## $\mathcal{O}(\alpha^3 \ln \alpha)$ corrections to muonium and positronium hyperfine splitting

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We compute  $\mathcal{O}(\alpha^3 \ln \alpha)$  relative corrections to the ground state hyperfine splitting of a QED two body bound state with different masses of constituents. The general result is then applied to muonium and positronium. In particular, a new value of the muon to electron mass ratio is derived from the muonium ground state hyperfine splitting.

36.10.Dr, 06.20.Jr, 12.20.Ds, 31.30.Jv

The perturbative series for binding energies of a QED bound state are non-analytic in the fine structure constant and the expansion contains powers of  $\alpha^{n_1} \ln^{n_2} \alpha$ , where  $n_1$  and  $n_2$  are some integer numbers. The appearance of logarithms of  $\alpha$  is best explained by the fact that different scales, such as the mass m, the momentum  $m\alpha$  and the typical energy  $m\alpha^2$  control dynamics of the bound state.

In a recent paper [1] we have explained how the nonrelativistic Quantum Electrodynamics (NRQED) regularized dimensionally can be efficiently used to extract all  $\ln \alpha$  corrections in a given order of the expansion in  $\alpha$ and applied this technique to compute  $\mathcal{O}(\alpha^3 \ln \alpha)$  corrections to the decay rates of para- and orthopositronium. The purpose of this Letter is to apply that methods to the calculation of the  $\mathcal{O}(\alpha^3 \ln \alpha)$  corrections to the hyperfine splitting (hfs) of a general QED two body system in a ground state with an eye on the hfs in muonium and positronium.

For both, muonium and positronium, there are good phenomenological reasons to consider  $\mathcal{O}(\alpha^3 \ln \alpha)$  contributions to the ground state hfs. The most precise measurement of this quantity in positronium gives [2]:

$$\nu_{\rm exp}^{\rm Ps} = 203 \; 389.10(74) \; {\rm MHz},$$
 (1)

while the theoretical prediction [3,4], which includes  $\mathcal{O}(\alpha^3 \ln^2 \alpha)$  terms computed in [5], is:

$$\nu_{\rm th}^{\rm Ps} = 203\ 392.01(46)$$
 MHz. (2)

Obviously, the theoretical and experimental results differ from each other by an uncomfortably large amount (given the claimed accuracy of the two), which indicates that further study of  $\mathcal{O}(\alpha^3)$  corrections to the hfs of the positronium ground state is warranted. The complete calculation of  $\mathcal{O}(\alpha^3)$  corrections is currently out of question because of tremendous technical difficulties; nevertheless, the  $\mathcal{O}(\alpha^3 \ln \alpha)$  corrections can be determined.

Before considering the case of two equal masses, we decided to study a bound state of two particles with masses m and M. For  $m = m_e$  and  $M = m_\mu$  this corresponds to the bound state of the electron and the anti-muon called muonium. Our technique provides an excellent tool to extract the  $\mathcal{O}(\alpha^3 \ln \alpha)$  corrections in this case keeping the full mass dependence and this result can be used in two ways. First, we will be able to check the correctness of our calculation against the known results for  $\mathcal{O}(\alpha^3 \ln \alpha)$ corrections obtained in an expansion in  $m_e/m_\mu$ . Second, we will derive some new results from our formula; in particular, we will give the complete  $\mathcal{O}(\alpha^3 m_e/m_\mu \ln \alpha)$ correction to the ground state hfs in muonium which is important for the extraction of the muon to electron mass ratio.

The Letter is organized as follows. We first review our method of calculation (for more details we refer to [1]). We then consider the unequal mass case (muonium) where virtual annihilation is not allowed. Later, we discuss phenomenological implications of our result for muonium and derive the new value of the muon to electron mass ratio. Finally, we describe how the calculation should be modified in order to accommodate the positronium case and its phenomenological consequences.

