Calculation of the Positronium Hyperfine Interval

Gregory S. Adkins
Franklin and Marshall College, Lancaster, Pennsylvania 17604

Richard N. Fell
Brandeis University, Waltham, Massachusetts 02254

Plamen M. Mitrikov
Franklin and Marshall College, Lancaster, Pennsylvania 17604

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We have completed the calculation of the one-photon-annihilation contribution to the positronium hyperfine interval at order $m\alpha^6$. Our result for this contribution is $-0.1256481(12)m\alpha^6 = -2.344$ MHz. The complete theoretical result for this interval is worked out, and comparison with experiment is discussed. [S0031-9007(97)04341-X]

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Positronium provides an important testing ground for our understanding of bound-state QED. The low mass and pointlike nature of its constituents minimize strong and weak interaction effects, so the structure is governed almost completely by QED. The equal masses of the constituents require that a field theory based bound-state formalism be used to go beyond the most basic nonrelativistic Schrödinger level of approximation. The annihilation channel leads to interesting effects not present in hydrogen or muonium. Positronium is accessible to high precision measurements of spectrum and decay rates. In particular, the measured values for the ground state (triplet minus singlet) hyperfine interval are

$$\Delta E_{\text{expt}} = 203\,387.5 \pm 1.6 \text{ MHz} \quad (7.9 \text{ ppm}),$$
$$= 203\,389.10 \pm 0.74 \text{ MHz} \quad (3.6 \text{ ppm}) \quad (1)$$

[1–3]. In order to achieve a comparable theoretical prediction, all order α^2 corrections to the lowest order interval must be computed. In this Letter we report the result for the final uncalculated contribution at this order.

For this calculation, we have used a new bound-state formalism [4], a quasipotential variant of the Bethe-Salpeter formalism [5]. Our approach is closely related to the methods of Barbieri, Remiddi, and Buchmüller [6–8] and Caswell and Lepage [9]. We write the bound-state equation for the e^-e^+ to e^-e^+ Green's function G as $G = S_0 + S_0KG$, where S_0 is a modified e^-e^+ propagator and K is the "quasipotential." For S_0 we use [10]

$$S_0(p) = 2\pi\delta(p_0)\frac{-i}{2(\omega_p - E/2 - i\epsilon)}[\Lambda_+(\vec{p})\gamma^0]^{(1)} \times [\Lambda_-(\vec{p})(-\gamma^0)]^{(2)T}, \quad (2)$$

where $\omega_p = (\vec{p}^{\,2} + m^2)^{1/2}$ and the $\Lambda_\pm(\vec{p})$ are projection operators. The reference bound-state equation has the form $G_0 = S_0 + S_0K_0G_0$, where K_0 is an approximation to K containing the dominant nonrelativistic physics and is chosen so that the reference equation can be solved exactly. The reference energy levels and wave functions can be found by studying the pole structure of the reference Green's function G_0. With the particular reference kernel K_0 that we are using, the reference energy levels are $E_n^0 = 2m(1 - \alpha^2/4n^2)^{1/2}$, where n is the principal quantum number. The $n = 1$ reference wave functions have the form

$$\Psi^0(p) = 2\pi\delta(p_0)\left(\frac{2\omega_p}{\omega_p + m}\right)\left(\frac{\omega_p + W}{2W}\right)^{1/2}\phi(\vec{p}) \times [\Lambda_+(\vec{p})\Gamma\Lambda_-(\vec{p})(-\gamma^0)], \quad (3)$$

where $W = E_1^0/2$, Γ is a 4×4 spin matrix, and $\phi(\vec{p})$ is the nonrelativistic momentum space wave function.

We used Coulomb gauge for our calculation. Coulomb gauge is certainly the best gauge to use for exchange photons since spurious lower order terms are absent. If a covariant gauge were used for radiative photons, a nontrivial gauge correction term would be required. Therefore, we found it simplest to use Coulomb gauge throughout. The extensive noncovariant algebraic calculations were done with routines written using MATHEMATICA [11] and MACSYMA [12]. We used dimensional regularization with $n = 4 - 2\epsilon$ dimensions of space-time to regulate the ultraviolet divergences that occurred in intermediate stages of our calculation. In a previous work, we showed how the on-shell renormalization scheme works in Coulomb gauge at two-loop order [13], and calculated the two-loop vertex renormalization constant that will be used here.

