Order $\alpha^7 \ln(1/\alpha)$ Contribution to Positronium Hyperfine Splitting

Bernd A. Kniehl[1] and Alexander A. Penin[1,2]

[1]*II. Institut für Theoretische Physik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany*
[2]*Institute for Nuclear Research, Russian Academy of Sciences, 60th October Anniversary Prospect 7a, Moscow 117312, Russia*

(Received 28 August 2000; revised manuscript received 16 October 2000)

The logarithmically enhanced $\alpha^7 \ln(1/\alpha)$ contribution to the hyperfine splitting of the positronium ground-state energy levels is calculated in the framework of dimensionally regularized nonrelativistic quantum electrodynamics. The correction is negative and amounts to about 1/3 of the leading logarithmic $\alpha^7 \ln^2(1/\alpha)$ one. The discrepancy between the experimental measurements and the theoretical prediction is reduced.

PACS numbers: 36.10.Dr, 12.20.Ds, 31.30.Jv

Positronium, which is an electromagnetic bound state of the electron e^- and the positron e^+, is the lightest known atom. Thanks to the smallness of the electron mass m_e, strong- and weak-interaction effects are negligible, and its properties can be calculated perturbatively in quantum electrodynamics (QED), as an expansion in Sommerfeld's fine-structure constant α, with very high precision, only limited by the complexity of the calculations. Positronium is thus a unique laboratory for testing the QED theory of weakly bound systems. However, the theoretical analysis is complicated due to annihilation and recoil effects.

The positronium hyperfine splitting (HFS) $\Delta\nu = E(1^3S_1) - E(1^1S_0)$, where $E(1^1S_0)$ and $E(1^3S_1)$ are the energy levels of para- and orthopositronium, respectively, is the most precisely measured quantity in positronium spectroscopy as far as the absolute precision is concerned. The most recent measurements of the HFS [1,2] yielded

$$\Delta\nu^{\rm exp} = 203.387\,5(16)\,\text{GHz}, \tag{1}$$

$$\Delta\nu^{\rm exp} = 203.389\,10(74)\,\text{GHz}, \tag{2}$$

respectively.

The present theoretical knowledge may be summarized as

$$\Delta\nu^{\rm th} = \Delta\nu_0^{\rm th}\left\{1 - \frac{\alpha}{\pi}\left(\frac{32}{21} + \frac{6}{7}\ln 2\right) + \frac{5}{14}\alpha^2\ln\frac{1}{\alpha} + \left(\frac{\alpha}{\pi}\right)^2\left[\frac{1367}{378} - \frac{5197}{2016}\pi^2 + \left(\frac{6}{7} + \frac{221}{84}\pi^2\right)\ln 2 - \frac{159}{56}\zeta(3)\right] - \frac{3}{2}\frac{\alpha^3}{\pi}\ln^2\frac{1}{\alpha} + C\frac{\alpha^3}{\pi}\ln\frac{1}{\alpha} + D\left(\frac{\alpha}{\pi}\right)^3\right\}, \tag{3}$$

where $\Delta\nu_0^{\rm th} = 7m_e\alpha^4/12$ is the leading-order result [3]. The first-order correction was calculated in Ref. [4]. The logarithmically enhanced $\alpha^6\ln(1/\alpha)$ term was found in Refs. [5,6]. The nonlogarithmic $\mathcal{O}(\alpha^6)$ term includes the contribution due to the radiative correction to the Breit potential [7], the three-, two-, and one-photon annihilation contributions [8], the nonannihilation radiative recoil contribution [9], and the pure recoil correction computed numerically in Ref. [10] and analytically in Ref. [11]. In $\mathcal{O}(\alpha^7)$, only the leading double-logarithmic $\alpha^7\ln^2(1/\alpha)$ term is available [12].

Including all the terms known so far, we have

$$\Delta\nu^{\rm th} = 203.392\,01\,\text{GHz}, \tag{4}$$

which exceeds Eqs. (1) and (2) by approximately 2.8 and 3.9 experimental standard deviations, respectively. In contrast to the well-known *orthopositronium lifetime puzzle* (for the most recent developments of this problem, see, for example, Ref. [13] and the references cited therein), the experimental situation for the HFS is unambiguous. In fact, the experimental error is compatible with a naive estimate of the theoretical uncertainty due to as-yet unknown higher-order corrections. Should this discrepancy persist after the dominant terms of the latter have been calculated, this would provide a signal for *new physics*. This makes the HFS one of the most interesting topics in positronium spectroscopy, both from the experimental and theoretical points of view.

