{a_0^3}{r^3} \begin{bmatrix} -\frac{3}{2} & 0 \\ 0 & 0 \end{bmatrix} \\ & -\alpha^4 mc^2 \frac{m}{4M} \left\{ g_{(1)} g_{(2)} \frac{W}{Mc^2} + g^{HS} \frac{w}{mc^2} \right\} \frac{a_0^3}{r^3} \begin{bmatrix} \frac{1}{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{bmatrix} \\ & + \alpha^6 mc^2 \frac{a_0^4}{r^4} g^{DT} \begin{bmatrix} \frac{1}{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{bmatrix} - \alpha^4 mc^2 \sqrt{2g^D + \frac{1}{3}g^{DS}} \frac{a_0^3}{r^2} \frac{d}{dr}. \quad (54) \end{aligned}$$

The solutions of (53) in $C^2 \otimes L^2(\mathbb{R}_+, r^2 dr)$ give rise, via (52), to solutions of (51) in $C^2 \otimes L^2(\mathbb{R}_+, r^2 dr)$. In (53), we can evaluate ϵ by standard first order perturbation methods, treating \mathcal{V}' given by (54) as a perturbation. The solutions of the corresponding unperturbed problem are obviously

$$\begin{bmatrix} R_{n2}(r) \\ 0 \end{bmatrix}, n = 3, 4, \dots \quad \text{and} \quad \begin{bmatrix} 0 \\ R_{n0}(r) \end{bmatrix}, \quad n = 1, 2, \dots \tag{55}$$

and the corresponding eigenvalues are

$$\epsilon_n^{(0)} = -\alpha^2 mc^2 \frac{\chi^2}{2n^2}$$

First order standard perturbation calculation consists in determining the eigenvalues of the restriction of \mathcal{V}' to the two-dimensional (one-dimensional if $n = 1, 2$) subspace of $C^2 \otimes L^2(\mathbb{R}_+, r^2 dr)$ generated by (55). In spite of the singular terms occurring in (54), such a restriction exists as it is easy to verify since $R_{nl}(r) = O(r^l)$ for $r \rightarrow 0$. The following term of \mathcal{V}'

$$\alpha^6 mc^2 \frac{a_0^4}{r^4} g^{DT} \begin{bmatrix} \frac{1}{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{bmatrix}$$

giving rise to a contribution of order α^6 in ϵ , can be neglected. On the other hand the only possible non-diagonal contribution of order α^4 , i.e.

$$\int_0^\infty R_{n2}^*(r) \mathcal{V}' R_{n0}(r) r^2 dr, \quad n > 2$$

comes from the third term in (54). However, such a contribution vanishes. Up to order α^4 , the restriction of \mathcal{V}' relative to the basis (55) is diagonal. Hence, up to order α^4 , states with $l = 0$ and 2 do not mix.

For states with $l = 2$ ($J = 1$) the contribution of order α^4 of \mathcal{V}' to ϵ is given by the diagonal element of \mathcal{V}' associated with

$$\begin{bmatrix} R_{n2}(r) \\ 0 \end{bmatrix}, \quad n > 2$$

i.e. by the mean value of

$$\begin{aligned} & -\frac{\alpha^4 mc^2}{2} \frac{a_0^2}{r^2} - \frac{3}{4} \alpha^4 mc^2 (g_{(1)}^{SO} + g_{(2)}^{SO}) \frac{a_0^3}{r^3} \\ & -\frac{\alpha^4 mc^2}{2} \frac{m}{4M} \left\{ g_{(1)} g_{(2)} \frac{W}{Mc^2} + g^{HS} \frac{w}{mc^2} \right\} \frac{a_0^3}{r^3} \\ & -\alpha^4 mc^2 \sqrt{2g^D + \frac{1}{3}g^{DS}} \frac{a_0^3}{r^2} \frac{d}{dr} \end{aligned}$$

with respect to $R_{n2}(r)$. But, in this expression, the last term does not contribute because:

$$\int_0^\infty R_{n2}^*(r) \frac{a_0^3}{r^2} \frac{dR_{n2}(r)}{dr} r^2 dr = 0$$

Finally, the mean value of the above sum of operators, for $w=0$ and $W=Mc^2$ ($\chi=1$) reads ($n>2$):

$$\Delta W_{n1} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{5} \left\{ 2 + \frac{g_{(1)}^{SO} + g_{(2)}^{SO}}{2} + \frac{m}{2M} \frac{g_{(1)} g_{(2)}}{6} \right\} \quad (56)$$

and gives the corresponding contribution of order α^4 to the energy-spectrum. It is important to note that this result coincides with (43) (for $j=j'=J+\frac{1}{2}$) where $J=1$.

