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On The Treatment of Möller and Breit-Potentials and the Covariant Two-Body Equation for Positronium and Muonium*

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Abstract

A consistent non-perturbative treatment of the relativistic Möller potential is proposed and the application of a covariant two-body equation derived from field theory to the spectra of positronium and muonium is discussed.

1. Introduction

Many authors have discussed the difficulties with the Breit or Möller-type of relativistic two-body potentials. Some of these difficulties stem from an additional external potential to the two-body problem. We shall discuss here the relativistic two-body problem only; systems like hydrogen, muonium and positronium. The purpose of this report is to show how a fully covariant two- (and many) body wave equation can be derived from field theory, how it can be solved and how it can be applied sucessfully to the description of precision spectra in relativistic systems. We shall explain a method of treatment of negative energy states in the Möller type relativistic potentials. Finally, we give a summary of numerical results obtained so far.

2. Covariant equations

Let P_μ be the total momentum of the two-body system, and $p_\mu = (1 - a)\, p_{1\mu} - a p_{2\mu}$, the relative momentum of the two particles with $a = m_1/(m_1 + m_2)$, for example. The covariant two-body equation is [1]

$$\{P_\| + (a\alpha_\perp^1 + (1 - a)\alpha_\perp^2) \cdot P_\perp + (\alpha_\perp^1 - \alpha_\perp^2) \cdot p_\perp - m_1\gamma_\|^1 - m_2\gamma_\|^2 - V(r_\perp)\}\Phi(x_1, x_2) = 0. \quad (1)$$

The notation is as follows. $P_\|$ and $P_\perp$ are the parallel and perpendicular components of P_μ relative to the normal n_μ to a space-like surface Σ: $P_\mu = (P \cdot n)n_\mu + P_{\perp\mu} = P_\| n_\mu + P_{\perp\mu}$. Note that for $n_\mu = (1000)$, $P_\|$ is just $P_0 = H$, the total Hamiltonian and $P_{\perp\mu} = (0, \boldsymbol{P})$. Further, $\alpha_\perp^\mu = (\gamma \cdot n)\gamma_\perp^\mu$ where $\gamma_\mu = (\gamma \cdot n)n_\mu + \gamma_{\perp\mu} \equiv \gamma_\| n_\mu + \gamma_{\perp\mu}$. The relativistic potentials V are functions of the relative distance $r_\perp$ only, where $r_\mu = x_{1\mu} - x_{2\mu} = (r \cdot n)n_\mu + r_{\perp\mu}$, hence the magnitude $r_\perp = ((r \cdot n)^2 - r_\mu^2)^{1/2}$. Only the perpendicular component of the relative momentum enters into the equation, hence it is a one-time equation, i.e., $\Phi(x_1, x_2)$ is independent of the relative time, or $\Phi = \Phi(P_\|, P_\perp; p_\perp)$ or $\Phi(R_\mu, r_\perp)$ where $R_\mu = a x_{1\mu} + (1 - a)x_{2\mu}$ is the centre-of-mass co-ordinate.

The separation of four vectors into their parallel and perpendicular components is Lorentz invariant. We can choose co-ordinates and Dirac matrices such that eq. (1) is of the form

$$\{P_0 - (a\boldsymbol{\alpha}_1 + (1 - a)\boldsymbol{\alpha}_2) \cdot \boldsymbol{P} - (\boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2) \cdot \boldsymbol{p} - m_1\beta_1 - m_2\beta_2 - V(\boldsymbol{r})\}\Phi = 0 \quad (2)$$

In the rest frame $\boldsymbol{P} = 0$, one obtains then a familiar two-body Hamiltonian.

Eq. (1) can be derived from the coupled Maxwell–Dirac equations for two fields $\psi_1(x)$, $\psi_2(x)$ by a variational principle which also gives us the form of the relativistic potentials [2]. For the minimal coupling of $\psi_i(x)$ to the electromagnetic potential $A_\mu(x)$ we obtain for the relativistic potential

$$V(r_\perp) = e_1 e_2 \frac{1 + \overset{(1)}{\alpha}{}_\perp^\mu \otimes \overset{(2)}{\alpha}{}_{\perp\mu}}{r_\perp} \to e_1 e_2 \frac{1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r} \quad (3)$$

The potentials arising from a Pauli coupling of the spinors ψ_1, ψ_2 to the electromagnetic field $F_{\mu\nu}$ have also been studied in detail [Refs. 2 and 3].