Thus, it is an urgent matter to improve the prediction of the HFS as much as possible, and one is faced with the task of analyzing the third-order correction, which is extremely difficult. However, there is a special subclass of the $\mathcal{O}(\alpha^7)$ contributions which can be analyzed separately, namely those which are enhanced by powers of $\ln(1/\alpha) \approx 5$. They may reasonably be expected to provide an essential part of the full $\mathcal{O}(\alpha^7)$ contributions. This may be substantiated by considering Eq. (3) in $\mathcal{O}(\alpha^6)$, where the logarithmic term is approximately 2.6 times larger than the nonlogarithmic one. While the leading double-logarithmic $\mathcal{O}(\alpha^7)$ contribution to Eq. (3) is known [12], the subleading single-logarithmic one is yet to be found. In fact, from the positronium lifetime calculation [13–15] we know that the subleading terms can be as important as the leading ones. The purpose of this Letter is to

 0031-9007/00/85(24)/5094(4)$15.00

complete our knowledge of the logarithmically enhanced terms of $\mathcal{O}(\alpha^7)$ by providing the coefficient C in analytic form.

The origin of the logarithmic corrections is the presence of several scales in the bound-state problem. The dynamics of the nonrelativistic e^+e^- pair near threshold involves four different scales: (i) the hard scale (energy and momentum scale like m_e); (ii) the soft scale (energy and momentum scale like βm_e); (iii) the potential scale (energy scales like $\beta^2 m_e$, while momentum scales like βm_e); and (iv) the ultrasoft scale (energy and momentum scale like $\beta^2 m_e$). Here β denotes the electron velocity in the center-of-mass frame. The logarithmic integration over a loop momentum between different scales yields a power of $\ln(1/\beta)$. Since positronium is approximately a Coulomb system, we have $\beta \propto \alpha$. This explains the appearance of powers of $\ln(1/\alpha)$ in Eq. (3). The leading logarithmic corrections may be obtained straightforwardly by identifying the regions of logarithmic integration [6,12]. The calculation of the subleading logarithms is much more involved because certain loop integrations must be performed exactly beyond the logarithmic accuracy.

In the following, we briefly outline the main features of our method developed previously in Ref. [13], where it was applied to the analysis of the subleading logarithmic third-order corrections to the positronium ground-state decay rates. This approach is similar to the one adopted in Ref. [15]. We work in nonrelativistic QED (NRQED) [16], which is the effective field theory that emerges by expanding the QED Lagrangian in β and integrating out the hard modes. If we also integrate out the soft modes and the potential photons, we arrive at the effective theory of potential NRQED [17], which contains potential electrons and ultrasoft photons as active particles. Thus, the dynamics of the nonrelativistic e^+e^- pair is governed by the effective Schrödinger equation and by its multipole interaction with the ultrasoft photons. The corrections from harder scales are contained in the higher-dimensional operators of the nonrelativistic Hamiltonian, corresponding to an expansion in β, and in the Wilson coefficients, which are expanded in α. In the process of scale separation, spurious infrared and ultraviolet divergences arise, which endow the operators in the nonrelativistic Hamiltonian with anomalous dimensions. In fact, these divergences completely determine the logarithmic corrections [13,18]. We use dimensional regularization, with $d = 4 - 2\epsilon$ space-time dimensions, to handle these divergences, which are of the form $1/\epsilon^n$ ($n = 1, 2, \ldots$) as $\epsilon \to 0$ [11,19,20]. Compared to the *traditional* NRQED approach, endowed with an explicit momentum cutoff and a fictitious photon mass to regulate the ultraviolet and infrared behavior [6,14,21], this scheme has the advantage that contributions from different scales are matched automatically.

