

## A NEW APPROACH TO BOUND-STATE QUANTUM ELECTRODYNAMICS

### II. SPECTRA OF POSITRONIUM, MUONIUM AND HYDROGEN

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The solutions of a covariant two-body equation are applied to the spectra of H, muonium and positronium. In order to compare with the standard results we have expanded the potentials, the recoil terms and the perturbation calculations up to order  $\alpha^5$ . The best known intervals, namely Hfs of H, muonium and positronium and the  $2^3S_1-1^3S_1$  interval of positronium are obtained to this order in agreement with standard results and experiments. Having thus verified the nonperturbative equation to order  $\alpha^5$ , the recoil and normal and anomalous magnetic moment terms can now be evaluated numerically to all orders.

One can divide the precision tests of quantum electrodynamics into three groups. First we have the high energy experiments, accurate to a few percent, but which test the electron and photon propagators and form factors at very high momentum transfers<sup>1</sup>), and involve only few higher order diagrams in perturbation theory. In the second group we may put the (g-2) experiments which involve at the moment diagrams up to eight order<sup>2</sup>). The theory is again pure perturbation theory although the number of graphs, the renormalization procedures, overlapping and nested divergences become considerably more difficult. In contrast, the third group of tests all involve nonperturbative bound state problems in hydrogen, positronium, muonium, . . . , namely the Lamb shifts, hyperfine splittings and decay rates. The nonperturbative starting point for this third type of calculations has been described as an “art”<sup>3</sup>) in contrast to the well-defined mechanical rules of perturbation theory. More and more accurate relativistic bound state wavefunctions are necessary to perform further perturbations on them. The development of the various starting points for QED-bound state problems has been reviewed recently by Bodwin, Yennie and Gregorio<sup>3</sup>). In the most recent works the starting point for the nonperturbative bound state problems has been a one-particle Dirac equation. In this work we take a recently discussed genuinely relativistic 2-body equation<sup>4,5</sup>) as

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a starting point for bound state problems. This equation has the following properties:

- i) It is relativistic and covariant;
- ii) it takes full account of spin and recoil of *both* particles (it is a  $16 \times 16$  spinor equation);
- iii) it is a one-time equation with relativistic potentials; relative coordinates are 3-dimensional ( $\mathbf{r}$ ). Since Poincaré invariance is built in, there is no retardation problem;
- iv) it is derived from the QED action by a variational principle on the configuration space wave function and the exchange of a massless particle is essential in the derivation;
- v) center of mass and relative coordinates are exactly separable;
- vi) angular and radial parts are exactly separable;
- vii) it provides relativistic good quantum numbers for positronium instead of  $L$  and  $S$ . Vertex radiative corrections are included partly by an anomalous magnetic moment Pauli coupling;
- viii) the potentials up to order  $\alpha^4$  are exactly soluble. This soluble part may be taken to be the basis for a Furry-picture perturbation theory both for scattering and bound state problems.

We believe this approach brings a conceptual and practical simplicity to relativistic bound state problems. The equation is

$$\left\{ (\gamma^{(1)\mu} p_{1\mu} - m_1) \otimes \gamma^{(2)} \cdot n + \gamma^{(1)} \cdot n \otimes (\gamma^{(2)\mu} p_{2\mu} - m_2) + e_1 e_2 \frac{\gamma^{(1)\mu} \gamma^{(2)}_{\mu}}{r_{\perp}} + V_{\text{magn}} + V_{\text{rad}} \right\} \Phi(x_1, x_2) = 0. \tag{1}$$