3. Mass conjugate equations

In this Section I discuss the negative energy solutions in the two-body rest frame Hamiltonian

$$H_{\text{real}} = (\boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2) \cdot \boldsymbol{p} + \beta_1 m_1 + m_2\beta_2 + e_1 e_2 \frac{1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r}. \quad (4)$$

The negative energy states of the single particle Dirac equation, in the first quantized theory, can be interpreted as follows. The negative energy states of the Hamiltonian $H_D = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m + (e_1 e_2)/r$ are identical with the positive energy states of the mass conjugate equation $H_D' = \boldsymbol{\alpha} \cdot \boldsymbol{p} - \beta m - (e_1 e_2/r)$ (change $m \to -m$). We can therefore consider *only positive energy solutions* of H_D and H_D' and interpret them as electron and positron motion in the field of another charge e_2; electron and positron thus differ by an "internal" quantum number [4]. The spectrum consists of discrete and continuum positive energy levels of H_D and positive continuum levels of H_D' (H_D' has no discrete spectrum) and these are all the physically interpretable states of the problem. For the two-body case, eq. (4), we have also two distinct mass conjugate Hamiltonian, eq. (4) and

$$H_{\text{rel}}' = (\boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2) \cdot \boldsymbol{p} + \beta_1 m_1 - \beta_2 m_2 - e_1 e_2 \frac{1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r}, \quad (5)$$

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where we have changed the sign of m_2. The case when the signs of both masses m_1 and m_2 are changed is equivalent to (4), and the case with $(-m_1)$, $(+m_2)$ is equivalent to (5). The negative energy solutions of (4) are identical to the positive energy solutions of (5). We shall now study the solutions of H and H'.

4. Solutions

We have analyzed the 16-component equation (4) or (5) by separating the angular part [3]. The 16 first order radial equations split into two groups of eight. There is a discrete symmetry transformation that does this splitting. In the set of eight equations four are algebraic so that four of the eight components of the wave functions can be eliminated. We can further reduce the remaining four first order equations into two coupled second-order Schrödinger type equations. We do the same procedure in the second set of eight equations.

For applications to atomic physics we expand the potentials as a power series in α/r. The major part of the coupled second-order equations turns out to be exactly soluble. The remaining potentials of order α^5 (in units of mc^2) we shall treat it as far as QED applications are concerned, as a perturbation. The exactly soluble equations are [5] for the first set ($M = m_1 + m_2$, $\Delta m = m_1 - m_2$)

$$\left\{\frac{1}{4}\left(E - \frac{M^2}{E}\right)\left(E - \frac{\Delta m^2}{E}\right) + \frac{\alpha}{r}\left(E - \frac{M^2 + \Delta m^2}{2E}\right) - \frac{j(j+1) - \alpha^2}{r^2} + \partial_r^2\right\}(ru_2) - 2\,\frac{\sqrt{j(j+1)}}{r^2}(rv_0) = 0$$

$$\left\{\frac{1}{4}\left(E - \frac{M^2}{E}\right)\left(E - \frac{\Delta m^2}{E}\right) + \frac{\alpha}{r}\left(E - \frac{M^2 + \Delta m^2}{2E}\right) - \frac{j(j+1) + 2 - \alpha^2}{r^2} + \partial_r^2\right\}(rv_0) - 2\,\frac{\sqrt{j(j+1)}}{r^2}(ru_2) = 0 \qquad (6)$$

and for the second set

$$\left\{\frac{1}{4}\left(E - \frac{M^2}{E}\right)\left(E - \frac{\Delta m^2}{E}\right) + \frac{\alpha}{r}\left(E - \frac{M^2 + \Delta m^2}{2E}\right) - \frac{j(j+1) - \alpha^2}{r^2} + \partial_r^2\right\}(ru_1) = 0$$

$$\left\{\frac{1}{4}\left(E - \frac{M^2}{E}\right)\left(E - \frac{\Delta m^2}{E}\right) + \frac{\alpha}{r}\left(E - \frac{M^2 + \Delta m^2}{2E}\right) - \frac{j(j+1) - \alpha^2\delta_E}{r^2} + \partial_r^2\right\}(rv_{00}) = 0$$

$$\delta_E = \frac{\Delta m^2 + M^2}{E^2} + \frac{M^2 \Delta m^2}{E^4} \qquad (7)$$