In the effective theory, the HFS is generated by spin-flip operators of the effective nonrelativistic Hamiltonian averaged over the bound-state wave function. The hard-scale corrections, which require fully relativistic QED calculations and are most difficult to find, do not depend on β and do not lead to logarithmic contributions by themselves. However, they can interfere with the logarithmic corrections from the softer scales. The only results from relativistic perturbation theory that enter our analysis are the one-loop renormalizations of the relevant operators in the effective nonrelativistic Hamiltonian. The missing ingredients can all be obtained in the nonrelativistic approximation. The leading-order $\mathcal{O}(\alpha^4)$ HFS is generated by the $\mathcal{O}(\beta^2)$ spin-flip part of the tree-level Breit potential, which consists of the Fermi operator V_F and the annihilation operator $V_{\rm ann}$. The $\alpha^7 \ln(1/\alpha)$ contribution, which we are interested in, arises from several sources. A part of it can be extracted from the positronium lifetime calculation [13]. This part corresponds to: (1) the second-order corrections in nonrelativistic Rayleigh-Schrödinger perturbation theory, which arise from (1a) the insertions of the tree-level $\mathcal{O}(\beta^2)$ spin-independent Breit potential and the one-loop hard corrections to the leading-order spin-flip operators and (1b) the insertions of the one-loop $\mathcal{O}(\alpha\beta^2)$ operators related to the hard [22], soft [19], or ultrasoft [13,23] scales [cf. Eqs. (13)–(15) of [13], respectively] and the leading-order spin-flip operators; (2) *irreducible* corrections to the leading-order spin-flip operators, which include (2a) $\mathcal{O}(\alpha\beta^2)$ and (2b) $\mathcal{O}(\alpha^2\beta)$ terms and can be obtained from the corresponding equations of Ref. [13] by replacing the leading-order decay operator $V_4(\mathbf{p}, \mathbf{p}', \mathbf{S})$ by $V_F + V_{\rm ann}$. The hard renormalization coefficients of the leading-order operators V_F and $V_{\rm ann}$ are 1 and $-(44/9 + 2\ln 2)$, respectively [21,24]. They replace the renormalization coefficients $A_{p,o}$ of $V_4(\mathbf{p}, \mathbf{p}', \mathbf{S})$ in Ref. [13]. Another nontrivial difference with respect to the positronium lifetime calculation [13] is that the Fermi operator can cause a $\Delta L = 2$ transition of the spin-triplet state, so that D-wave intermediate states contribute to second order in nonrelativistic perturbation theory, by double insertion of V_F. This gives an additional contribution of $5/42$ to the coefficient C. Finally, there is a modification of the soft part of contribution (1b) due to the spin-dependent part of the transverse-photon-exchange contribution, which vanishes for the annihilation channel. This gives an additional contribution of $68/63$ to the coefficient C. Using the results of Ref. [13] and taking these modifications into account, we obtain the following contribution to the coefficient C from the sources enumerated above

$$\begin{aligned} C_{\rm I} &= \left[-\frac{64}{21} - \frac{12}{7}\ln 2\right]_{1a} + \left[-\frac{8}{15} + \frac{8}{3}\ln 2\right]_{1b} + \left[\frac{4}{3}\right]_{2a} \\ &\quad + \left[\frac{41}{6} - \frac{32}{3}\ln 2\right]_{2b} + \left[\frac{5}{42}\right]_{D\text{-wave}} + \left[\frac{68}{63}\right]_{\rm soft} \\ &= \frac{1822}{315} - \frac{68}{7}\ln 2\,, \end{aligned} \tag{5}$$

where the various contributions are given separately. Note that contribution (1b) also includes the entire

double-logarithmic term not presented in Eq. (5). The structure of the overlapping divergences resulting in the double-logarithmic contribution to the HFS is similar to the positronium lifetime analysis [13].

Another part of the $\alpha^7 \ln(1/\alpha)$ contribution is produced in the first order of the nonrelativistic Rayleigh-Schrödinger perturbation theory by the one-loop hard corrections to the $\mathcal{O}(\beta^4)$ and $\mathcal{O}(\alpha\beta^3)$ spin-flip operators, which give rise to the $\alpha^6 \ln(1/\alpha)$ contribution to the HFS. The relevant operators are generated by the relativistic correction to the Coulomb-photon exchange, the relativistic correction to the transverse-photon exchange, the kinematical retardation, and the one-loop correction involving *seagull* vertex diagrams with one Coulomb and one transverse photon. For our calculation, we only need the three hard renormalization coefficients, usually denoted as c_F, c_S, and $c_{pp'}$, which are related to the anomalous magnetic moment of the electron and are finite and scheme independent. By gauge invariance, the coefficients c_F and c_S are the same as for the $\mathcal{O}(\beta^2)$ operators, while the coefficient $c_{pp'}$ parametrizes the new $\mathcal{O}(\alpha\beta^4)$ operator contribution to the transverse-photon exchange [21]. The resulting contributions to the coefficient C are

$$C_{\rm II} = \left[\frac{1}{14}\right]_{\rm Cou} + \left[-\frac{5}{14}\right]_{\rm tra} + \left[\frac{2}{7}\right]_{\rm ret} + \left[-\frac{12}{7}\right]_{\rm sea} = -1\,. \tag{6}$$