Corrections for the energy levels can be calculated from a systematic perturbation series [7,9,14]. For those terms from this series involving virtual annihilation to a single photon, we have shown that all ultraviolet divergences vanish. The several graphs that contribute are represented in Fig. 1. We describe the contributions of these graphs in turn, and tabulate the results in Table I.

The first contribution, shown in Fig. 1(a), involves a renormalized one-loop vertex part on either end of the annihilation photon. The (unrenormalized) amplitude for positronium to annihilate into a single photon with a

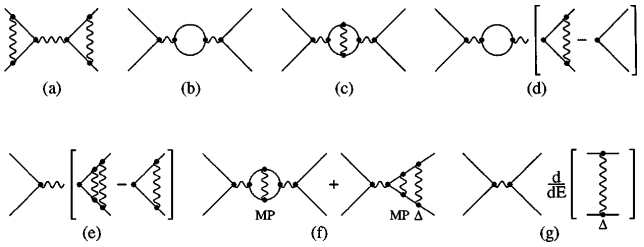

FIG. 1. The set of all one-photon-annihilation graphs that contribute at order $m\alpha^6$. The vertex corrections and vacuum polarization bubbles are renormalized. The bubble in (c) represents full two-loop vacuum polarization. The two-rung ladder diagram of (e) represents all two-loop corrections to the annihilation vertex diagram. The "MP" in (f) stands for many potential: the exchange of two or more photons with the ground state pole subtracted out. The "Δ" in (f) and (g) represents the difference between a Coulomb gauge photon and a reference photon. The asymmetric graphs (d), (e), and the second part of (f) must be doubled.

one-loop vertex correction, in our formalism, is $A_1^m = B^m I_1$, where

$$I_1 = 1 + L_1 I_0 - 2\frac{\alpha}{\pi} + \frac{5}{8}\alpha^2 \ln\left(\frac{1}{\alpha}\right) + \alpha^2[-0.247\,065\,7(9)] + O(\alpha^3). \quad (4)$$

The uncorrected decay amplitude is $A_0^m = B^m I_0$, where $B^m = \sqrt{2}\, ie\phi_0 \epsilon^m$, $\phi_0 = [m^3\alpha^3/(8\pi)]^{1/2}$ is the wave function at contact, $\vec{\epsilon}$ is the positronium spin vector, and $I_0 = 1 + \alpha/6 + O(\alpha^2)$ [7]. The one-loop renormalization constant is $L_1 = (\alpha/4\pi)\Omega^\epsilon \Gamma(\epsilon)$, where $\Omega = 4\pi\mu^2/m^2$ with μ the arbitrary mass introduced in the process of dimensional regularization. The renormalized one-rung decay amplitude is just $A_{1R}^m = B^m I_{1R}$ where $I_{1R} = I_1 - L_1 I_0$, so that the energy shift due to the graph of Fig. 1(a), through terms of order $m\alpha^6$, is

$$\Delta E_a = m\alpha^4\left\{\frac{1}{4} - \frac{\alpha}{\pi} + \frac{5}{16}\alpha^2 \ln\left(\frac{1}{\alpha}\right) + \alpha^2[0.040\,288\,3(5)]\right\}. \quad (5)$$

The one-loop vacuum polarization contribution of Fig. 1(b) is easy to evaluate. The value of this graph is just $-\Pi_R(4W^2)$ times the lowest order annihilation contribution, where $\Pi_R(k^2)$ is the renormalized scalar vacuum polarization function. The relativistic expansion of the wave function also leads to a contribution at $O(m\alpha^6)$. One has

$$\Delta E_b = \frac{m\alpha^4}{4}\left\{-\frac{8}{9}\frac{\alpha}{\pi} + \frac{\alpha^2}{4} + \ldots\right\} I_0^2 = m\alpha^4\left\{-\frac{2}{9}\frac{\alpha}{\pi} + \frac{\alpha^2}{16} - \frac{2}{27}\frac{\alpha^2}{\pi}\right\}. \quad (6)$$

TABLE I. One-photon-annihilation contributions to the positronium hyperfine interval. The corresponding diagrams are shown in Figs. 1(a)–1(g). Each contribution is the sum of parts of orders α^4, α^5/π, $\alpha^6\ln(1/\alpha)$, and α^6. The energy in MHz of the pure α^6 contribution is shown in the final column. Note that the numerically uncertain $O(\alpha^6)$ part of I_1 cancels between (a) and (e), so the final uncertainty is just that of Eq. (9).