Here  $\gamma^{(1)}_{\mu}$  and  $\gamma^{(2)}$  are the Dirac matrices for each particle,  $n_{\mu}$  a unit vector in the direction of the total momentum  $P_{\mu} = p_{1\mu} + p_{2\mu}$  and  $r_{\perp} = [(x, n)^2 - x^2]^{1/2}$  is the relativistic distance perpendicular to  $n$ . For  $n_{\mu} = (1000)$ ,  $r_{\perp} = r$ , the ordinary radial distance. It follows that the equation is independent of the “time” component of the relative momentum  $p_{\parallel}$ , where  $p_{\mu} = [m_2/(m_1 + m_2)]p_{1\mu} + [m_1/(m_1 + m_2)]p_{2\mu}$ . In the center of mass frame  $P_{\mu} = (M000)$ , the mass operator becomes

$$\mathbb{M} = (\alpha_1 - \alpha_2) \cdot \mathbf{p} + \beta_1 m_1 + \beta_2 m_2 + e_1 e_2 \frac{1 - \alpha_1 \cdot \alpha_2}{\tau} + U_{\text{magn}} + U_{\text{rad}}, \tag{2}$$

where the potential due to anomalous magnetic moment,  $U_{\text{magn}}$ , has been given elsewhere<sup>4-8</sup>). The potentials due to other radiative processes,  $U_{\text{rad}}$ , including the Uehling and self-energy potentials which we have treated

separately<sup>9-11</sup>), will be included perturbatively. In previous papers we discussed in detail the explicit separation of the radial equations in (1) and (2)<sup>6</sup>), the exactly soluble part of (2)<sup>7</sup>) and the calculation of perturbations due to  $U_{\text{mag}}$ <sup>8</sup>). The main exactly soluble spectrum for arbitrary masses  $m_1, m_2$  is<sup>6</sup>)

$$E_{\pm}^2 = \frac{M^2 + \Delta m^2}{2} \pm \frac{M^2 - \Delta m^2}{2} \left[ 1 + \frac{\alpha^2}{(n_r + l)^2} \right]^{-1/2}, \quad M = m_1 + m_2, \\ \Delta m = m_1 - m_2, \quad (3)$$

where  $\pm$  refer to levels just below the positive continuum, and just above the negative continuum, respectively; the treatment and interpretation of the latter solutions are given in ref. 8.

We pass to the principle quantum number  $n$  and total angular momentum; by using  $l(l+1) = j(j+1) - \alpha^2$ ,  $(j-1)(j) - \alpha^2$ ,  $(j+1)(j+1)\alpha^2$ , respectively and setting  $n_r + l = n - \alpha^2/2(j + \frac{1}{2}) + \mathcal{O}(\alpha^4)$ , etc.

Eq. (3), when expanded, gives then for small  $m_1/m_2$ ,

$$E_+(n, l) = (m_1 + m_2) - \frac{m_1 \alpha^2}{2n^2(1 + m_1/m_2)} - \frac{m_1 \alpha^4}{2n^3(1 + m_1/m_2)(l + \frac{1}{2})} \\ + \frac{3}{8} \frac{m_1 \alpha^4}{(1 + m_1/m_2)n^4} - \frac{1}{8} \frac{m_1^2/m_2 \alpha^4}{(1 + m_1/m_2)^2 n^4} + \mathcal{O}(\alpha^6) \\ (l = j \pm 1, j). \quad (4)$$

It will turn out, as we shall see, that eq. (3) is exact for para-positronium up to order  $\alpha^4$  because the normal and anomalous spin terms will be zero for this case; and we obtain in this case

$$E_{(l=j)}^{\text{paraps.}} = 2m - \frac{m\alpha^2}{4n^2} - \frac{m\alpha^4}{2n^3(2j+1)} + \frac{11}{64} \frac{m\alpha^4}{n^4} + \mathcal{O}(\alpha^5). \quad (5)$$

Eq. (4) should be compared with Lepage<sup>12</sup>). There the third term is written as  $[m_1 \alpha^4 / (1 + m_1/m_2)n^3] / 2(j + \frac{1}{2})$ . The reason for this difference is that in ref. 12,  $j$  is half integer because a one-body equation is used for the electron. In our case, we shall use  $j$  for the total angular momentum of the two-body system: our  $j$  is integer, but  $l \cong j, j-1, j+1$  to order  $\alpha^2$ , so that both results are numerically the same. The energy shifts due to fine and hyperfine splittings both for normal and anomalous magnetic moment interactions calculated as perturbations to the exact part (3) to order  $\alpha^5$  and  $\alpha^6$  are<sup>8</sup>)