The remaining part of the $\alpha^7 \ln(1/\alpha)$ contribution also corresponds to the first order of the nonrelativistic Rayleigh-Schrödinger perturbation theory and is related to the relativistic corrections to the operators contributing to the HFS in lower orders. The relevant operators are generated by the diagrams with one or two transverse-photon exchanges, where the momentum of the photon with spin-independent interaction can be soft or ultrasoft, and by the soft diagrams with one or two seagull vertices involving either one Coulomb and one transverse photon or two transverse photons. The resulting contribution to the coefficient C reads

$$C_{\rm III} = -\frac{41}{63}\,. \tag{7}$$

Adding Eqs. (5)–(7), we obtain

$$C = \frac{62}{15} - \frac{68}{7}\ln 2 \approx -2.6001\,. \tag{8}$$

Thus, the $\alpha^7 \ln(1/\alpha)$ term in Eq. (3) has the same sign as the $\alpha^7 \ln^2(1/\alpha)$ one and amounts to about 1/3 of the latter. It reduces $\Delta\nu$ by 323 kHz, while the $\alpha^7 \ln^2(1/\alpha)$ term reduces $\Delta\nu$ by 918 kHz. For comparison, we recall that, in the counterpart of Eq. (3) appropriate for the muonium HFS, the coefficient of the $\alpha^7 \ln^2(1/\alpha)$ correction reads $-8/3$ and $C = 281/180 - (8/3)\ln 2 \approx -0.2873$ [25]. Our final prediction for the HFS reads

$$\Delta\nu^{\rm th} = 203.391\,69(41)\,{\rm GHz}. \tag{9}$$

Here, the uncertainty due to the unknown nonlogarithmic $\mathcal{O}(\alpha^7)$ term in Eq. (3) is estimated by using the value $D = 16.233\pi^2$ of the analogous coefficient in the case of the HFS of muonium [21,26].

The unknown nonlogarithmic $\mathcal{O}(\alpha^7)$ term in Eq. (3) receives contributions from three-loop QED diagrams with a considerable number of external lines, which are still beyond the reach of presently available computational techniques. In this sense, we expect Eq. (9) to remain the best prediction for the foreseeable future.

The new theoretical value in Eq. (9) exceeds the experimental values in Eqs. (1) and (2) by approximately 2.6 and 3.5 experimental standard deviations, respectively. Thus, the discrepancy between experiment and theory is somewhat reduced by the inclusion of the $\alpha^7 \ln(1/\alpha)$ term, but it still remains sizable.

We may speculate about the magnitude of the coefficient D in Eq. (3). Note that two powers of α in the nonlogarithmic $\mathcal{O}(\alpha^7)$ term can be of nonrelativistic origin. Each of them should be accompanied by the characteristic factor π, which happens for the logarithmic terms. Thus, a plausible estimate of the coefficient D is a few units times π^2. In order to bring the theoretical estimate into agreement with Eqs. (1) and (2), we need $D \approx -100\pi^2$ and $D \approx -70\pi^2$, respectively. On the other hand, the logarithmic terms of the positronium HFS exhibit a structure similar to the muonium case, so that it is not unreasonable to expect the nonlogarithmic terms of the positronium and muonium HFS's to be of the same magnitude. This would imply a significant contradiction between the current experimental measurements and the theoretical prediction. However, although this may seem unlikely, one cannot completely exclude the possibility that the residual discrepancy will be removed by the inclusion of the nonlogarithmic $\mathcal{O}(\alpha^7)$ term. We conclude that both the calculation of the coefficient D as well as improved experimental measurements are necessary in order to establish or remove the residual discrepancy. Although there is no conceptual problem on the theoretical side, from the technical point of view, such a calculation represents a challenge for QED bound-state perturbation theory.

Finally we would like to note that the technique developed in Ref. [13] and here can be applied to the analysis of QCD heavy quark-antiquark bound states, where the logarithmically enhanced corrections are known to be essential [18,27].

We are indebted to K. Melnikov and A. Yelkhovsky for useful discussions. This work was supported in part by the Deutsche Forschungsgemeinschaft through Grant No. KN 365/1-1, by the Bundesministerium für Bildung und Forschung through Grant No. 05 HT9GUA 3, and

by the European Commission through the Research Training Network *Quantum Chromodynamics and the Deep Structure of Elementary Particles* under Contract No. ERBFMRX-CT98-0194. The work of A. A. P. was supported in part by the Volkswagen Foundation through Grant No. I/73611.