Contribution	α^4	$\frac{\alpha^5}{\pi}$	$\alpha^6\ln(1/\alpha)$	α^6	ΔE (MHz)
a	$\frac{1}{4}$	-1	$\frac{5}{16}$	0.040 288 3(5)	0.752
b	0	$-\frac{2}{9}$	0	0.038921490	0.726
c	0	0	$-\frac{1}{8}$	0.038327738	0.715
d	0	0	0	0.113641784	2.120
e	0	0	$-\frac{7}{48}$	−0.124 035 5(13)	−2.314
f	0	0	0	−0.201541896	−3.760
g	0	0	0	−0.031250000	−0.583
Total	$\frac{1}{4}$	$-\frac{11}{9}$	$\frac{1}{24}$	−0.1256481(12)	−2.344

The $\alpha^2/16$ from the expansion of the one-loop vacuum polarization function was noted by Karshenboim [15] and Hoang [16].

The two-loop vacuum polarization contribution of Fig. 1(c) was done many years ago by Barbieri *et al.* [17] and by Samuel [18]. The result, given in Table I, includes the reducible product of two one-loop vacuum polarization parts, but does not include the "Coulomb distortion" part of [17], which we take to be part of the "many-potential" contribution of Fig. 1(f).

The contribution of Fig. 1(d) comes from combining the one-loop vacuum polarization and vertex corrections. It is

$$\Delta E_d = m\alpha^4\left\{\frac{8}{9}\left(\frac{\alpha}{\pi}\right)^2 + \frac{2}{27}\frac{\alpha^2}{\pi}\right\}. \quad (7)$$

The α^2/π contribution comes from the relativistic expansion of the wave function and cancels against a similar term in ΔE_b. The other contribution here was worked out by Karshenboim [15].

The heart of our calculation is contained in the two-loop annihilation vertex of Fig. 1(e). The five two-loop vertex graphs are shown in Fig. 2. All divergent contributions and lower order contributions were obtained analytically. The $O(\alpha^2)$ correction to the decay amplitudes was obtained numerically [19], except for the vacuum polarization contribution, which was found analytically. Our result for the unrenormalized two-loop correction is

$$A_2^m = L_1 A_1^m + B^m\left\{1 - 2\frac{\alpha}{\pi} + \frac{1}{3}\alpha^2\ln\left(\frac{1}{\alpha}\right) + \left(\frac{\alpha}{\pi}\right)^2(\Omega e^{-\gamma_E})^{2\epsilon}\left[\frac{1}{96\epsilon^2} + \frac{1}{\epsilon}\left(\frac{3}{8}\zeta(2) - \frac{391}{576}\right) - 3.73\,122\,7(23)\right] + O(\alpha^3)\right\}. \quad (8)$$

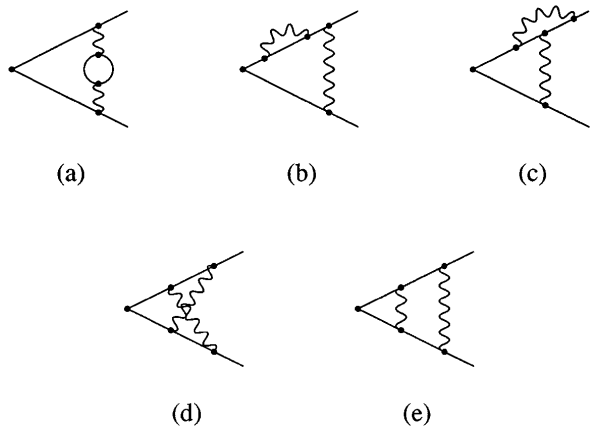

FIG. 2. The two-loop annihilation vertex contributions. They are (a) the vacuum polarization (VP) graph, (b) self-energy (SE) graph, (c) side-vertex (SV) graph, (d) crossed ladder (CL) graph, and (e) two-rung double ladder (DL) graph.

