$\alpha(Z\alpha)^2 E_F$ correction to hyperfine splitting in hydrogenic atoms

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The electron self-energy correction of the order $\alpha(Z\alpha)^2 E_F$ to the ground-state hyperfine splitting in hydrogenic atoms is calculated using a semianalytical method. The correction is divided into three parts by introducing two auxiliary parameters. The low-energy part corresponds to the nonrelativistic limit, where photon energy is of the order $m\alpha^2$, and the effective hyperfine interaction is given by $\delta^3(r)$. In the middle-energy part electron and photon momenta are of the order $m\alpha$ and m, respectively. This part is calculated using on-shell electron form factors. The high-energy part corresponds to the *S*-matrix amplitude for the forward scattering. The final value does not depend on auxiliary parameters and amounts to $\Delta E = (\alpha/\pi)(Z\alpha)^2 E_F \times 17.122$. It is larger than the previous value of Sapirstein ~15.10(29) and significantly alters theoretical predictions. [S1050-2947(96)08209-1]

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I. INTRODUCTION

The hyperfine structure (hfs) of hydrogenic atoms, behind the Lamb shift, is one of the stringent tests of quantum electrodynamics (QED). The high precision of the measurement of the hfs in hydrogen [1],

$$E_{\text{expt}} = 1420.405\ 751\ 766\ 7(9)$$
 MHz, (1)

stimulates theorists to improve QED predictions and to calculate higher-order corrections. Unfortunately, uncertainties in the low-energy proton form factors limit the possibility of significant progress in QED tests based on the hfs in hydrogen. The leading nuclear structure correction [2] as given by

$$\Delta E = \frac{64}{3} \frac{(Z\alpha)^5 \mu^3}{\pi m_p} \int_0^\infty \frac{dp}{p^2} \times [G_M(-p^2)G_E(-p^2) - G_M(0)G_E(0)]$$
(2)

could not be calculated precisely, because G_E and G_M are determined from the experiment. These problems do not appear in muonium, which consists of the electron and the approximately 200 times heavier muon. This pure leptonic atom is the ideal system for theorists, since all non-QED effects could be accounted for. The current experimental value of muonium hfs is [3]

$$E_{\text{expt}} = 4\,463\,302.88(16)\,\text{ kHz}.$$
 (3)

On the other hand, the theoretical predictions are mostly limited by the electron-muon mass ratio. An improved measurement [4] of this mass ratio and muonium hfs is in preparation, making the evaluation of higher-order QED corrections more attractive. The review of hfs in hydrogenic systems is presented in [5] and [6]. Recently a large class of two-loop corrections has been calculated in [6] and [7]. In this paper we present an improved calculation of the one-loop contribution in the order of $\alpha(Z\alpha)^2$. The first calculation by Brodsky and Ericson [8] brings a rough value of 18.36(500); later Sapirstein [9], applying his method used for the analogous problem in the hydrogen Lamb shift, obtained the value 15.10(29). Our result is

$$\Delta E = \frac{\alpha}{\pi} (Z\alpha)^2 E_F \times 17.122. \tag{4}$$

Although it differs from the Sapirstein result, it is in much better agreement with the recent calculation of Nio and Kinoshita [10].

It is the purpose of this paper to present a method that we think could be extended to intrinsic two-body problems. A widely used Bethe-Salpeter equation allows for the derivation of appropriate formulas and the subsequent calculation. The problem appears in the $O(\alpha^6)$ and higher-order corrections to energy levels where the large number of terms make the calculation less tractable. There are several other techniques, which eliminate relative time from the Bethe-Salpeter equation by introducing an effective interaction Hamiltonian. It is worth mentioning here the Lepage formulation of nonrelativistic quantum electrodynamics (NRQED) [11] which simplifies the treatment of bound states. We have introduced an approach [12], which is similar in some aspects to the Lepage NRQED. In this approach, one calculates separately corrections at different energy scales, choosing a photon gauge and performing simplifications, which are proper for that scale. Higher-order electron self-energy and recoil corrections to the Lamb shift in hydrogenic atoms [12] were calculated in this way.