Significant differences appear for states with $l=0$ ($J=1$). The contribution of order α^4 of \mathcal{V}' to ε is given by the diagonal element of \mathcal{V}' associated with

$$\begin{bmatrix} 0 \\ R_{n0}(r) \end{bmatrix} \quad n=1, 2, \dots$$

i.e. the mean value of the operators

$$-\frac{\alpha^4 mc^2}{2} \frac{a_0^2}{r^2} - \alpha^4 mc^2 \sqrt{2g^D + \frac{1}{3}g^{DS}} \frac{a_0^3}{r^2} \frac{d}{dr}$$

relative to $R_{n0}(r)$. The above mean value, for $w=0$ and $W=Mc^2$ ($\chi=1$) reads

$$\Delta W_{n1} = -\frac{\alpha^4 mc^2}{2n^3} \{2 - 4\sqrt{2g^D + \frac{1}{3}g^{DS}}\} \quad (57)$$

and gives the corresponding contribution of order α^4 to the energy-spectrum. This result completes (61) in the case $j=j'=J-\frac{1}{2}$ for $J=1$.

Let us now summarize. The spectrum, up to order α^4 , associated to solutions of the form (34) is given by the expansion (31) for $W_n^{(0)}$ up to the same order, where the contributions of (42) or (49) have to be added. For such states l is a good quantum number but j is not (except if $J=0$ with then $j=\frac{1}{2}$).

The spectrum, up to order α^4 , associated to solutions of the form (35) is given by the expansion (31) for $W_n^{(0)}$ where contributions given by ((43), (56) or (57)) have to be added. For these states l and j are approximate good quantum numbers in the sense that there exists a mixing between $l=J\pm 1$ -components in terms of order α^6 and higher. Exceptionally, l (and j) are good quantum numbers when $J=0$ and then $l=1$, $j=\frac{1}{2}$.

3. An application to the hydrogen atom

In this application, particle (1) is a proton and particle (2) is an electron. We may thus suppose $M_{(2)} \ll M_{(1)}$, i.e. $m/M \ll 1$.

Our aim is to determine, from the previous results, the energy-spectrum of the hydrogen atom up to terms of order α^4 and up to terms in m/M . This implies from (11)

$$\left. \begin{aligned} g_{(1)}^{SO} &\cong g_{(1)} \frac{m}{M}, & g_{(2)}^{SO} &\cong \frac{g_{(2)}}{2} \\ \text{and from (16)} & & & \\ g^D &\cong \frac{1}{32} \left\{ h_{(2)}^2 + \frac{m}{M} (2g_{(2)}^2 - 3h_{(2)}^2) \right\}, & g^{DS} &= g_{(1)} g_{(2)} \frac{m}{8M} \end{aligned} \right\} \quad (58)$$

The other dimensionless constants play no role at all because of (42), (43), (49) and (57). As a consequence of the above expression for $g_{(1)}^{SO}$ we note that the non diagonal elements in (42) are of order m/M and thus contribute to the eigenvalues of the 2×2 matrices $\mathcal{V}_{jj'}^{nJM}$, through terms of order $(m/M)^2$ (whenever the corresponding trace does not vanish). So, the diagonal elements in (42) lead to $\Delta W_{n,J}$ up to terms in m/M . This result together with (43), (49), and (57) gives directly $\Delta W_{n,J} \dots$.

For convenience, we express $\Delta W_{n,J} \dots$ as a sum of a so-called "fine structure term" $\Delta W_{n,J}^{FS}$ and a so-called "hyperfine structure structure term" $\Delta W_{n,J}^{HS}$

$$\Delta W_{n,J} = \Delta W_{n,J}^{FS} + \Delta W_{n,J}^{HS} \tag{59}$$

The energy levels of the atom are labelled by n, J, j, l . As follows from the previous comments, j and l may be assumed to be good quantum numbers since the mixing between states of different j and l is very small.

