

# PHYSICAL REVIEW A

## GENERAL PHYSICS

THIRD SERIES, VOLUME 37, NUMBER 11

JUNE 1, 1988

### New calculation of the three-photon-annihilation contribution to the positronium hyperfine interval

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(Received 24 December 1987)

The three-photon-annihilation contribution to the positronium hyperfine interval is obtained in analytic form. This contribution is of order  $m\alpha^6$ , and has the value  $-0.969$  MHz. The result of a previous calculation of this contribution is shown to be incomplete because of a subtlety in the regularization of infrared divergences.

#### I. INTRODUCTION

The comparison of experimental and theoretical results for the ground-state hyperfine interval of positronium has for many years been considered an important test of our understanding of bound-state physics. This interval was first measured by Deutsch and Dulit in 1951.<sup>1,2</sup> Several other determinations were made over the years, the latest being<sup>3</sup>

$$\Delta E = 203\,389.10 \pm 0.74 \text{ MHz} . \quad (1)$$

The theoretical result for this splitting is<sup>4-7</sup>

$$\begin{aligned} \Delta E &= m\alpha^4 \left\{ \frac{7}{12} - \frac{\alpha}{\pi} \left( \frac{8}{9} + \frac{1}{2} \ln 2 \right) + \frac{5}{24} \alpha^2 \ln(1/\alpha) + O(\alpha^2) \right\} \\ &= 203\,400 \text{ MHz} . \end{aligned} \quad (2)$$

With a coefficient of 1, the uncalculated term of  $O(m\alpha^6)$  would contribute 18.7 MHz to  $\Delta E$ . This theoretical uncertainty is much larger than the present experimental uncertainty. As early as 1975 the experimental uncertainty was only a few megahertz.<sup>8</sup> The completion of the calculation of the  $O(m\alpha^6)$  contribution to  $\Delta E$  is long overdue.

Graphs containing three photons from electron-positron annihilation as intermediate states (see Fig. 1) form one class of contributions to the positronium hyperfine interval. These graphs contribute at order  $m\alpha^6$ . An analytic evaluation of this contribution has been carried through by Cung, Devoto, Fulton, and Repko<sup>9</sup> (hereafter referred to as CDFR), with the result

$$\begin{aligned} \Delta E &= \frac{m\alpha^6}{2\pi^2} \left\{ \frac{3}{4} \zeta(3) - \frac{1}{3} \zeta(2) \ln 2 - \frac{19}{6} \zeta(2) - 4 \ln 2 + \frac{13}{2} \right. \\ &\quad \left. + (-i\pi) \left[ \frac{4}{3} \zeta(2) - 2 \right] \right\} . \end{aligned} \quad (3)$$

The imaginary part of this energy shift is related to the orthopositronium decay rate, which is

$$\Gamma(\text{ortho-Ps}) = -2 \text{Im}(\Delta E) = \frac{2}{9\pi} (\pi^2 - 9) m\alpha^6 , \quad (4)$$

a result first obtained by Ore and Powell.<sup>10</sup> The real part of (3) is the calculated contribution to the hyperfine interval,

$$\text{Re}(\Delta E) = -0.907 \text{ MHz} . \quad (5)$$

In this paper we show that Eq. (3) for the energy shift is not correct. The correct result is

$$\begin{aligned} \Delta E &= \frac{m\alpha^6}{2\pi^2} \left\{ \frac{3}{4} \zeta(3) - \frac{1}{3} \zeta(2) \ln 2 - \frac{1}{6} \zeta(2) - 4 \ln 2 + \frac{3}{2} \right. \\ &\quad \left. + (-i\pi) \left[ \frac{4}{3} \zeta(2) - 2 \right] \right\} , \end{aligned} \quad (6)$$

which makes a contribution of

$$\text{Re}(\Delta E) = -0.969 \text{ MHz} \quad (7)$$

to the hyperfine interval. We have traced the discrepancy between (3) and (6) to a subtlety in the regularization of infrared singular integrals.

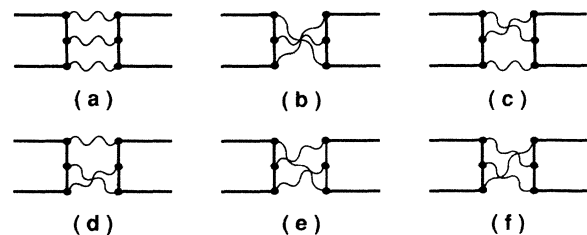


FIG. 1. These six three-photon annihilation graphs contribute to the positronium hyperfine interval at order  $m\alpha^6$ .