1)

$$\begin{aligned}
 E^1(n, l = j + 1, S = 1) = & -\frac{2\alpha^4(M^2 - \Delta m^2)/2M}{4^2 n^3(j+1)(j+\frac{3}{2})} - \frac{\alpha^4(M^2 - \Delta m^2)^2/2M^3}{4^2 n^3(j+\frac{1}{2})(j+\frac{3}{2})} \\
 & \times \left(1 + \frac{(4j+3)\lambda M - \tau\Delta m}{2\alpha(j+1)}\right) \\
 & - \tilde{a}_1 \tilde{a}_2 \frac{(M^2 - \Delta m^2)^3 \alpha^3/2M^3}{2 \cdot 4n^3(j+\frac{1}{2})(j+1)(j+\frac{3}{2})};
 \end{aligned}$$

2)

$$\begin{aligned}
 E^1(n, l = j - 1, S = 1) = & \left\{ \frac{2\alpha^4(M^2 - \Delta m^2)/2M}{4^2 n^3(j-\frac{1}{2})j} + \frac{\alpha^4(M^2 - \Delta m^2)^2/2M^3}{4^2 n^3(j-\frac{1}{2})(j+\frac{1}{2})} \right. \\
 & \times \left(1 + \frac{(4j+1)\lambda M + \tau\Delta m}{2j\alpha}\right) \\
 & \left. - \tilde{a}_1 \tilde{a}_2 \frac{\alpha^3(M^2 - \Delta m^2)^3/2M^3}{2 \cdot 4^3 n^3(j-\frac{1}{2})j(j+\frac{1}{2})} \right\} (1 - \delta_{j1});
 \end{aligned} \tag{6}$$

and

3)

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

4)

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

where

$$\begin{aligned}
 \Delta_{\pm} & \equiv A \pm [A^2 + 4j(j+1)B^2]^{1/2}, \\
 A & \equiv 1 + \frac{\lambda M + \tau\Delta m}{2\alpha} \frac{(M^2 - \Delta m^2)}{M^2} - \frac{\tilde{a}_1 \tilde{a}_2}{2M^2 \alpha} (M^2 - \Delta m^2)^2, \\
 B & \equiv \frac{\Delta m}{M} + \frac{\tau(M^2 - \Delta m^2)}{\alpha M}.
 \end{aligned}$$

For positronium, in particular, we find

$$\Delta_+ = 2 \left(1 + \frac{\lambda M}{2\alpha} - \frac{\tilde{a}_1 \tilde{a}_2 M^2}{2\alpha}\right), \quad \Delta_- = 0. \tag{7}$$

Here  $\tilde{a}_1, \tilde{a}_2$  are the anomalous magnetic moments and we shall put  $\tilde{a}_1 = (e_1/2m_1)a_1$ ,  $\tilde{a}_2 = (e_2/2m_2)a_2$ ,

$$\lambda = e_1 \bar{a}_2 + e_2 \bar{a}_1, \quad \tau = e_1 \bar{a}_2 - e_2 \bar{a}_1. \quad (8)$$