In this way we obtain the following $\Delta W_{n,J}^{FS}$ and $\Delta W_{n,J}^{HS}$, for $l \neq 0$ (from (42) and (43)). We have

$$\Delta W^{FS} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{j+\frac{1}{2}} \left\{ 1 \pm \frac{g_{(2)}/2-1}{2l+1} \right\} \tag{60}$$

for $l = j \pm \frac{1}{2}$ respectively

$$\Delta W^{HS} = -\frac{\alpha^4 mc^2}{2n^3} \frac{m}{M} \frac{2g_{(1)}}{(2J+1)(2l+1)} \left\{ \pm 1 \pm \frac{g_{(2)}/2-1}{2j+1} \right\} \tag{61}$$

for $j = J \pm \frac{1}{2}$ respectively for the first sign and for $l \neq J$ or $l = J$ respectively for the second sign.

For $l = 0$ (from (49) and (57)), we have

$$\Delta W^{FS} = -\frac{\alpha^4 mc^2}{2n^3} \left\{ 1 - \left[h_{(2)} - 1 + \frac{m}{M} \left(\frac{2g_{(2)}^2 - 3h_{(2)}^2}{2h_{(2)}} \right) \right] \right\} \tag{62}$$

and

$$\Delta W^{HS} = -\frac{\alpha^4 mc^2}{2n^3} \frac{m}{M} \frac{2g_{(1)}}{2J+1} \left\{ \pm 1 \pm \frac{g_{(2)}/2-h_{(2)}}{h_{(2)}} \right\} \tag{63}$$

depending on whether $J = 0$ or 1 .

The above results need some comments.

The first terms in the expressions (60) and (62) of ΔW^{FS} , i.e.

$$-\frac{\alpha^4 mc^2}{2n^3} \frac{1}{j+\frac{1}{2}} \tag{64}$$

are the same as the fine structure terms of the Dirac spectrum [6] where the mass of the electron has been replaced by the reduced mass m . These terms exhibit the well known degeneracy relatively to l for fixed j . In our model this degeneracy is removed by the second terms in (60) and (62). These terms contribute thus to the Lamb shifts of the fine structure spectrum. Usually the Lamb shifts are obtained as radiative corrections to the Dirac results. The energy shifts terms obtained by such a procedure [7] may be compared with the corresponding energy shifts terms resulting from expressions (60) and (62) of ΔW^{FS} . Both types of expressions, ours,

which read

$$\left. \begin{aligned} & \mp \frac{\alpha^4 mc^2}{2n^3} \frac{g_{(2)} - 2}{(2j+1)(2l+1)} \\ & \text{for } l = j \pm \frac{1}{2} \neq 0 \text{ respectively and} \\ & \frac{\alpha^4 mc^2}{2n^3} \left(h_{(2)} - 1 + \frac{m}{M} \frac{2g_{(2)}^2 - h_{(2)}^2}{2h_{(2)}} \right) \end{aligned} \right\} \quad (65)$$

for $l=0$, and the ones obtained from radiative corrections are rather similar, particularly in what concerns their n -dependence. (For a comparison, see also Ref. [17] Section 2.)

Actually, in the hydrogen atom, where

$$g_{(2)} \cong 2.0023$$

is the gyromagnetic factor of the electron, and where we put

$$h_{(2)} = 1.048$$

our fine structure terms ΔW^{FS} exhibit Lamb shifts with good numerical agreement. For the ${}^nS_{1/2} - {}^nP_{1/2}$ energy separations ($n \geq 2$) we have the expression

$$\frac{\alpha^4 mc^2}{2n^3} \left(h_{(2)} - 1 + \frac{m}{M} \frac{2g_{(2)}^2 - 3h_{(2)}^2}{2h_{(2)}} + \frac{g_{(2)} - 2}{6} \right) \quad (66)$$

corresponding in the hydrogen atom (where $\alpha^4 mc^2/h = 350.19$ [GHz] and $m/M = 0.5440 \cdot 10^{-3}$) to the frequencies $8.464/n^3$ [GHz]. The above value of $h_{(2)}$ has been chosen to reproduce the experimental value 1.058 [GHz] for the ${}^2S_{1/2} - {}^2P_{1/2}$ energy separation [8]. The predicted numerical values for $n > 2$ may then be compared with the experimental results [9].

n	theory [GHz]	experiment [GHz] *)
3	0.314	0.315
4	0.132	0.133
5	0.068	0.065

*) Experimental data are reproduced up to the last significant figure.

In the above cases where $j = \frac{1}{2}$, the line width is always smaller than the Lamb shifts, but for $j = \frac{3}{2}$ it is larger than the predicted energy splitting.