II. THE METHOD OF CALCULATION

The one-loop correction to the hyperfine structure in the nonrecoil limit and Feynman gauge are given by the following formulas:

$$\Delta E = E_1 + E_2 + E_3, \tag{5}$$

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$$E_{2} = -2 e^{2} \int \frac{d^{4}k}{(2\pi)^{4}i} \frac{1}{k^{2}} \times \left\langle \left. \vec{\psi} \right| \gamma^{\mu} \frac{1}{\not{p} - \not{k} - \gamma^{0}V - m} \gamma_{\mu} \frac{1}{(\not{p} - \gamma^{0}V - m)'} \gamma \mathbf{A} \right| \psi \right\rangle,$$
(7)

$$E_{3} = -E_{F}e^{2} \int \frac{d^{4}k}{(2\pi)^{4}i} \frac{1}{k^{2}} \times \left\langle \left. \vec{\psi} \right| \gamma^{\mu} \frac{1}{\not{p} - \not{k} - \gamma^{0}V - m} \gamma_{0} \frac{1}{\not{p} - \not{k} - \gamma^{0}V - m} \gamma_{\mu} \right| \psi \right\rangle.$$
(8)

For its calculation we divide ΔE into three parts, E_L , E_M , and E_H , by introducing two auxiliary parameters, ϵ and ρ . The most important thing is that, after the expansion in α , the expansions in ρ and next in ϵ are performed. This allows one to perform an appropriate simplification, which is specific for any part. It also preserves the gauge independence. The parameter ϵ is the cutoff of the photon frequency ω on the branch cut from the photon propagator. In the part E_L we have $0 \le \omega \le \epsilon$. We may use here a nonrelativistic approximation, where the effective hyperfine interaction is given by the $\delta^3(r)$ function. We chose a Coulomb gauge and calculate the radiative correction to the energy shift due to this $\delta^3(r)$ function. In the remaining two parts ϵ plays the role of infrared cutoff. It is safe now to expand the electron propagator in the Coulomb field; all nonperturbative effects are contained in E_L . We introduce here a second parameter ρ in the following way:

$$\mathbf{A}(\mathbf{q}) = -i\frac{\boldsymbol{\mu} \times \mathbf{q}}{q^2} = -i\boldsymbol{\mu} \times \mathbf{q} \left(\frac{1}{q^2} - \frac{1}{q^2 + \rho^2}\right) - i\frac{\boldsymbol{\mu} \times \mathbf{q}}{q^2 + \rho^2}.$$
(9)

The magnetic field from the nucleus magnetic moment is split into two pieces. The first piece, which will correspond to the E_M part, forces the electron momenta to be small, namely, to be of the order $m\alpha$. In this domain radiative corrections are described only by the modification of electron form factors F_1 and F_2 ,

$$F_1(q^2) = 1 + \frac{\alpha q^2}{3 \pi m^2} \bigg[\ln \bigg(\frac{m}{\mu} \bigg) - \frac{3}{8} \bigg], \tag{10}$$

$$F_2(q^2) = \frac{\alpha}{2\pi} \left(1 + \frac{q^2}{6m^2} \right).$$
(11)

The F_1 is infrared divergent. It depends on the photon mass μ . We use a formula

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$$\ln(\mu) = \ln(2\epsilon) - \frac{5}{6} \tag{12}$$

to convert this dependence to ϵ . The second term in (9), which corresponds to E_H , forces electron momenta to be large, of the order of the electron mass. We may put here external momenta on mass shell, and calculate the corresponding *S*-matrix element for the forward-scattering amplitude. This matrix element is infrared divergent due to the presence of lower-order terms, but they can be easily subtracted out. The remaining term is finite due to the presence of ρ . The sum of three parts,

$$\Delta E = E_L + E_M + E_H, \qquad (13)$$

does not depend on ϵ and ρ and gives the required correction.

III. LOW-ENERGY PART E_L

In the nonrelativistic limit the effective hyperfine interaction V_F for S states is

$$V_F = \frac{e^2 g_p}{3 m_e m_p} \delta^3(r), \qquad (14)$$

where g_p is defined by

$$\boldsymbol{\mu}_p = -\frac{g_p e}{2 m_p} \frac{\boldsymbol{\sigma}_p}{2}.$$
 (15)

Here and in the following we put Z=1. The Z dependence is restored in the final formulas. The radiative corrections take a form

$$E_L = E_{L1} + E_{L2}, (16)$$

$$E_{L1} = 2 \frac{2 \alpha}{3 \pi m^2} \int_0^{\epsilon} \omega d\omega \left\langle \phi \left| \mathbf{p} \frac{1}{H - E + \omega} \mathbf{p} \frac{1}{(H - E)'} V_F \right| \phi \right\rangle,$$
(17)

$$E_{L2} = -E_F \frac{2 \alpha}{3\pi m^2} \int_0^{\epsilon} \omega d\omega \left\langle \phi \left| \mathbf{p} \frac{1}{(H - E + \omega)^2} \mathbf{p} \right| \phi \right\rangle,$$
(18)