Taking the recoil and the spin parts together the final results are

$$\begin{aligned}
 &1) \\
 &E_{n,j+1,1} = E_{(+)} - \frac{\mu\alpha^4}{4n^3(j+1)(j+\frac{3}{2})} \left[ 1 + \frac{2(a_1 + \xi^2 a_2)}{(1+\xi)^2} - 2a_1 a_2 \frac{\xi}{1+\xi} \right] \\
 &\quad - \frac{(\mu^2/M)\alpha^4}{2n^3(j+\frac{1}{2})(j+\frac{3}{2})} [1 + a_1 + a_2 + a_1 a_2]; \\
 &(\ ^3P_0, \ ^3D_1, \ ^3F_2, \dots) \\
 &2) \\
 &E_{n,j-1,1} = E_{(+)} + \frac{\mu\alpha^4}{4n^3(j-\frac{1}{2})j} \left[ 1 + \frac{2(a_1 + \xi^2 a_2)}{(1+\xi)^2} - 2a_1 a_2 \frac{\xi}{1+\xi} \right] \\
 &\quad + \frac{(\mu^2/M)\alpha^4}{2n^3(j-\frac{1}{2})(j+\frac{1}{2})} [1 + a_1 + a_2 + a_1 a_2]; \\
 &(\ ^3S_1, \ ^3P_2, \ ^3D_3, \dots) \quad (9) \\
 &3) \\
 &E_{n,j,0} = E_{(+)} - \frac{\mu\alpha^4}{4n^3(j+\frac{1}{2})(j+1)} \left[ 1 + \frac{2a_1 + 2a_2 \xi^2 - 2a_1 a_2 \xi}{(1+\xi)^2} \right] \\
 &\quad - \frac{(\mu^2/M)\alpha^4}{2n^3(j+\frac{1}{2})^2} \left( 1 + a_1 + a_2 + a_1 a_2 - \xi a_2^2 + \frac{a_1 a_2}{(1+\xi)^2} \right), \quad (j \neq 0); \\
 &(\ ^1S_0, \ ^1P_1, \ ^1D_2, \dots) \\
 &4) \\
 &E_{n,j,1} = E_{(+)} - \frac{\mu\alpha^4}{8n^3 j(j+\frac{1}{2})(j+1)} \left( 1 + \frac{2a_1 2a_2 \xi^2 - 2a_1 a_2 \xi}{(1+\xi)^2} \right) \\
 &\quad + \frac{(\mu^2/M)\alpha^4}{2n^3(j+\frac{1}{2})^2} \left( 1 + a_1 + a_2 + a_1 a_2 - \xi a_2^2 + \frac{a_1 a_2}{(1+\xi)^2} \right), \\
 &\quad \left( \mu = \frac{m_1 m_2}{M}, \xi = \frac{m_1}{m_2} \right). \\
 &(\ ^3P_1, \ ^3D_2, \ ^3F_3, \dots)
 \end{aligned}$$

We now apply these results to the following important special intervals:

### 1. Hydrogen and muonium ground-state hyperfine splitting

This is the interval between the  $n = 1$ ,  $F = 0$  and  $F = 1$  levels, or

$$\Delta E^{\text{Hfs}} = E(n = 1, l = j - 1 = 0, S = 1) - E(n = 1, l = j = 0, S = 0).$$

All terms in our expansions cancel except for the last one in eqs. (9) and we obtain

$$\begin{aligned} \Delta E^{\text{Hfs}} = & \frac{(\mu^2/M)\alpha^4}{2n^3(j - \frac{1}{2})(j + \frac{1}{2})} (1 + a_1 + a_2 + a_1 a_2) \Big|_{j=1} \\ & + \frac{(\mu^2/M)\alpha^4}{2n^3(j + \frac{1}{2})^2} \left( 1 + a_1 + a_2 + a_1 a_2 - \xi a_2^2 + \frac{a_1 a_2}{(1 + \xi)^2} \right) \Big|_{j=0}, \end{aligned}$$

which gives finally with  $\xi = m_1/m_2$

$$\Delta E^{\text{Hfs}} = \frac{8}{3} \frac{\xi}{(1 + \xi)^3} m_e \alpha^4 \left[ (1 + a_e)(1 + a_2) - \frac{3}{4} \xi a_2^2 + \frac{3}{4} a_e \frac{a_2}{(1 + \xi)^2} \right], \quad (10)$$

where  $a_2$  is the anomalous magnetic moment of the proton or moun. It is interesting to note that Fermi's effective dipole-dipole interaction formula emerges at the end with proper recoil correction and a sum of both normal and anomalous magnetic moment contributions. Numerical values obtained from eq. (8) are