We now consider the hyperfine structure contribution ΔW^{HS} given in (61) and (63). The first terms in these expressions of ΔW^{HS} can be written in the unified form

$$\mp \frac{\alpha^4 mc^2}{2n^3} \frac{m}{M} \frac{2g_{(1)}}{(2J+1)(2l+1)} \quad (67)$$

which, (for the gyromagnetic factor of the proton $g_{(1)} \cong 5.585$), corresponds to the hyperfine energy shifts for the hydrogen obtained from the Breit equation [10]. These results are in agreement with the experimental ones.

Finally, the second terms in the expressions (61) and (63) of ΔW^{HS} are small corrections in the present case as $g_{(2)}$ is very close to 2 and $h_{(2)}$ close to 1. For $l \neq 0$

these correcting terms are negligible but for $l=0$ their contributions are about 4% of the hyperfine energy shift. For experimental data on the ground state hyperfine structure of hydrogen we refer to [11].

4. The particle-antiparticle system. The positronium

In this particular case

$$M_{(1)} = M_{(2)} = 2m = M/2$$

Moreover, we assume that

$$g_{(1)} = g_{(2)} \equiv g \quad \text{and} \quad h_{(1)} = h_{(2)} \equiv h_F$$

Then, from (11), (13) and (16) we have

$$\left. \begin{aligned} g_{(1)}^{SO} = g_{(2)}^{SO} \equiv g^{SO} = \frac{3}{8}g, \quad g^{HS} = 0 \\ g^D = \frac{g^2 + h_F^2/2}{64}, \quad g^{DT} = -\frac{1}{64} = -\frac{1}{64} \frac{g^2}{3}, \quad g^{DS} = \frac{g^2}{32} \end{aligned} \right\} \quad (68)$$

We evaluate the energy spectrum (up to terms in α^4) by a perturbative treatment of (23). As previously we assume the terms (27) to be a perturbation \mathcal{V} in (23). In this particular case (from (22) and (68)),

$$\left. \begin{aligned} \mathcal{V}^{(1)} &= \frac{\alpha^4 mc^2}{16} 3g\hbar^{-1} \frac{a_0^3}{r^3} \mathbf{LS} \\ \mathcal{V}^{(2)} &= -\frac{\alpha^4 mc^2}{16} \frac{W}{Mc^2} g^2 \frac{a_0^3}{r^3} T(\mathbf{x}) \\ \mathcal{V}^{(3)} &= \frac{\alpha^6 mc^2}{16} \left(\frac{h_F^2}{8} - \frac{g^2}{12} T(\mathbf{x}) + \frac{g^2}{6} \mathbf{S}^2 \right) \frac{a_0^4}{r^4} \end{aligned} \right\} \quad (69)$$

where \mathbf{S} stands for the total spin operators

$$\mathbf{S} = \mathbf{S}_{(1)} + \mathbf{S}_{(2)}$$

From this definition it follows that (18) also reads

$$T(\mathbf{x}) = \frac{1}{2} \left(\mathbf{S}^2 - 3 \frac{(\mathbf{xS})^2}{r^2} \right) \quad (70)$$

The following procedure and the basic considerations are quite similar as in Section 2 except that now, the total spin \mathbf{S}^2 obviously commutes with \mathcal{H}_0 and with $\mathcal{H}_0 + \mathcal{V}$. As a set of normalized eigenfunctions corresponding to the unperturbed energy spectrum (45), we thus take

$$R_{nl}(r) \mathcal{Y}_{JMS}^M(\theta, \phi) \quad (71)$$

where $\mathcal{Y}_{JMS}^M(\theta, \phi) \in \mathbb{C}^4$ denote the angular eigenfunctions of \mathbf{J}^2 , J_3 , \mathbf{L}^2 and \mathbf{S}^2 for the eigenvalues $J(J+1)\hbar^2$, $M\hbar$, $l(l+1)\hbar^2$ and $S(S+1)$ respectively.