Our calculation is based on dimensionally regularized nonrelativistic QED with  $d = 3 - 2\epsilon$  being the number of spatial dimensions. In the NRQED framework two different contributions to the final result should be distinguished. The first one is the hard contribution, which is sensitive to relativistic momenta only. This contribution is not capable to produce any non-analytic dependence on  $\alpha$ . The second contribution is the soft one. It is sensitive to nonrelativistic scales and for this reason can produce a non-analytic dependence on the fine structure constant. The main idea that permits a simple extraction of the logarithmic terms is the following. In dimensionally regularized NRQED, the matrix elements of the nonrelativistic operators are the uniform functions of the fine structure constant. This implies that, when written in proper units, the dependence on  $\alpha$  can be scaled out

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<sup>\*</sup>Work supported by DOE Contract DE-AC03-76SF00515.

of any matrix element. We refer to our recent paper [1] for additional details on this approach; here we remind the reader that the relative momentum  $\boldsymbol{p}$ , the relative coordinate  $\boldsymbol{r}$  and the binding energy E scale as  $\boldsymbol{p} \to \gamma \boldsymbol{p}$ ,  $\boldsymbol{r} \to \gamma^{-1} \boldsymbol{r}, E \to \gamma^2 \mu^{-1} E$ , with the scaling parameter  $\gamma = (\mu Z \alpha)^{1/(1+2\epsilon)}$  [1]. Here  $\mu = mM/(m+M)$  is the reduced mass of the bound state. We also assign the charge Z to the particle of mass M to distinguish recoil and radiative recoil contributions, as it is customary in bound state calculations. To illustrate how the scaling arguments help to compute the  $\ln \alpha$  corrections, let us consider the matrix element of a nonrelativistic operator O that delivers  $\mathcal{O}(\alpha^3)$  correction to the lowest order hfs kernel  $V_{\text{Born}}$  ( $\boldsymbol{\sigma}$  and  $\boldsymbol{\Sigma}$  are the spin operators of the two particles),

$$V_{\text{Born}} = -\frac{Z\alpha}{mM} \frac{[\sigma_i, \sigma_j][\Sigma_i, \Sigma_j]}{4d} \pi \delta(\boldsymbol{r}).$$
(3)

We consider relative correction to the hfs:

$$\frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | V_{\text{Born}} | \Psi \rangle} = \frac{\alpha^3}{\pi} \left( \Delta_O \ln(Z\alpha) + \text{const} \right). \tag{4}$$

The operator O is a function of r and p. Performing the rescaling of all the quantities on the left hand side of Eq.(4) according to the rules given above, we extract the dependence on  $\alpha$ :

$$\frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | V_{\text{Born}} | \Psi \rangle} = \frac{\gamma^{3-n+j\epsilon}}{\mu^{l+k\epsilon}} \left. \frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | V_{\text{Born}} | \Psi \rangle} \right|_{\gamma=1}$$

where n = 2, 3 is a power of  $\alpha$  that explicitly enters the operator O and j, l, k are some integers. If the matrix element is finite, we can put  $\epsilon = 0$  and then the relative correction to the hfs is  $\alpha^3$  times the  $\alpha$ -independent function and hence no logarithms of  $\alpha$  appear. Therefore, after the rescaling, the *only* place where  $\ln \alpha$  can come from is the expansion of the factor  $\gamma^{3-n+j\epsilon}$  in powers of  $\epsilon$ ; this implies that, in order to generate the  $\ln \alpha$ corrections, the nonrelativistic matrix elements should diverge and only divergent pieces of the matrix elements are needed to determine the  $O(\ln \alpha)$  corrections. Note also, that since the hard  $O(\alpha^3)$  contributions to the hfs are not needed, it is straightforward to keep the mass dependence exactly in our calculation.