*Hydrogen:*  $(1 + a_p) = 2.7928456$ ,  $(1 + a_e) = 1.001159652$

$$\xi = 5.446174 \times 10^{-4}$$

$$\Delta E_{\text{Hfs}} = 1420.348 \dots \text{ MHz}$$

$$(\Delta E_{\text{exp}} = 1420.405752)$$

*Muonium:*  $(1 + a_\mu) = 1.001165924$ ,  $(1 + a_e) = 1.001165652$

$$\xi = 10^{-3} \times 4.8363305$$

$$\Delta E_{\text{Hfs}} = 4.463.0601 \text{ MHz}$$

$$(\Delta E_{\text{exp}} = 4463.302)$$

## 2. Hydrogen and muonium $n = 1$ , $n = 2$ splitting

From eqs. (9) and (4) we have

$$\begin{aligned} \Delta E(2^3S_1 - 1^3S_1) = & -\frac{m_1\alpha^2}{2(1+\xi)}\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right) - \frac{m_1\alpha^4}{2(1+\xi)(l+\frac{1}{2})}\left(\frac{1}{n_2^3} - \frac{1}{n_1^3}\right) \\ & + \frac{3}{8}\frac{m_1\alpha^4}{(1+\xi)}\left(\frac{1}{n_2^4} - \frac{1}{n_1^4}\right) - \frac{1}{8}\frac{m_1\xi\alpha^4}{(1+\xi)^2}\left(\frac{1}{n_2^4} - \frac{1}{n_1^4}\right) \\ & + \frac{\mu\alpha^4}{4(j-\frac{1}{2})j}\left(1 + \frac{2(a_1 + \xi^2a_2)}{(1+\xi)^2} - 2a_1a_2\frac{\xi}{(1+\xi)}\right)\left(\frac{1}{n_2^3} - \frac{1}{n_1^3}\right) \\ & + \frac{(\mu^2/M)\alpha^4}{2(j-\frac{1}{2})(j+\frac{1}{2})}(1+a_1+a_2+a_1a_2)\left(\frac{1}{n_2^3} - \frac{1}{n_1^3}\right)\Bigg|_{\substack{j=1 \\ n_1=1, n_2=2}} \end{aligned}$$

or

$$\begin{aligned} \Delta E = & \frac{3}{8}\mu\alpha^2 + \frac{7}{128}\mu\alpha^4 + \frac{15}{128}\mu\alpha^4\frac{\xi}{1+\xi} \\ & - \frac{7}{16}\mu\alpha^4\left(1 + \frac{2(a_1 + \xi^2a_2)}{(1+\xi)^2} - 2a_1a_2\frac{\xi}{1+\xi}\right) \\ & - \frac{7}{12}\frac{\mu^2}{M}\alpha^4(1+a_1+a_2+a_1a_2). \end{aligned} \tag{11}$$

## 3. Positronium hyperfine splitting

Since in this case  $\Delta_- = 0$  in eqs. (6), there is no spin shift in  $1S_0$ -level (para-positronium) to order  $\alpha^4$ . Hence the Hfs-splitting is

$$\begin{aligned} \Delta E_{\text{Hfs}} = & \frac{\mu\alpha^4}{4n^3j(j-\frac{1}{2})}\left[1 + \frac{2(a_1 + \xi^2a_2)}{(1+\xi)^2} - 2a_1a_2\frac{\xi}{(1+\xi)}\right] \\ & + \frac{(\mu^2/M)\alpha^4}{2n^3(j-\frac{1}{2})(j+\frac{1}{2})}(1+a_1+a_2+a_1a_2)\Bigg|_{j=1}, \end{aligned}$$

which gives

$$\Delta E_{\text{Hfs}} = \frac{4}{12} m\alpha^2 + \frac{5}{12} m\alpha^4 \left(\frac{\alpha}{2\pi}\right) - \frac{1}{6} m\alpha^4 \left(\frac{\alpha}{2\pi}\right)^2. \tag{12}$$

To this we must add the annihilation contribution, evaluated by a function potential both for normal and anomalous magnetic moments. For these we take the standard results<sup>13)</sup> namely  $\frac{3}{12}m\alpha^4$  and  $(-\alpha/2\pi)(\frac{13}{9} + \ln 2)m\alpha^4$ , respectively. Thus in total

$$\Delta E_{\text{Hfs}} = \frac{7}{12} m\alpha^4 + \frac{5}{12} m\alpha^4 \left(\frac{\alpha}{2\pi}\right) - \frac{\alpha}{2\pi} \left(\frac{13}{9} + \ln 2\right) m\alpha^4 + \dots. \tag{12'}$$