This implies that J , M and $S=0, 1$ are good quantum numbers for the system. On the other hand, for what concerns l , we note that the operators

$$\mathbf{LS}, T(\mathbf{x}) \quad \text{and} \quad \mathbf{S}^2$$

occurring in the expression of \mathcal{V} and acting on the angular part of (71), do not change the parity. Then, for given J , M and S , the eigenfunctions $\phi_{J,S}^M(\mathbf{x})$ of $\mathcal{H}_0 + \mathcal{V}$, i.e. verifying (23), necessarily have the following forms:

For $S = 0$ (singlet state)

$$\phi_{J0}^M(\mathbf{x}) = R(r) \mathcal{Y}_{JJ0}^M(\theta, \phi) \quad (72)$$

For $S = 1$ (triplet state) and $J \neq 0$

$$\phi_{J1}^M(\mathbf{x}) = R(r) \mathcal{Y}_{JJ1}^M(\theta, \phi) \quad (73)$$

(i.e. a wave function for $l = J$) or

$$\phi_{J1}^M(\mathbf{x}) = R_+(r) \mathcal{Y}_{JJ+11}^M(\theta, \phi) + R_-(r) \mathcal{Y}_{JJ-11}^M(\theta, \phi) \quad (74)$$

(i.e. a superposition of wave functions for $l = J + 1$ and $l = J - 1$). For the special case where $J = 0$, the corresponding form is

$$\phi_{01}^0(\mathbf{x}) = R(r) \mathcal{Y}_{011}^0(\theta, \phi) \quad (75)$$

Let us now denote by $E_{n,J,M,S}$ the one-dimensional sub-spaces of $\mathbb{C}^4 \otimes L^2(\mathbb{R}^3, d^3x)$ generated by

$$R_{nl}(r) \mathcal{Y}_{JlS}^M(\theta, \phi), \quad l = J \quad (76)$$

for $n > J$, M and S fixed. ($J \neq 0$ if $S = 1$).

We denote by $F_{n,J,M,1}$ the two-dimensional (one-dimensional if $J = 0$ or if $n = J + 1$, J) subspaces of $\mathbb{C}^4 \otimes L^2(\mathbb{R}^3, d^3x)$ generated by

$$R_{nl}(r) \mathcal{Y}_{JlS}^M(\theta, \phi), \quad l = J \pm 1 \quad (77)$$

for $n \geq J$, M fixed and $S = 1$ ($J \neq 0$).

As previously, because of the ‘‘Darwin’’ like term $\mathcal{V}^{(3)}$ in (69), which introduces a singular potential of r^{-4} behaviour, the perturbative treatment depends on whether we consider an eigenvalue associated to an eigenfunction with a $l = 0$ -component or without such a component. In other words the perturbation from unperturbed solutions in $E_{n,J,M,S}$ with $J \neq 0$ and in $F_{n,J,M,1}$ with $J \neq 1$ can be performed in the standard way: the eigenvalues of the corresponding restrictions of \mathcal{V} leads, with (40), to the contributions of order α^4 of \mathcal{V} to the spectrum.

The special cases of perturbations from unperturbed solutions in $E_{n,0,0,0}$, $n \geq 1$ and in $F_{n,1,M,1}$, $n \geq 1$ will be treated as previously in Section 2.

We separately consider the singlet $S = 0$ and the triplet $S = 1$ cases.

The singlet states. Then $S = 0$, $\mathcal{V}^{(1)}$ and $\mathcal{V}^{(2)}$ do not contribute since

$$\mathbf{LS} \mathcal{Y}_{JJ0}^M = 0 \quad \text{and} \quad T(\mathbf{x}) \mathcal{Y}_{JJ0}^M = 0$$

On the other hand, $\mathcal{V}^{(3)}$ gives rise to a contribution of order α^6 for perturbations from $E_{n,J,M,0}$, $J \neq 0$. Then, up to order α^4 , the contribution of \mathcal{V} comes from the first term in (27). The corresponding contributions to the spectrum are given by

$$\Delta W_{nJ} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{l + \frac{1}{2}}, \quad l = J \neq 0, \quad n > J \quad (78)$$

For $E_{n,0,0,0}$, the solution of (23) reads

$$R(r)\mathcal{Y}_{000}^0(\theta, \phi)$$

and the radial function $R(r)$ verifies the eigenvalue equation

$$\left\{ \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \chi \alpha^2 mc^2 \frac{a_0}{r} - \frac{\alpha^4 mc^2 a_0^2}{2 r^2} + \frac{\alpha^6 mc^2 h_F^2 a_0^4}{2 \cdot 64 r^4} \right\} R(r) = \epsilon R(r)$$

which is similar to (44). Then in analogy to (49) we have

$$\Delta W_{n0} = -\frac{\alpha^4 mc^2}{2n^3} \left\{ 2 - \frac{h_F}{2} \right\}, \quad l = J = 0, \quad n \geq 1 \tag{79}$$

Finally, for singlet states, we note that l is a good quantum number.