This article is organized as follows. In Sec. II we give the derivation of an integral expression for the energy shift  $\Delta E$ . In Sec. III we discuss the ir regularization of terms in the integral for  $\Delta E$ . In Sec. IV we describe the evaluation of the integral for  $\Delta E$ . Finally, in Sec. V we give a discussion of our results.

## II. DERIVATION OF AN INTEGRAL EXPRESSION FOR $\Delta E$

The energy levels of positronium are determined by the positions of the poles of the electron-positron-to-electron-positron propagator  $G$ . Near its poles,  $G$  takes the form<sup>11–13</sup>

$$G(P; p, q) \rightarrow \frac{i \sum_j \psi_{nj}(p) \bar{\psi}_{nj}(q)}{E - E_n}, \quad (8)$$

where  $P$  is the center-of-mass momentum,  $p$  and  $q$  are the relative momenta of the outgoing and incoming pairs of particles, and the index  $j$  labels degenerate states. The propagator  $G$  satisfies the Bethe-Salpeter equation<sup>14–16</sup>

$$G = S + SKG, \quad (9)$$

where  $S$  is the product of two one-particle propagators and  $K$  is the two-particle irreducible kernel. In order to set up a perturbation scheme for the energies, we imagine an approximation  $K_0$  to  $K$  which allows the Bethe-Salpeter equation to be solved for  $G$ ,

$$G_0 = S + SK_0 G_0. \quad (10)$$

Then  $G_0$  has poles at known energies  $E_n^0$ , and satisfies

$$G_0(P; p, q) \rightarrow \frac{i \sum_j \psi_{nj}^0(p) \bar{\psi}_{nj}^0(q)}{E - E_n^0} \quad (11)$$

near its poles. The propagator  $G$  can be expressed in terms of  $G_0$  as

$$G = G_0 + G_0 \delta K G_0 + \dots, \quad (12)$$

where  $\delta K = K - K_0$ . Then bound-state perturbation theory<sup>17</sup> gives

$$\Delta E = i \bar{\psi}^0 \delta K \psi^0 \quad (13)$$

$$\begin{aligned} \Delta E = & i(-1)^{\frac{1}{3}} \sum_{\epsilon} \int (dk_1)' (dk_2)' (dk_3)' (2\pi)^4 \delta(P - k_1 - k_2 - k_3) (\phi_0^2/2) \\ & \times \text{tr} \left[ \begin{pmatrix} 0 & 0 \\ \sigma \cdot \hat{\epsilon}^* & 0 \end{pmatrix} (-ie\gamma^{\mu_1}) \frac{i}{\gamma(\frac{1}{2}P - k_1) - m} (-ie\gamma^{\mu_2}) \frac{i}{\gamma(-\frac{1}{2}P + k_3) - m} (-ie\gamma^{\mu_3}) \right] \\ & \times \frac{-i}{k_1^2} \frac{-i}{k_2^2} \frac{-i}{k_3^2} \sum_{\sigma \in S_3} \text{tr} \left[ (-ie\gamma_{\mu_{\sigma(3)}}) \frac{i}{\gamma(-\frac{1}{2}P + k_{\sigma(3)}) - m} (-ie\gamma_{\mu_{\sigma(2)}}) \right. \\ & \left. \times \frac{i}{\gamma(\frac{1}{2}P - k_{\sigma(1)}) - m} (-ie\gamma_{\mu_{\sigma(1)}}) \begin{pmatrix} 0 & \sigma \cdot \hat{\epsilon} \\ 0 & 0 \end{pmatrix} \right]. \quad (16) \end{aligned}$$

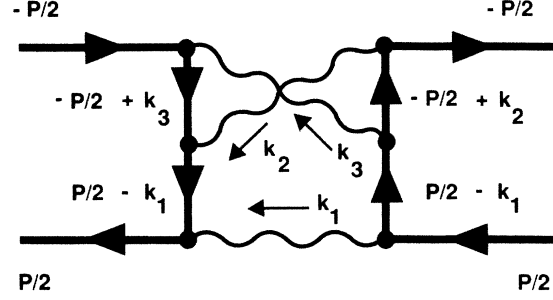


FIG. 2. This three-photon annihilation graph is shown with complete momentum labeling. Directions of fermion lines are also shown, and fermion momenta are given relative to those directions. The relative momenta of the incoming fermions (on the right) and the outgoing fermions (on the left) are taken to be zero.