Let us now list all the contributions to the hfs in muonium and positronium relevant at  $\mathcal{O}(\alpha^3 \ln \alpha)$ . We begin with discussing the irreducible contributions, i.e. those that arise as average values of some local operators. The first of those is the operator that corresponds to a Taylor expansion of  $\mathcal{O}(\alpha)$  hard scale contributions in powers of the relative momenta of the bound state constituents up to  $\mathcal{O}(\mathbf{p}^2)$ . For both radiative and annihilation corrections this contribution can be related to the divergences in real radiation [1]. For the recoil contributions things are more complicated and the easiest way to extract the  $\mathcal{O}(\alpha \mathbf{p}^2)$ piece of the hard scattering amplitudes is to actually expand the box diagrams to the required order. This results in the following contribution to the muonium hfs:

$$\Delta_{\text{real rad}} = Z^2 \mu^2 \left( \frac{4}{3} \left( \frac{Z}{M} + \frac{1}{m} \right)^2 + \frac{Z}{Mm} \right).$$
 (5)

Other irreducible corrections at this order are produced due to, loosely speaking, the magnetic moment renormalization of the  $\mathcal{O}(\alpha^2)$  corrections to the hfs and in many cases the result can be simply obtained by generalizing the calculation of Ref. [4] to the unequal mass case. We then derive:

$$\Delta_{\rm rad\ ret} = -Z^2 (1 + \xi Z^2) \frac{\mu^2}{mM},$$
 (6)

$$\Delta_{\text{rad 1loop}} = Z^2 \mu \left( \frac{2 + \xi Z^2}{m} + \frac{1 + 2\xi Z^2}{M} \right).$$
(7)

for the contributions of the retardation and the "oneloop" operators, respectively (see [4] for the nomenclature). Parameter  $\xi = 1$  distinguishes the contributions due to anomalous magnetic moment of the particle with the mass M.

Two additional irreducible contributions originate from relativistic corrections to the single Coulomb or magnetic exchange when we account for the Pauli form factor in one of the vertices:

$$\Delta_C = -\frac{Z^2(1+\xi Z^2)}{4} \frac{\mu^2}{mM},$$
(8)

$$\Delta_M = -\frac{Z^2 \mu^2}{4} \left( \frac{3 + 2\xi Z^2}{m^2} + \frac{2 + 3\xi Z^2}{M^2} \right).$$
(9)

The last set of irreducible corrections can be loosely described as the effect of the retardation on all the relevant operators that generate non-radiative corrections at lower orders. This includes: the third order retardation, the retardation in the one-loop operator, the irreducible exchange of two magnetic photons, the retardation in the graph with magnetic seagull operator on one line, the graph with two magnetic-Coulomb seagull vertices on both lines and, finally, the graph with the magnetic seagull vertex on each line. The resulting correction reads:

$$\Delta_{\rm irr\ ret} = \frac{22}{3} Z^3 \frac{\mu^2}{mM}.$$
 (10)

Several reducible contributions appear in the second order of time-independent perturbation theory. The first of them is generated by the so-called double seagull effective potential. This contribution is very similar to the case of  $\mathcal{O}(\alpha^3 \ln \alpha)$  corrections to the positronium decay rate considered in [1] and it can be easily generalized on the unequal mass case:

$$\Delta_{\rm s} = \frac{Z^3 \mu^2}{mM} \left( 6\ln(Z\alpha\mu^2) - \frac{2}{\epsilon} + \frac{20}{3}(\ln 2 - 1) \right).$$
(11)

The reducible retardation correction can also be derived as a simple generalization of the result in [1]. The only difference is that the spin parts of the magnetic currents also give non-zero contribution to the hfs. For unequal masses, the result reads:

$$\Delta_{\rm ret} = \frac{Z^3 \mu^2}{mM} \left( 8\ln(Z\alpha\mu^2) - \frac{8}{3\epsilon} + \frac{64\ln 2}{3} - \frac{82}{3} \right).$$
(12)

Also, the so-called ultrasoft contribution [1] should be considered. We find:

$$\Delta_{\rm us} = -\frac{4Z^2\mu^2}{3} \left(\frac{Z}{M} + \frac{1}{m}\right)^2 \left(4\ln(Z\alpha\mu^{\frac{3}{2}}) - \frac{1}{\epsilon} - \frac{5}{3}\right).$$