The triplet states. We first consider the one-dimensional subspaces $E_{n,J,M,1}$ (where the case $l = J = 0$ does not occur). To perform a standard perturbation calculation we have to determine the action of the operators $\hbar^{-1}\mathbf{LS}$ and $T(\mathbf{x})$ on the angular functions $\mathcal{Y}_{JJ1}^M(\theta, \phi)$. We obtain

$$\hbar^{-1}\mathbf{LS}\mathcal{Y}_{JJ1}^M = -\mathcal{Y}_{JJ1}^M \quad \text{and} \quad T(\mathbf{x})\mathcal{Y}_{JJ1}^M = -\frac{1}{2}\mathcal{Y}_{JJ1}^M \tag{80}$$

Since in this case $\mathcal{V}^{(3)}$ gives rise to a contribution of order α^6 we neglect this term in the following integral

$$\int_0^\infty r^2 dr \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi R_{nJ}^*(r)\mathcal{Y}_{JJ1}^M(\theta, \phi) + \mathcal{V} R_{nJ}(r)\mathcal{Y}_{JJ1}^M(\theta, \phi) \\ \cong -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J+1} \left\{ 2\chi^2 + \left(\frac{3}{4}g - \frac{1}{8} \frac{W}{Mc^2} g^2 \right) \frac{\chi^3}{J(J+1)} \right\}$$

The previous expression follows from (69) taking into account (80). Because of (40) we finally have for the contribution of order α^4 of \mathcal{V} , with $W = mc^2$ and $\chi = 1$ in the above expression.

$$\Delta W_{nJ} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J+1} \left\{ 2 + \frac{3}{4} \frac{g}{J(J+1)} - \frac{1}{8} \frac{g^2}{J(J+1)} \right\} \tag{81}$$

for $J \geq 1$ and $n > J$.

Consider now the subspaces $F_{n,J,M,1}$, for $J \neq 1$ and determine the corresponding restriction of \mathcal{V}' (i.e. \mathcal{V} where $\mathcal{V}^{(3)}$ has been neglected).

The non-diagonal elements of the restrictions of \mathcal{V}' to F_{nJM1} relative to the basis (77), vanish. For diagonal elements we have the following results, from (69). We have set $W = Mc^2$ and $\chi = 1$ (see (40))

$$\left. \begin{aligned} \Delta W_{nJ} &= -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J+3} \left\{ 2 + \frac{3}{4} \frac{g}{J+1} + \frac{1}{8} \frac{g^2}{(J+1)(2J+1)} \right\} \\ \Delta W_{nJ} &= -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2J-1} \left\{ 2 - \frac{3}{4} \frac{g}{J} + \frac{1}{8} \frac{g^2}{J(2J+1)} \right\} \end{aligned} \right\} \tag{82}$$

for $l = J + 1$ and $n > l$, and

for $l = J - 1$ and $n > l$.

Furthermore we have to consider the particular situations where a $l = 0$ -component occurs. This corresponds to the subspaces $F_{n,1,M,1}$. In this case the solutions of (23) are of the form (74) for $J = 1$.

$$\phi_{J1}^M(\mathbf{x}) = R_+(r)\mathcal{Y}_{J21}^M(\theta, \phi) + R_-(r)\mathcal{Y}_{J01}^M(\theta, \phi)$$

From (23) and (69), we obtain the following coupled radial equations for $R_+(r)$ and $R_-(r)$.

$$\begin{aligned} & \left\{ \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{\hbar^2}{2mr^2} \begin{bmatrix} 6 & 0 \\ 0 & 0 \end{bmatrix} - \chi \alpha^2 mc^2 \frac{a_0}{r} \right. \\ & \quad - \frac{\alpha^4 mc^2}{2} \frac{a_0^2}{r^2} + \frac{\alpha^4 mc^2}{2} \frac{3g}{4} \frac{a_0^3}{r^3} \begin{bmatrix} -\frac{3}{2} & 0 \\ 0 & 0 \end{bmatrix} \\ & \quad - \frac{\alpha^4 mc^2}{16} \frac{W}{Mc^2} g^2 \frac{a_0^3}{r^3} \begin{bmatrix} \frac{1}{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{bmatrix} \\ & \quad \left. + \alpha^6 mc^2 \frac{a_0^4}{r^4} \left\{ \left(\frac{h_F^2}{128} + \frac{g^2}{48} \right) - \frac{g^2}{12} \begin{bmatrix} \frac{1}{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{bmatrix} \right\} \right\} \begin{bmatrix} R_+(r) \\ R_-(r) \end{bmatrix} = \epsilon \begin{bmatrix} R_+(r) \\ R_-(r) \end{bmatrix} \quad (83) \end{aligned}$$