4. Positronium  $n = 2, n = 1$  transition

This is the newly measured<sup>14)</sup> interval

$$\Delta E_{12} = E(2, j = l + 1 = 1, S = 1) - E(1, j = l + 1 = 1, S = 1).$$

In this energy shift we have

a) a recoil part

$$\begin{aligned} \Delta E_{12}^{\text{recoil}} &= -\frac{m\alpha^4}{4} \left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right) - \frac{m\alpha^4}{2} \left(\frac{1}{n_2^3} - \frac{1}{n_1^3}\right) + \frac{11}{64} m\alpha^4 \left(\frac{1}{n_3^4} - \frac{1}{n_1^4}\right) \\ &= \frac{3}{8} \text{Ry} + \alpha^2 \text{Ry} \left(\frac{7}{8} - \frac{11 \cdot 15}{8 \cdot 64}\right); \\ &\qquad\qquad\qquad 0.875 \quad 0.3222656 \end{aligned}$$

b) the normal magnetic moment term does not contribute because of the  $\delta_{\mu}$ -terms in eqs. (6);

c) the annihilation part gives

$$\Delta E_{12}^{\text{annih}} = \alpha^2 \text{Ry} \frac{7}{6} \left(\frac{1}{n_2^3} - \frac{1}{n_1^2}\right) = -\alpha^2 \text{Ry} \frac{49}{48}. \tag{1.020833}$$

Thus up to order  $\alpha^4$  in total

$$\Delta E_{21} = \frac{3}{8} \text{Ry} - 0.468093\alpha^2 \text{Ry}; \tag{13}$$

d) anomalous magnetic moment contribution from eq. (10) to order  $\alpha^3 \text{Ry}$  is

$$\Delta E_{21}^{(a)} = -\frac{\alpha^3 \text{Ry}}{2\pi} \frac{35}{96}.$$



### 5. Hydrogen and positronium fine splittings

Finally we give the hydrogen fine structure splitting

$$\begin{aligned} \Delta E(2P_{3/2} - 2P_{1/2}) = & -\frac{\alpha^2 \text{Ry}}{16} \frac{1}{(1+\xi)} \left( 1 + \frac{2a_1 + 2a_1\xi^2}{(1+\xi)^2} - 2a_1a_2 \frac{\xi}{1+\xi} \right) \\ & + \frac{\alpha^2 \text{Ry}}{9} \frac{\xi}{(1+\xi)} (1 + a_1 + a_2 + a_1a_2), \end{aligned} \quad (14)$$

and the measured<sup>15)</sup> positronium splitting

$$\begin{aligned} \Delta E^{\text{ps}}(2^3S_1 - 2^3P_2) = & -\frac{1}{12}\alpha^2 \text{Ry} + \frac{7}{48}\alpha^2 \text{Ry} - \frac{7}{480}\alpha^2 \text{Ry} + \mathcal{O}(\alpha^5) \\ & \text{(recoil)} \quad \text{(annihilation)} \quad \text{(normal magn.} \\ & \qquad \qquad \qquad \text{moment)} \\ = & \frac{23}{480}\alpha^2 \text{Ry} + \mathcal{O}(\alpha^5). \end{aligned} \quad (15)$$

Eqs. (13) and (14) agree with the result of Fulton and Martin<sup>16)</sup> and Fulton<sup>17)</sup>, but now are obtained from a 2-body one-time wave equation.

Our results agree with the standard ones to order  $\alpha^4$  and to order  $\alpha^5$  for terms coming from the anomalous magnetic moment<sup>18)</sup>. There are however other self energy terms to order  $\alpha^5$  which for the moment we take over from standard results, but which eventually may be included dynamically as a potential in eq. (2) as we have indicated.

There are a large number of terms to order  $\alpha^6 \sim \alpha^2 \text{Ry}$ :

- i) those coming from the expansion of the recoil term (3);
- ii) those coming from the expansion potentials;
- iii) those coming from the evaluation of the perturbation averages. We have taken here, in order to compare with standard results terms up to order  $\alpha^5$  (and some up to order  $\alpha^6$ ). But, now that we know that the wave equation is correct up to order  $\alpha^5$ , it is of course more appropriate to evaluate the  $\alpha^6$  term nonperturbatively and directly by numerical methods.

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