For the last reducible contribution to the hfs, the corresponding nonrelativistic operator O is of the form  $BGV_{\rm hl} + V_{\rm hl}GB$ , where G is the reduced Green function of the Coulomb Hamiltonian, B is the Breit Hamiltonian and  $V_{\rm hl}$  is the hard radiative correction to B. The Breit Hamiltonian in d dimensions has been derived in [4] for M = m. For different masses, it reads:

$$B = -\frac{p^4}{8} \left( \frac{1}{m^3} + \frac{1}{M^3} \right) + \left( \frac{1}{2\mu^2} + \frac{d-2}{mM} \right) \pi Z \alpha \delta(\mathbf{r}) + \frac{d-1}{4} \left\{ \frac{p^2}{mM}, C \right\} - \frac{\left[ [\boldsymbol{\sigma} \nabla, \boldsymbol{\sigma}] [\boldsymbol{\Sigma} \nabla, \boldsymbol{\Sigma}], C \right]}{16mM}, \quad (13)$$

where C is the Coulomb potential in d dimensions  $C(r) = -Z\alpha\Gamma(d/2-1)/(\pi^{d/2-1}r^{d-2}).$ 

The potential  $V_{\rm hl}$  is the sum of four contributions [6]:

$$V_{\rm hl} = V_{\rm ff} + V_{\rm magn} + V_{\rm box} + V_{\rm vp}, \qquad (14)$$

where the first one arises from the Coulomb photon exchange with one of the vertices being either the one-loop slope of the Dirac form factor or the Pauli form factor,

$$V_{\rm ff} = \frac{2Z\alpha^2}{3} \left[ \frac{1}{m^2} \left( -\frac{1}{\epsilon} + 2\ln m \right) + \frac{Z^2}{M^2} \left( -\frac{1}{\epsilon} + 2\ln M - \frac{3}{4} \left( 1 - \xi \right) \right) \right] \delta(\mathbf{r}), \quad (15)$$

the second one is due to the one-loop anomalous magnetic moments,

$$V_{\text{magn}} = -(1 + \xi Z^2) \frac{\alpha}{2\pi} \frac{[[\boldsymbol{\sigma} \nabla, \boldsymbol{\sigma}][\boldsymbol{\Sigma} \nabla, \boldsymbol{\Sigma}], C]}{16mM}, \quad (16)$$

the third one comes from the hard one-loop box diagrams,

$$V_{\text{box}} = \frac{(Z\alpha)^2}{mM} \left(\frac{1}{\epsilon} - \ln(mM) - \frac{1}{3} + \frac{M + m - 2\mu(1 + \boldsymbol{\sigma}\boldsymbol{\Sigma})}{M - m} \ln\frac{M}{m}\right) \delta(\boldsymbol{r}), \quad (17)$$

and the last one accounts for the one-loop vacuum polarization (hadronic vacuum polarization is not included):

$$V_{\rm vp} = -\frac{4Z\alpha^2}{15} \left(\frac{1}{m^2} + \frac{Z^2}{M^2}\right) \delta(\mathbf{r}).$$
 (18)

The structure of  $V_{\rm hl}$  is very similar to the structure of the Breit Hamiltonian and so the corresponding calculation goes along the lines of [4]. On this way one recognizes that both D wave and S wave contributions should be considered.

Since the *D* wave part of the new perturbation (16) differs from that of the original Breit perturbation (13) only by the overall factor, we can read off the *D* wave contribution to the  $\mathcal{O}(\alpha^3 \ln \alpha)$  correction to the hfs from the corresponding  $\mathcal{O}(\alpha^2)$  correction in positronium (see [4]):

$$\Delta_D = -\frac{5}{12}(1 + \xi Z^2) \frac{\mu^2}{mM}.$$
 (19)

To find the contribution of the intermediate S states, we first project both B and  $V_{\rm hl}$  on to the S wave and then proceed along the lines described in [4]. Since all the steps in this calculation have their counterparts in the calculation described in detail in [4] and since the intermediate formulas for the different mass case are lengthy, we refrain from presenting them here.