where *E* is the nonrelativistic energy $E = -m\alpha^2/2$. The term that comes from the expansion of Schrödinger propagator $1/(H-E+\omega)$ in V_F does not contribute after the angle average. By 1/(H-E)' one denotes the reduced propagator (i.e., without 1*S* state contribution) with angular momentum l=0. We use the formula

$$R(r_2, r_1) = \langle r_2 | \frac{1}{(H - E)'} | r_1 \rangle,$$
(19)

$$R(r,0) = \frac{m^2 \alpha}{\pi} e^{-m\alpha r} \left[\frac{5}{2} - C - m\alpha r + \frac{1}{2 m\alpha r} - \ln(2 m\alpha r) \right]$$
(20)

to convert our matrix elements to the form that is the combination of

$$P(\gamma) = \langle \phi | \mathbf{p} \frac{1}{H - E + \omega} (m \, \alpha r)^{\gamma} \mathbf{p} | \phi \rangle \tag{21}$$

$$= 64 \frac{\nu^{5+\gamma}}{(1+\nu)^{8+\gamma}} \Gamma(4+\gamma) \int_0^1 dx \ x^{1-\nu} \ (1-\eta x)^{\gamma} \ (1-\eta^2 x)^{-(4+\gamma)}, \tag{22}$$

where

$$\eta = \frac{\nu - 1}{\nu + 1} \quad \text{and} \quad \nu = -\frac{m\,\alpha^2}{2(E - \omega)}.\tag{23}$$

For the ω integration we subtract the terms that are divergent in ϵ and calculate them analytically:

$$\Delta E = E_F \frac{\alpha}{\pi} \alpha^2 F,$$

$$F_L = \frac{1156}{27} + \frac{25\pi^2}{18} - \frac{166\ln(2)}{3} - \frac{2\ln(2)^2}{3} - 4\ln(\alpha) + 8\ln(2)\ln(\alpha) - \frac{8\ln(\alpha)^2}{3}$$
(24)

$$+2\ln(\epsilon) - 4\ln(2)\ln(\epsilon) + \frac{8\ln(\alpha)\ln(\epsilon)}{3} - \frac{2\ln(\epsilon)^2}{3} + n_1 + n_2,$$
(25)

where $E_F = 8\alpha^4 m_r^3 / (3 m_e m_\mu)$ and m_r is a reduced mass. The remaining terms n_1 and n_2 are integrated numerically with the results

$$n_{1} = \int_{0}^{1} d\nu \int_{0}^{1} dx \left[-\frac{128 h(1-\nu)^{2} \nu}{3 (1+\nu)^{6}} + \frac{16 g(1-\nu)^{2}(3+5 \nu)}{3 (1+\nu)^{5}} + \frac{16 f(1-\nu)(-1+5 \nu-31 \nu^{2}+19 \nu^{3})}{3 (1+\nu)^{6}} \right] = -0.085 740 3, \quad (26)$$

$$n_{2} = \int_{0}^{1} d\nu \frac{128 (1-\nu)\nu^{3}}{3 (1+\nu)^{7}} \frac{{}_{2}F_{1}(1,2-\nu,3-\nu,\eta^{2})}{2-\nu} = 0.067 496 9, \quad (27)$$

where

$$f = \frac{x^{1-\nu} - x}{\nu} \frac{1}{1 - \eta^2 x},$$
(28)

$$g = \frac{x^{1-\nu} - x}{\nu} \frac{1}{1 - \eta x},$$
 (29)

$$h = \frac{x^{1-\nu}}{1-\eta^2 x} \ln \left[\frac{1-\eta^2 x}{(1-\eta x)(1+\eta)} \right].$$
 (30)

This calculation was very similar to the nonrelativistic Lamb shift calculation with one difference due to the presence of the $\delta^3(r)$ function.

IV. MIDDLE-ENERGY PART E_M

In this part ω is bounded from below by ϵ and the magnetic field from the nucleus magnetic moment is regularized according to (9). All electron momenta are of the order $m\alpha$. In this domain radiative corrections are described effectively by on-shell electron form factors F_1 and F_2 ,

$$j^{\mu} = \gamma^{\mu} F_1(q^2) + \frac{i}{2m} \sigma^{\mu\nu} q_{\nu} F_2(q^2), \qquad (31)$$

where F_1 and F_2 are given by (10) and (11). It is in agreement with the Lepage formulation of NRQED, where the effective Hamiltonian is obtained from the *S*-matrix amplitude. This part E_L is in turn split into four subparts calculated as follows. E_{M1} is a correction due to the anomalous magnetic moment $\alpha/(2\pi)$ on the relativistic wave function:

$$E_{M1} = e \frac{\alpha}{2\pi} \frac{i}{2m} \langle \overline{\psi} | \sigma^{kj} [p^j, A^k] | \psi \rangle.$$
(32)