Here (u_2, v_0) and (u_1, v_{00}) are certain components of the wave function. Equations (7) of the second set are uncoupled. The first set (6) corresponds to states $l = j \mp 1$, $S = 1$ ($^3P_0$, $^3D_1$, $^3F_2$, ... and $^3S_1$, $^3P_2$, $^3D_2$, in nonrelativistic notation) and the second set (7) to $l = j$, $S = 0, 1$ ($^1S_0$, $^1P_1$, $^1D_2$, ... and $^3P_1$, $^3D_2$, $^3F_3$, ...). The discrete spectrum of eqs. (6) is given by [59

$$E_n^2 = \frac{M^2 + \Delta m^2}{2} \pm \frac{M^2 - \Delta m^2}{2}\left[1 + \frac{\alpha^2}{n^2}\right]^{-1/2} \qquad (8)$$

where $n = n_r + l$ with n_r = relativistic radial quantum number and

$$l(l + 1) = j(j + 1) - \alpha^2 \qquad (9)$$

(the non-relativistic label l_0 is equal to $(j - 1)$ or $(j + 1)$, for the two states in eq. (6)). The physically acceptable discrete solutions correspond to (+) sign in (8) with energy values just below the positive continuum $E < M$.

The second set of equations, (7), have also the same discrete spectrum (8), but now in the second equation of (7) we have

$$l(l + 1) = j(j + 1) - \alpha^2\delta_E \qquad (10)$$

For physical solutions near the positive continuum, $E \approx M$, δ_E is close to -1 (for $\Delta m \sim 0$) and (10) gives $l(l + 1) = j(j + 1) + \alpha^2$. This results in a wrong mass spectrum, for example, for parapositronium, already in terms of the order α^4. The inadequacy of the Breit interaction for parapositronium has been discussed by many authors [6]. We therefore use the mass conjugate, eq. (5), for the second set. Under the change $m_2 \to -m_2$, we have $M = m_1 + m_2 \to \Delta m = m_1 - m_2$ and the first set of equations is invariant. In the second set, the only change is $\delta_E \to 2(M^2\Delta m^2)/E^4 - \delta_E$, hence for solutions near the positive continuum again we now get $\delta_E \approx +1$. We propose therefore to use eq. (6) and eq. (7) with

$$\delta_E \to \delta'_E = \frac{M^2 - \Delta m^2}{E^2} + \frac{M^2 \Delta m^2}{E^4}. \qquad (11)$$

The eigenfunctions of eqs. (6) or (7) are the same as the one-body Coulomb–Dirac functions with the appropriate kinematical change of the parameters. But eqs. (6) and (7) contain full recoil of both particles and correct spin properties so that they can be used as a two-body starting point to make calculations in the Furry-picture of the two-body problems [7].

The remaining part of the potentials up to order α^5 for the coupled set (6) are given by

$$\Delta V_{11} = \left(\frac{2\alpha/r^2 - 8j(j+1)/Er^3}{(E - \Delta m^2/E)}\right)\partial_r$$

$$\Delta V_{12} = \sqrt{j(j+1)}\left[\frac{2}{r^2}\frac{E - M}{M} + \frac{6\alpha}{Er^3} + \frac{1}{r}\,\frac{2\alpha/r^2 - 8j(j+1)/Er^3}{(E - \Delta m^2/E)}\right]$$

$$\Delta V_{21} = \sqrt{j(j+1)}\left[\frac{2}{r^2}\frac{E - M}{M} + \frac{1}{r}\,\frac{4\alpha/r^2 - 2\alpha\Delta m^2/r^2E^2 - 8j(j+1)/Er^3}{(E - \Delta m^2/E)}\right]$$

$$\Delta V_{22} = \frac{2\alpha(2 - \Delta m^2/E^2)/r^2 - 8j(j+1)/Er^3}{(E - \Delta m^2/E)}\left(\partial_r + \frac{1}{r}\right) \qquad (12)$$

A coupled channel perturbation theory in E^2 leads to the following energy shifts [8]

$$\Delta E(n, l_0 = j+1, S=1) = -\frac{2\alpha^4(M^2-\Delta m^2)/2M}{16n^3(j+1)(j+\frac{3}{2})} - \frac{\alpha^4(M^2-\Delta m^2)^2/2M^3}{16n^3(j+\frac{1}{2})(j+\frac{3}{2})}$$

$$\Delta E(n, l_0 = j-1, S=1) = \frac{2\alpha^4(M^2-\Delta m^2)/2M}{16n^3(j-\frac{1}{2})j} + \frac{\alpha^4(M^2-\Delta m^2)^2/2M^3}{16n^3(j-\frac{1}{2})(j+\frac{1}{2})}$$