Summing up all the relevant contributions, we obtain the final result for the  $\mathcal{O}(\alpha^3 \ln \alpha)$  correction to the hfs of the ground state in the unequal mass case (we put  $\xi = 1$ below):

$$\Delta_{\text{tot}} = \frac{Z^2 \mu^2}{m^2} \left( \frac{8}{3} \ln \frac{4m}{\mu Z \alpha} - \frac{281}{180} \right) - \frac{Z^2 \mu^2}{mM} - \frac{Z^4 \mu^2}{mM} - \frac{Z^3 \mu^2}{mM} \left( 2 \ln \frac{mM}{\mu^2} + \frac{2 \ln(Z\alpha)}{3} - 20 \ln 2 + \frac{101}{9} \right)$$
(20)
$$+ \frac{Z^3 \mu}{M - m} \left( 5 + \frac{4\mu^2}{mM} \right) \ln \frac{M}{m} + \frac{Z^4 \mu^2}{M^2} \left( \frac{8}{3} \ln \frac{4M}{\mu Z \alpha} - \frac{281}{180} \right).$$

Eq.(20) is one of the principal results of this Letter. If we identify m with the electron mass and M with the muon mass, Eq.(20) provides the result for the  $\mathcal{O}(\alpha^3 \ln \alpha)$ correction to muonium hfs. Muonium has been studied extensively over the years and much is known about this system. In particular, there are certain limits of Eq.(20) that can be checked against known results. To this end, it is instructive to expand Eq.(20) in powers of m/M up to the first non-trivial order:

$$\Delta^{\mathrm{Mu}} = \frac{2Z^2}{3} \ln(Z\alpha) \left( -4 + \frac{m_e}{m_{\mu}} (8 - Z) \right) + Z^2 \left\{ \frac{16}{3} \ln 2 - \frac{281}{180} + \frac{m_e}{m_{\mu}} \left[ -Z^2 - \frac{32}{3} \ln 2 + \frac{431}{90} \right] + Z \left( 3 \ln \frac{m_{\mu}}{m_e} - \frac{101}{9} + 20 \ln 2 \right) \right\}.$$
(21)

The last equation shows that our result, Eq.(20), correctly reproduces the  $\ln^2(Z\alpha)$  terms [7,8,5], as well as the  $Z^2 \ln(Z\alpha)$  single logarithmic term [7,8] and the  $(m_e/m_\mu)Z^3 \ln(Z\alpha) \ln(m_\mu/m_e)$  term [9,10] which are all available in the literature.

We now proceed to the discussion of what this result implies for the phenomenology of the muonium hfs. We first note that in this case Eq.(21) can be used since higher powers in the expansion in  $m_e/m_{\mu}$  have a negligible impact. Since the  $\ln(m_{\mu}/m_e)$  enhanced part of the

 $\mathcal{O}(m_e/m_\mu\alpha^3\ln\alpha)$  corrections has been properly taken into account in a recent compilation of all theoretical results for muonium hfs [12], we disregard it here. Setting Z = 1, we then obtain the  $\mathcal{O}(m_e/m_\mu\alpha^3\ln\alpha)$  hfs shift:

$$\delta\nu^{\rm Mu} = E_{\rm F} \frac{m_e}{m_\mu} \frac{\alpha^3}{\pi} \left(\frac{28}{3}\ln 2 - \frac{223}{30}\right) \ln \alpha.$$
(22)

Numerically, it evaluates to 0.013 kHz; this should be compared with a similar contribution  $\delta' \nu^{\text{Mu}} = -0.265(64)$  kHz, originating from the incomplete calculation in [11], that has been accounted for in the theoretical value for muonium hfs in [12].