The result in required order, expressed in terms of corresponding F, is

$$F_{M1} = \frac{1}{2} \left[1 - \ln\left(\frac{2\alpha}{\rho}\right) \right]. \tag{33}$$

 E_{M2} is coming from V_F and the radiative correction to the Coulomb interaction V_{RC} as given by F_1 and F_2 :

$$V_{\rm RC} = \frac{4\alpha^2}{3m^2} \ln\left(\frac{m}{\mu}\right) \delta^3(r), \qquad (34)$$

and could be expressed as

$$E_{M2} = 2\left\langle \phi \left| V_F \frac{1}{(E-H)'} V_{\rm RC} \right| \phi \right\rangle.$$
(35)

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Using (14), (34), and (35) one obtains

$$F_{M2} = -\frac{8}{3} \left[\frac{1}{2} - \ln\left(\frac{2\alpha}{\rho}\right) \right] \ln\left(\frac{m}{\mu}\right). \tag{36}$$

 E_{M3} is due to q^2 dependence of magnetic interaction between the electron and the nucleus as given by F_1 and F_2 . The hyperfine potential V_F is modified by δV_F :

$$\delta V_F = -\frac{e^2 g_p}{3 m_e m_p} \left\{ \frac{\alpha}{3 \pi m^2} \left[\ln \left(\frac{m}{\mu} \right) - \frac{3}{8} \right] + \frac{\alpha}{2 \pi} \frac{1}{6m^2} \right\} \\ \times q^4 \left(\frac{1}{q^2} - \frac{1}{q^2 + \rho^2} \right).$$
(37)

The expectation value, after expanding in ρ , is

$$F_{M3} = 4 \ln\left(\frac{m}{\mu}\right) - \frac{1}{2}.$$
 (38)

 E_{M4} is a correction analogous to E_{M2} but with negative energy states between the hyperfine V_F and the radiatively corrected Coulomb interactions. One could not use here the nonrelativistic approximation V_F and V_{RC} as in E_{M2} . The correct relativistic expression is $V_F = -e \gamma A$, and the relevant part for the Coulomb interaction is

$$V_{\rm RC} = -\frac{\alpha}{2\pi} \alpha \frac{\alpha^i}{2m} \left[p^i, \frac{1}{r} \right]. \tag{39}$$

The value of this correction is

$$F_{M4} = \ln\left(\frac{2\alpha}{\rho}\right). \tag{40}$$

The complete value for the middle-energy part using (33), (36), (38), and (40) is

$$E_{M} = \frac{8}{3} \ln\left(\frac{m}{\mu}\right) + \frac{3}{4} \ln\left(\frac{2\alpha}{\rho}\right) + \frac{8}{3} \ln\left(\frac{m}{\mu}\right) \ln\left(\frac{2\alpha}{\rho}\right).$$
(41)

V. HIGH-ENERGY PART E_H

This part is calculated from the corresponding *S*-matrix forward-scattering amplitude. The magnetic potential **A** is regularized by ρ . It eliminates logarithmic infrared divergences that could appear, putting external momenta on mass shell. This amplitude is a one-loop radiative correction to the scattering on the magnetic field and two Coulomb fields coming from the nucleus, described by 13 nonequivalent Feynman diagrams. It contains the terms that contribute to the lower-order hfs, and they are subtracted out by removing the pole in the relevant momentum. An expression for an example diagram is

$$\delta E = e^{2} \int_{\epsilon} \frac{d^{4}k}{(2\pi)^{4}i} \frac{1}{k^{2}} \int \frac{d^{3}p_{1}}{(2\pi)^{3}} \frac{d^{3}p_{2}}{(2\pi)^{3}} \times \operatorname{Tr} \left[\gamma^{0} \frac{4\pi\alpha}{p_{1}^{2}} \frac{1}{\not{p}_{1}-m} \gamma^{\mu} \frac{1}{\not{p}_{1}-\not{k}-m} (-ie) \frac{\not{\mu}_{p} \times \mathbf{q}}{q^{2}+\rho^{2}} \cdot \gamma \frac{1}{\not{p}_{2}-\not{k}-m} \gamma^{0} \frac{4\pi\alpha}{p_{2}^{2}} \frac{1}{\not{l}-\not{k}-m} \gamma^{\mu} \psi(0) \overline{\psi}(0) \right], \quad (42)$$