The perturbations in the second set (7) are

$$\Delta V_{11} = \frac{\frac{d}{dr}(1+2\alpha/Er-\Delta m^2/E^2)}{(1+2\alpha/Er-\Delta m^2/E^2)}\frac{d}{dr}$$

$$\Delta V_{12} = \frac{\Delta m}{E}\sqrt{j(j+1)}\,\frac{-d/dr\,(1+2\alpha/Er-\Delta m^2/E^2)}{r(1+2\alpha/Er-\Delta m^2/E^2)}$$

$$\Delta V_{21} = \Delta V_{12}/(1+2\alpha/Er)$$

$$\Delta V_{22} = 0$$

and these give the following energy shifts:

$$\Delta E(n, l_0 = j, S=0) = -\frac{\alpha^4(M^2-\Delta m^2)/2M}{16n^3 j(j+\frac{1}{2})(j+1)}\Delta_-$$

$$\Delta E(n, l_0 = j, S=1) = -\frac{\alpha^4(M^2-\Delta m^2)/2M}{16n^3 j(j+\frac{1}{2})(j+1)}\Delta_+ \qquad (j \neq 0) \tag{15}$$

where

$$\Delta_\pm = 1 \pm \left[1+4j(j+1)\frac{\Delta m^2}{M^2}\right]^{1/2}$$

For positronium, in particular, we find

$$\Delta_- = 0$$

$$\Delta_+ = 2. \tag{16}$$

It is also possible to study the anomalous magnetic moment potentials coming from a Pauli coupling in eq. (4). Let the anomalous magnetic moments of the particle be a_1 and a_2. We then obtain to order α^5 the following mass formulae [8]:

$$(1)\ E_{n,j+1,1} = E_+ - \frac{\mu\alpha^4}{4n^3(j+1)(j+\frac{3}{2})} \times \left(1+\frac{2(a_1+\xi^2 a_2)}{(1+\xi)^2} - 2a_1a_2\frac{\xi}{1+\xi}\right) - \frac{(\mu^2/M)\alpha^4}{2n^3(j+\frac{1}{2})(j+\frac{3}{2})}(1+a_1+a_2+a_1a_2)$$

$({}^3P_0, {}^3D_1, {}^3F_2, \ldots)$

$$(2)\ E_{n,j-1,1} = E_+ + \frac{\mu\alpha^4}{4n^3(j-\frac{1}{2})j} \times \left(1+\frac{2(a_1+\xi^2 a_2)}{(1+\xi)^2} - 2a_1a_2\frac{\xi}{1+\xi}\right) + \frac{(\mu^2/M)\alpha^4}{2n^3(j-\frac{1}{2})(j+\frac{1}{2})}(1+a_1+a_2+a_1a_2)$$

$({}^3S_1, {}^3P_2, {}^3D_3, \ldots)$

$$(3)\ E_{n,j,0} = E_+ - \frac{\mu\alpha^4}{4n^3(j+\frac{1}{2})(j+1)} \times \left(1+\frac{2a_1+2a_2\xi^2-2a_1a_2\xi}{(1+\xi)^2}\right) - \frac{(\mu^2/M)\alpha^4}{2n^3(j+\frac{1}{2})^2}\left(1+a_1+a_2+a_1a_2 - \xi a_2^2 + \frac{a_1a_2}{(1+\xi)^2}\right);\quad j\neq 0$$

$({}^1S_0, {}^1P_1, {}^1D_2, \ldots)$

$$(4)\ E_{n,j,1} = E_+ - \frac{\mu\alpha^4}{8n^3 j(j+\frac{1}{2})(j+1)} \times \left(1+\frac{2a_1+2a_2\xi^2-2a_1a_2\xi}{(1+\xi)^2}\right) + \frac{(\mu^2/M)\alpha^4}{2n^3(j+\frac{1}{2})^2}\left(1+a_1+a_2+a_1a_2 - \xi a_2^2 + \frac{a_1a_2}{(1+\xi)^2}\right)$$

$({}^3P_1, {}^3D_2, {}^3F_3, \ldots)$

$$\mu \equiv \frac{m_1m_2}{m_1+m_2}, \qquad \xi \equiv m_1/m_2. \tag{17}$$

Here E_+ is the spectrum independent of normal and anomalous magnetic moments, from (8)

$$E_+ \equiv (m_1+m_2) - \frac{\mu\alpha^2}{2n^2} - \frac{\mu\alpha^4}{2n^3(l+\frac{1}{2})} + \frac{3}{8}\frac{\mu\alpha^4}{n^4} - \frac{1}{8}\frac{\mu^2\alpha^4}{n^4 m_2} + O(\alpha^6) \tag{18}$$