as the first-order expression for  $\Delta E = E - E^0$ . If we make the relative momentum integrals explicit, this is

$$\Delta E = i \int (dp)' (dq)' \bar{\psi}^0(p) \delta K(p, q) \psi^0(q), \quad (14)$$

where  $(dp)' = d^4p/(2\pi)^4$ . The three-photon annihilation contributions to  $\delta K$  are shown in Fig. 1. They involve internal momenta on the scale of the electron mass  $m$ . On the other hand, the lowest-order wave functions are largest at small momentum, and are effectively proportional to four-dimensional momentum-space  $\delta$  functions. Since charge-conjugation invariance limits the effects of three-photon annihilation to orthopositronium, the lowest-order wave functions are effectively given by<sup>18</sup>

$$\psi^0(p) \cong (2\pi)^4 \delta(p) (\phi_0/\sqrt{2}) \begin{pmatrix} 0 & \sigma \cdot \hat{\epsilon} \\ 0 & 0 \end{pmatrix}, \quad (15a)$$

$$\bar{\psi}^0(p) \cong (2\pi)^4 \delta(p) (\phi_0/\sqrt{2}) \begin{pmatrix} 0 & 0 \\ \sigma \cdot \hat{\epsilon}^* & 0 \end{pmatrix}, \quad (15b)$$

where  $\hat{\epsilon}$  is the orthopositronium spin vector and where  $\phi_0 = [m^3 \alpha^3 / (8\pi)]^{1/2}$  is the value of the nonrelativistic wave function at  $\mathbf{x} = \mathbf{0}$ .

We will now obtain an explicit expression for the energy-level shift due to the three-photon annihilation graphs shown in Fig. 1. One of these graphs is shown with complete momentum labeling in Fig. 2. The expression for  $\Delta E$  due to all six graphs is

The traces come from the outgoing and incoming fermion loops. The  $-1$  factor arises because these graphs have an extra fermion loop compared to nonannihilation graphs. The integration is over the three internal photon momenta subject to overall energy-momentum conservation. The sum over the permutations  $\sigma$  in the permutation group  $S_3$  gives the six graphs of Fig. 1. For instance, the graph shown in Fig. 2 has  $\sigma(1)=1$ ,  $\sigma(2)=3$ , and  $\sigma(3)=2$ . We choose to average the formula over the three degenerate spin states specified by  $\epsilon$ . This spin average is easy to perform using

$$\sum_{\epsilon} \epsilon_{\mu} \epsilon_{\nu}^* = n_{\mu} n_{\nu} - g_{\mu\nu}, \quad (17)$$

$$\begin{aligned} \Delta E = & \frac{-16\pi^2}{3} m \alpha^6 \int (dk_1)' (dk_2)' (dk_3)' (2\pi)^4 \delta(2n - k_1 - k_2 - k_3) \\ & \times \sum_{\sigma \in S_3} \frac{1}{k_1^2 k_2^2 k_3^2 [(k_1 - n)^2 - 1] [(k_3 - n)^2 - 1] [(k_{\sigma(1)} - n)^2 - 1] [(k_{\sigma(3)} - n)^2 - 1]} \\ & \times \frac{1}{4} \text{tr} \{ \gamma^{\mu_3} [\gamma(-n + k_3) + 1] \gamma^{\mu_2} [\gamma(n - k_1) + 1] \gamma^{\mu_1} (\gamma n + 1) \gamma_{\lambda} \} (g^{\lambda\kappa} - n^{\lambda} n^{\kappa}) \\ & \times \frac{1}{4} \text{tr} \{ \gamma_{\mu_{\sigma(3)}} [\gamma(-n + k_{\sigma(3)}) + 1] \gamma_{\mu_{\sigma(2)}} [\gamma(n - k_{\sigma(1)}) + 1] \gamma_{\mu_{\sigma(1)}} (\gamma n + 1) \gamma_{\kappa} \}. \end{aligned} \quad (19)$$