where t = (m, 0, 0, 0), $p_i = \gamma^0 m - \mathbf{p}\gamma$, and $q = p_1 - p_2$. A similar integration is described in detail in [12]. First, the twomomentum integral p_1 and p_2 is performed. The linear divergence at $p_1 = 0$ is simply removed, because it corresponds exactly to the lower-order term. The result could be expressed in terms of logarithmic, dilogarithmic, and rational functions. Next, the integrals with respect to k and afterwards in respect to ω are performed, leading to the result

$$F_{H} = -\frac{943}{108} - \frac{2\pi^{2}}{3} + \frac{190\ln(2)}{9} + \frac{2\ln(2)^{2}}{3} + \frac{2\ln(\epsilon)}{3} + \frac{20\ln(2)\ln(\epsilon)}{3} + \frac{2\ln(\epsilon)^{2}}{3} + \frac{107\ln(\rho)}{3} - \frac{8\ln(2)\ln(\rho)}{3} - \frac{8\ln(\epsilon)\ln(\rho)}{3} - \frac{5\zeta(3)}{4}.$$
(43)

The final result is the sum

$$F = F_L + F_M + F_H = n_1 + n_2 + \frac{1307}{36} + \frac{13\pi^2}{18} - \frac{407\ln(2)}{12} - \frac{8\ln(2)^2}{3} - \frac{37\ln(\alpha)}{36} + \frac{16\ln(2)\ln(\alpha)}{3} - \frac{8\ln(\alpha)^2}{3} - \frac{5\zeta(3)}{4}.$$
 (44)

The constant term is equal to (4).

VI. CONCLUSIONS

The one-loop electron self-energy and vacuum polarization contributions to the muonium hyperfine splitting are

$$E = E_F \left[1 + \frac{\alpha}{2\pi} + \alpha(Z\alpha) \left(\ln(2) - \frac{5}{2} \right) - \frac{8 \alpha(Z\alpha)^2}{3 \pi} \ln(Z\alpha) \left(\ln(Z\alpha) - \ln(4) + \frac{281}{480} \right) + \frac{\alpha(Z\alpha)^2}{\pi} \left(17.122 - \frac{8}{15} \ln(2) + \frac{34}{225} \right) \right].$$
(45)

The new result alters theoretical predictions by 1.1 kHz in respect to the previous value and it is about seven times larger than the experimental error. The uncertainty in the theoretical predictions, apart from the electron-muon mass ratio, is due to the unknown terms of order $\alpha^4 E_F$ and $\alpha^3 m_e/m_\mu E_F$, which are enhanced by $\ln(\alpha)$ and $\ln(m_\mu/m_e)$. They could contribute by about 1 kHz. These corrections have been partially treated in [6] and [13]. Since they are currently being evaluated by Nio and Kinoshita we postpone drawing the final conclusions, until their calculation is finished.

We think the method presented here is general, and could be used to calculate the recoil corrections, and to study other systems as well. Our principal interest is in the energy levels of positronium and the helium atom. In both cases, there is lack of some effective method like this one, which will simplify the calculation compared to the Bethe-Salpeter formalism and its derivatives.

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- [1] E.R. Cohen and B.N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).
- [2] G.T. Bodwin and D.R. Yennie, Phys. Rev. D 37, 498 (1988).
- [3] F.G. Mariam et al., Phys. Rev. Lett. 49, 993 (1982).
- [4] K. Jungmann (private communication).
- [5] J. R. Sapirstein and D. R. Yennie, in *Quantum Electrodynamics*, edited by T. Kinoshita (World Scientific, Singapore, 1990).
- [6] T. Kinoshita and M. Nio, Phys. Rev. Lett. 72, 3803 (1995).
- [7] M. Eides and V. Shelyuto, Phys. Rev. A 52, 954 (1995).

- [8] S.J. Brodsky and G.W. Eriskson, Phys. Rev. 148, 26 (1966).
- [9] J.R. Sapirstein, Phys. Rev. Lett. 51, 985 (1983).
- [10] M. Nio and T. Kinoshita (private communication).
- [11] G.P. Lepage, in *Atomic Physics 14*, Proceedings of the Fourteenth International Conference on Atomic Physics, Boulder, Colorado, edited by D. J. Wihelard, C. E. Wieman, and S. J. Smith, AIP Conf. Proc. No. 323 (AIP, Woodbury, NY, 1996).
- [12] K. Pachucki, Ann. Phys. (N.Y.) 226 1 (1993); K. Pachucki and H. Grotch, Phys. Rev. A 51, 1854 (1995).
- [13] S.G. Karshenboim, Z. Phys. D 36, 11 (1996).