The analogy of these coupled radial equations with (51) is obvious. Our problem is similar to the one we had treated in Section 2 and we can use this formal analogy to express the result for $l = J + 1$ using (56).

$$\Delta W_{n1} = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{5} \left\{ 2 + \frac{3}{8} g + \frac{1}{8} \frac{g^2}{6} \right\}, \quad l = J + 1 = 2 \quad (84)$$

i.e. the same expression as (82) for $J = 1$ in the case $l = J + 1$.

The result for $l = J - 1 = 0$ is obtained similarly from (57)

$$\Delta W_{n1} = -\frac{\alpha^4 mc^2}{2n^3} \left\{ 2 - \frac{1}{2} \sqrt{h_F^2 + \frac{8}{3} g^2} \right\}, \quad l = J - 1 = 0 \quad (85)$$

Collecting the results (78) and (79) for $S = 0$ and the results (81), (82), (84) and (85) for $S = 1$ we obtain the following formula for the contribution ΔW of order α^4 of \mathcal{V} . For $l \neq 0$

$$\Delta W = -\frac{\alpha^4 mc^2}{2n^3} \frac{1}{2l+1} \left[2 + \frac{g}{2} \left\{ \begin{array}{ll} 0 & \text{for } S = 0, J = l \\ \frac{-3(l+\frac{3}{2}) + g/4}{(l+1)(2l+3)} & \text{for } S = 1, J = l+1 \\ \frac{\frac{3}{2} - g/4}{l(l+1)} & \text{for } S = 1, J = l \\ \frac{3(l-\frac{1}{2}) + g/4}{l(2l-1)} & \text{for } S = 1, J = l-1 \end{array} \right. \right] \quad (86)$$

For $l = 0$

$$\Delta W = -\frac{\alpha^4 mc^2}{2n^3} \left[2 - \frac{1}{2} \left\{ \begin{array}{ll} h_F & \text{for } S = 0 \\ \sqrt{h_F^2 + \frac{8}{3} g^2} & \text{for } S = 1 \end{array} \right. \right]$$

whereas the unperturbed spectrum is given by

$$W_n^{(0)} = Mc^2 - mc^2 \left\{ \frac{\alpha^2}{2n^2} - \frac{15}{32} \frac{\alpha^4}{n^4} + O(\alpha^6) \right\} \quad (87)$$

These results call for some comments. First, for $l \neq 0$ and $g = 2$, the formula (86) corresponds to the fine and hyperfine structure of the positronium as obtained from the Breit equation [12]. Consequently, for $g = 2.0023$, the gyromagnetic factor of the electron (and positron), our results are very close to the predictions of Breit. For theoretical predictions from Bethe-Salpeter equation and QED techniques applied on bound state problems we also refer to [12], [13] and [14].

Second, for $l = 0$, to compare our results with the other theoretical predictions and with the experimental data [15], [16], we obviously have to take into account the energy shifts due to the instability of the positronium. In this way we have to add an energy shift term

$$\frac{1}{2} \frac{\alpha^4 mc^2}{n^3}$$

(from the Breit equation) to the energy level $n^3 S_1$ of the positronium and which is due to the virtual electron-positron annihilation. In (86), taking for $h_F = h_{(1)} = h_{(2)}$ the value 1.048 as for the electron in the hydrogen atom, we then find the following hyperfine energy separation for the S-states of the positronium

$$W(n^3 S_1) - W(n^1 S_0) = 1.095 \frac{\alpha^4 mc^2}{n^3} \quad (88)$$

which corresponds to the frequencies $191.81/n^3$ [GHz]. For the ground state $n = 1$, the measurements of E. R. Carlston, V. W. Hugues and I. Lindgren give the frequency 203.4 [GHz]. (This result is reproduced up to the last significant figure.)

Acknowledgements

I would like to express my gratitude to H. Beck and N. Giovannini for their suggestions and comments on the subject. Furthermore, my gratefulness goes to P. Huguenin and C. Piron for several helpful discussions.

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