5. Applications

5.1. *Positronium*

For parapositronium ($S = 0, l = j$) there are no normal or anomalous magnetic spin–orbit and spin–spin interactions up to order α^5 and α^6, respectively, and we obtain the formula

$$E = 2m - \frac{m\alpha^2}{4n^2} - \frac{m\alpha^4}{2n^3(2j+1)} + \frac{11}{64}\frac{m\alpha^4}{n^4} + O(\alpha^6)$$

except for Lamb shift contributions. There are only three measured positronium intervals:

(a) For the positronium hyperfine splitting we obtain from eqs. (17)

$$\Delta E_{\mathrm{Hfs}} = \tfrac{3}{4}m\alpha^2 - \tfrac{1}{6}m\alpha^4(\alpha/2\pi) + \cdots + \tfrac{5}{12}m\alpha^4(\alpha/2\pi)$$

The third term comes from the anomalous magnetic moment. To this we must add the annihilation contribution. Thus in total

$$\Delta E_{\mathrm{Hfs}} = \tfrac{7}{12}m\alpha^4 + \tfrac{5}{12}m\alpha^4(\alpha/2\pi) + \ldots$$

The self-energy corrections (Lamb shift) will be treated separately [10].

(b) For the positronium $n = 2$, $n = 1$ transition which has recently been measured we find

$$\Delta E_{12} = \tfrac{3}{8}R_y - 0.468093R_y - \frac{35}{96}\frac{\alpha^3 R_y}{2\pi}$$

(c) For the positronium ($2^3S_1 - 2^3P_2$) fine splitting

$$\Delta E = \tfrac{23}{480}\alpha^2 R_y$$

These results agree with those of Fulton *et al.* [9].

5.2. *Hydrogen and muonium*

(i) Ground state hyperfine splitting

$$\Delta E_{\mathrm{Hfs}} = \frac{8}{3}\frac{\xi}{(1+\xi)^3} m_e\alpha^4 \left\{(1 + a_e)(1 + a_2) - \tfrac{3}{4}\xi a_2^2 + \tfrac{3}{4}a_e \frac{a_2}{(1+\xi)^2}\right\}$$

(ii) $n = 1$, $n = 2$ splitting

$$\Delta E_{12} = \tfrac{3}{8}\mu\alpha^2 - \tfrac{7}{128}\mu\alpha^4 + \tfrac{15}{128}\mu\alpha^4 \frac{\xi}{1+\xi} - \tfrac{7}{16}\mu\alpha^4 \times \left(1 + \frac{2(a_1 + \xi^2 a_2)}{(1+\xi)^2} - 2a_1a_2\frac{\xi}{1+\xi}\right) - \frac{7}{12}\frac{\mu^2}{M}\alpha^4(1 + a_1 + a_2 + a_1a_2)$$

(iii) $2P_{3/2} - 2P_{1/2}$ splitting

$$\Delta E = -\frac{\alpha^2 R_y}{16}\frac{1}{(1+\xi)}\left(1 + \frac{2a_1 + 2a_2\xi^2}{(1+\xi)^2} - 2a_1a_2\frac{\xi}{1+\xi}\right) + \frac{\alpha^2 R_y}{9}\frac{\xi}{(1+\xi)}(1 + a_1 + a_2 + a_1a_2)$$

6. Conclusions

The purpose of our work is to develop non-perturbative and covariant equations with relativistic potentials for two and many-body problems in quantum electrodynamics including radiative corrections. Here we discussed the two-body problem with the mutual Möller and anomalous magnetic moment potentials. The self energy terms will be given elsewhere [10]. In particular, we addressed ourselves to the question of negative energy states in the solutions of the bound state equations. We found an exactly soluble genuine relativistic two-body potential and have treated the small remaining potentials up to order α^5 by perturbation. Having shown that the equations are tractable, they can now be solved completely numerically. *When the self energy terms are included* it should be possible to obtain precise tests of QED in positronium, muonium and hydrogen to order α^6 (and more) directly from a wave equation instead of calculating separate Feynman diagrams of each radiative correction.

Most of this lecture is based on Refs. [5] and [8], work done in collaboration with N. Ünal whom I thank for many fruitful discussions.

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