The renormalized two-loop annihilation vertex has the form [20] $A^m_{2R} = A^m_2 - L_1 A^m_1 - L_2 A^m_0 + L_1^2 A^m_0$, where L_2 is the two-loop renormalization constant [13] and L_1^2 is the square of the one-loop constant. The renormalized two-loop annihilation amplitude is

$$A^m_{2R} = B^m\left\{1 - 2\frac{\alpha}{\pi} + \frac{1}{3}\alpha^2 \ln\left(\frac{1}{\alpha}\right) + \left(\frac{\alpha}{\pi}\right)^2 [-4.88\,680\,4(24)]\right\}, \quad (9)$$

which is ultraviolet finite. The subtracted two-loop minus one-loop amplitude is

$$A^m_{2R} - A^m_{1R} = B^m\left\{-\frac{7}{24}\alpha^2 \ln\left(\frac{1}{\alpha}\right) + \alpha^2[-0.248\,071\,1(26)]\right\}, \quad (10)$$

and the energy contribution is

$$\Delta E_e = m\alpha^4\left\{-\frac{7}{48}\alpha^2 \ln\left(\frac{1}{\alpha}\right) + \alpha^2[-0.124\,035\,5(13)]\right\}. \quad (11)$$

The VP contribution was worked out earlier [15,21,22]. Our new calculation agrees with the earlier work on this graph.

The many-potential (MP) terms of Fig. 1(f) are similar to the MP contributions in other related formalisms. Corresponding contributions were worked out by Caswell and Lepage [9], where it was noted that the contributions having two annihilation photons and an annihilation photon with a transverse exchange photon should be formalism independent, while the term involving the exchange of a Coulomb minus lowest order photon should be formalism dependent. We found this to be the case, although our result for the Coulomb minus lower order contribution agrees with that of Buchmüller and Remiddi [8], which underscores the closeness of the formalisms. The total energy shift from MP contributions is $\Delta E_f = m\alpha^6[(5/16) - (5/16)\zeta(2)]$.

The final contribution from Fig. 1(g) is the derivative term. This is similar to the derivative term calculated by Caswell and Lepage [9], except for a formalism dependent sign and the fact that only the one-photon-annihilation part contributes here. The derivative term is $\Delta E_g = -m\alpha^6/32$.

The total result for the coefficient of $m\alpha^6$ coming from all one-photon-annihilation contributions, from Table I, is $-0.125\,648\,1(12)$. This agrees with the analytic result

$$\Delta E = \frac{m\alpha^6}{\pi^2}\left\{\frac{13}{32}\zeta(3) + \frac{27}{8}\zeta(2)\ln(2) - \frac{1183}{192}\zeta(2) + \frac{1477}{324}\right\} \quad (12)$$

of Hoang *et al.* [23] reported in the companion Letter. The numerical value of the analytic result is -0.1256487.

All contributions to the hyperfine interval are tabulated in Table II. The total coefficient at order $m\alpha^6$ is $K = -0.597(34)$, where the uncertainty is from the numerical integration in the three-photon-exchange contribution. The complete theoretical result for the hyperfine interval has the form [14,33]

$$\Delta E_{\rm th} = m\alpha^4\left\{\frac{7}{12} - \frac{\alpha}{\pi}\left(\frac{1}{2}\ln 2 + \frac{8}{9}\right) + \frac{5}{24}\alpha^2 \ln\left(\frac{1}{\alpha}\right) + K\alpha^2 - \frac{7}{8}\frac{\alpha^3}{\pi}\ln^2\left(\frac{1}{\alpha}\right) + \ldots\right\}. \quad (13)$$

With a coefficient of 1, the $m\alpha^6$ term would contribute 18.658 MHz. The complete theoretical prediction is

$$\Delta E_{\rm th} = 203\,388.22 \pm 0.63\ \text{MHz}, \quad (14)$$

in agreement with the combined experimental result of

$$\Delta E_{\rm expt} = 203\,388.82 \pm 0.67\ \text{MHz}. \quad (15)$$

However, Pachucki [34] has recently reported a new result for the three-photon-exchange contribution of 7.03(3) MHz, in disagreement with the old value given in Table II. This would give a difference between theory and experiment of 3.32 ± 0.67 MHz. The three-photon-exchange discrepancy will have to be resolved before final conclusions can be drawn.

TABLE II. Contributions to the positronium hyperfine interval at order $m\alpha^6$.

Contribution	K	ΔE (MHz)
Three-photon-annihilation [24–26]	−0.05194	−0.969
Two-photon-annihilation [27,28]	−0.03248	−0.606
One-photon-annihilation [this work]	−0.12565	−2.344
One-photon-exchange [21,29,30]	−0.01374	−0.256
Two-photon exchange [21,31]	−0.5394(14)	−10.06(3)
Three-photon-exchange [32]	0.167(34)	3.11(62)
Total	−0.596(34)	−11.13(63)

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