The difference between the two numbers has significant impact on the electron to muon mass ratio determination. It is easy to see, that it amounts to the relative shift of  $6.2 \times 10^{-8}$  in this ratio (compare with the quoted relative theoretical uncertainty  $2.7 \times 10^{-8}$  [12]) and, if we use the central value from [12], Eq.(161), the new result reads:

$$\frac{m_{\mu}}{m_e} = 206.768\ 2784(30)(23). \tag{23}$$

Here the first error is related to the error in the theoretical prediction for the muonium hfs and the second is the experimental one. The theoretical error in the hfs was estimated following [12]; the only difference is that we estimated the uncalculated non-logarithmic  $\mathcal{O}(m_e/m_{\mu}\alpha^3)$ recoil and radiative-recoil corrections as half of their ln  $\alpha$ enhanced counterparts in Eq.(21). The uncertainty in the muonium hfs due to uncalculated higher order corrections we have obtained in this way is 0.07 kHz, compared to 0.12 kHz in [12].

For positronium, the calculation goes essentially unchanged, although two facts have to be noticed. First, since there is an annihilation contribution to the leading order hfs in positronium, the relative weight of different corrections changes. Second, one has to take into account additional annihilation contributions to the Breit and  $V_{\rm hl}$  operators. These annihilation operators read (**S** is the spin of positronium):

$$B_{\rm ann} = \frac{\pi \alpha S^2}{m^2} \delta(\boldsymbol{r}), \qquad (24)$$

and

$$V_{\rm ann} = \frac{4\alpha^2}{m^2} \left[ -1 + \ln 2 - \left(\frac{13}{18} + \frac{\ln 2}{2}\right) S^2 \right] \delta(\boldsymbol{r}), \quad (25)$$

and they should be added to B and  $V_{\rm hl}$ , respectively. Finally, for obvious reasons, one should disregard the  $\mathcal{O}(1/M^2)$  contribution in Eq.(18). Proceeding along the lines described for the unequal mass case, we derive the result for the  $\mathcal{O}(m\alpha^7)$  hfs in positronium:

$$\delta\nu^{\rm Ps} = \frac{7m\alpha^7}{12\pi} \ln \alpha \left( -\frac{3}{2}\ln \alpha + \frac{68}{7}\ln 2 - \frac{62}{15} \right).$$
(26)

Numerically, the new  $\mathcal{O}(m\alpha^7 \ln \alpha)$  term gives an additional shift of -0.32 MHz to the theoretical value of the

positronium ground state hfs, so that the theoretical prediction becomes:

$$\nu_{\rm th}^{\rm Ps} = 203 \ 391.69(16) \ {\rm MHz}.$$
 (27)

The theoretical prediction moves closer to the experimental result in Eq.(1), however the difference is still significant. Since the value of the new  $\mathcal{O}(m\alpha^7 \ln \alpha)$  contribution turns out to be roughly one third of the  $\mathcal{O}(m\alpha^7 \ln^2 \alpha)$ one, the series look reasonably convergent. For this reason we estimate the nonlogarithmic  $\mathcal{O}(\alpha^3)$  contribution to the positronium hfs as being one half of the logarithmic one. This is the origin of the uncertainty estimate in Eq.(27).

In conclusion, we have computed  $\mathcal{O}(\alpha^3 \ln \alpha)$  corrections to the hyperfine splitting of the general QED bound state keeping the full mass dependence. We then applied this result to the hfs of the muonium and positronium. The new value for the muon to electron mass ratio is extracted from the ground state hyperfine splitting in muonium. As for the positronium ground state hfs, the computed correction slightly reduces the discrepancy between theory and experiment. However, it is hard to imagine that higher order corrections can further significantly shift the theoretical value. In this circumstances, one should perhaps start taking the discrepancy between the theory and experiment in the positronium ground state hfs seriously.

Acknowledgments: This work was supported in part by DOE under grant number DE-AC03-76SF00515, and by the Russian Foundation for Basic Research grant 00-02-17646. We are indebted to R. Hill for useful conversations and communicating to us his results [13] on  $\mathcal{O}(\alpha^3 \ln \alpha)$  corrections to the hfs prior to publication. Discussions with A. Penin are gratefully acknowledged.

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