[1] A. P. Mills, Jr. and G. H. Bearman, Phys. Rev. Lett. **34**, 246 (1975); A. P. Mills, Jr., Phys. Rev. A **27**, 262 (1983).
[2] M. W. Ritter, P. O. Egan, V. W. Hughes, and K. A. Woodle, Phys. Rev. A **30**, 1331 (1984).
[3] J. Pirenne, Arch. Sci. Phys. Nat. **29**, 265 (1947); V. B. Berestetski and L. D. Landau, Zh. Eksp. Teor. Fiz. **19**, 673 (1949); R. A. Ferrell, Phys. Rev. **84**, 858 (1951).
[4] R. Karplus and A. Klein, Phys. Rev. **87**, 848 (1952).
[5] G. T. Bodwin and D. R. Yennie, Phys. Rep. **43**, 267 (1978).
[6] W. E. Caswell and G. P. Lepage, Phys. Rev. A **20**, 36 (1979).
[7] S. J. Brodsky and G. W. Erickson, Phys. Rev. **148**, 26 (1966); R. Barbieri, J. A. Mignaco, and E. Remiddi, Nuovo Cimento Soc. Ital. Fis. **11A**, 824 (1972).
[8] G. S. Adkins, M. H. T. Bui, and D. Zhu, Phys. Rev. A **37**, 4071 (1988); G. S. Adkins, Y. M. Aksu, and M. H. T. Bui, Phys. Rev. A **47**, 2640 (1993); G. S. Adkins, R. N. Fell, and P. M. Mitrikov, Phys. Rev. Lett. **79**, 3383 (1997); A. H. Hoang, P. Labelle, and S. M. Zebarjad, Phys. Rev. Lett. **79**, 3387 (1997).
[9] J. R. Sapirstein, E. A. Terray, and D. R. Yennie, Phys. Rev. D **29**, 2290 (1984); K. Pachucki and S. G. Karshenboim, Phys. Rev. Lett. **80**, 2101 (1998).
[10] K. Pachucki, Phys. Rev. A **56**, 297 (1997); G. S. Adkins and J. Sapirstein, Phys. Rev. A **58**, 3552 (1998); **61**, 069902(E) (2000); A. P. Burichenko, Report No. hep-ph/0004063.
[11] A. Czarnecki, K. Melnikov, and A. Yelkhovsky, Phys. Rev. Lett. **82**, 311 (1999); Phys. Rev. A **59**, 4316 (1999).
[12] S. G. Karshenboim, Zh. Eksp. Teor. Fiz. **103**, 1105 (1993) [Sov. Phys. JETP **76**, 541 (1993)].
[13] B. A. Kniehl and A. A. Penin, Phys. Rev. Lett. **85**, 1210 (2000); **85**, 3065(E) (2000).
[14] R. Hill and G. P. Lepage, Report No. hep-ph/0003277 v2, 2000.
[15] K. Melnikov and A. Yelkhovsky, Report No. SLAC-PUB-8557; hep-ph/0008099.
[16] W. E. Caswell and G. P. Lepage, Phys. Lett. **167B**, 437 (1986).
[17] A. Pineda and J. Soto, Nucl. Phys. (Proc. Suppl.) **64**, 428 (1998).
[18] B. A. Kniehl and A. A. Penin, Nucl. Phys. **B577**, 197 (2000).
[19] A. Pineda and J. Soto, Phys. Lett. B **420**, 391 (1998); Phys. Rev. D **59**, 016005 (1999).
[20] M. Beneke and V. A. Smirnov, Nucl. Phys. **B522**, 321 (1998).
[21] T. Kinoshita and M. Nio, Phys. Rev. D **53**, 4909 (1996).
[22] A. V. Manohar, Phys. Rev. D **56**, 230 (1997); A. Pineda and J. Soto, Phys. Rev. D **58**, 114 011 (1998).
[23] B. A. Kniehl and A. A. Penin, Nucl. Phys. **B563**, 200 (1999).
[24] P. Labelle, S. M. Zebarjad, and C. P. Burgess, Phys. Rev. D **56**, 8053 (1997).
[25] D. E. Zwanziger, Bull. Am. Phys. Soc. **6**, 514 (1961); Nuovo Cimento **XXXIV**, 77 (1964); A. J. Layzer, Bull. Am. Phys. Soc. **6**, 514 (1961); Nuovo Cimento **XXXIII**, 1538 (1964).
[26] T. Kinoshita and M. Nio, Phys. Rev. Lett. **72**, 3803 (1994); M. I. Eides and V. A. Shelyuto, Pis'ma Zh. Eksp. Teor. Fiz. **61**, 465 (1995) [JETP Lett. **61**, 478 (1995)]; Phys. Rev. A **52**, 954 (1995); K. Pachucki, Phys. Rev. A **54**, 1994 (1996); M. Nio and T. Kinoshita, Phys. Rev. D **55**, 7267 (1997).
[27] N. Brambilla, A. Pineda, J. Soto, and A. Vairo, Phys. Lett. B **470**, 215 (1999).