As pointed out by CDFR, charge-conjugation symmetry can be used to reduce the number of independent contributing diagrams. The charge-conjugation matrix  $C$ , which satisfies<sup>19</sup>

$$C \gamma_{\mu}^T C^{-1} = -\gamma_{\mu}, \quad (20)$$

can be used to show that the indices 1 and 3 in either of the traces in (19) can be interchanged without changing the value of the corresponding trace. Diagrammatically this implies that a graph is unchanged when either the outgoing or incoming fermion line, with photon lines attached, is reflected top to bottom. One sees that graphs (a) and (b) in Fig. 1 are equivalent, as are (c), (d), (e), and (f). The sum of all six graphs can be written as twice (a)

$$\begin{aligned} M_{\text{I}} = & \frac{1}{2} T(3, 2, 1, \lambda) (g^{\lambda\kappa} - n^{\lambda} n^{\kappa}) T(3, 2, 1, \kappa) \\ = & 10(X_{11} + X_{33}) + 6X_{22} - 4(X_1^2 + X_3^2) + 13X_{11}X_{33} - 16(X_{11}X_3 + X_{33}X_1) \\ & - 2(X_{11}X_3^2 + X_{33}X_1^2) - 4X_{13} + 4X_{13}X_1X_3 + 2X_{13}^2 + 16X_1X_3 + 4(X_1 + X_3)X_{13}, \end{aligned} \quad (22a)$$

$$\begin{aligned} M_{\text{II}} = & T(3, 2, 1, \lambda) (g^{\lambda\kappa} - n^{\lambda} n^{\kappa}) T(2, 3, 1, \kappa) \\ = & 4X_{11} - 24(X_2 + X_3) + 8X_1^2 - 8X_2X_3 + 32X_{23} - 16X_{11}(X_2 + X_3) + 14X_{11}X_{23} - 4X_1(X_{12} + X_{13}) \\ & - 32X_1X_{23} + 4(X_2X_{13} + X_3X_{12}) - 8X_1^2X_{23} - 8(X_{12} + X_{13}) + 32X_1(X_2 + X_3) + 8X_1^2(X_2 + X_3). \end{aligned} \quad (22b)$$

We can use these results in (19) to write

$$\Delta E = \frac{m \alpha^6}{12\pi^2} \int (dk_1)'' (dk_3)'' \left[ \frac{M_{\text{I}}}{D_{\text{I}}} + \frac{M_{\text{II}}}{D_{\text{II}}} \right], \quad (23)$$

which implies

$$\begin{aligned} \sum_{\epsilon} \begin{bmatrix} 0 & 0 \\ \sigma \cdot \hat{\epsilon}^* & 0 \end{bmatrix}_{ab} \begin{bmatrix} 0 & \sigma \cdot \hat{\epsilon} \\ 0 & 0 \end{bmatrix}_{cd} \\ = [\gamma_{\lambda}^{\frac{1}{2}} (1 + \gamma^0)]_{ab} (g^{\lambda\kappa} - n^{\lambda} n^{\kappa}) [\frac{1}{2} (1 + \gamma^0) \gamma_{\kappa}]_{cd}. \end{aligned} \quad (18)$$

We also factor an  $m$  out of each  $k$ :  $k_i \rightarrow mk_i$ , where the new  $k$ 's are dimensionless. The center-of-mass momentum is given approximately by  $P = 2mn$ , where  $n$  is the timelike unit vector  $n = (1, 0)$ . After inverting the order of the  $\gamma$  matrices in the first trace, we find that

plus four times (c).

The traces were performed by computer. This was done in two ways: using REDUCE,<sup>20</sup> and using a routine written by one of us (D.Z.) in the muMATH/muSIMP (Ref. 21) language for personal computers. Using the abbreviation

$$\begin{aligned} T(i, j, k, \lambda) = & \frac{1}{4} \text{tr} \{ \gamma^{\mu_i} [\gamma(-n + k_i) + 1] \gamma^{\mu_j} \\ & \times [\gamma(n - k_k) + 1] \gamma^{\mu_k} (\gamma n + 1) \gamma_{\lambda} \} \end{aligned} \quad (21)$$

and the definitions  $X_i = k_i \cdot n$  and  $X_{ij} = k_i \cdot k_j$ , we found that

where

$$D_I = k_1^2 k_2^2 k_3^2 (k_1^2 - 2k_1 \cdot n)^2 (k_3^2 - 2k_3 \cdot n)^2, \quad (24a)$$

$$D_{II} = k_1^2 k_2^2 k_3^2 (k_1^2 - 2k_1 \cdot n)^2 (k_2^2 - 2k_2 \cdot n)(k_3^2 - 2k_3 \cdot n). \quad (24b)$$

We have used the definition  $(dk)' = d^4k / (2\pi)^4 = i(dk)'' / (4\pi)^2$  to write

$$\int (dk_1)'(dk_2)'(dk_3)'(2\pi)^4 \delta(2n - k_1 - k_2 - k_3) F(k_1, k_2, k_3) = \frac{-1}{(4\pi)^4} \int (dk_1)''(dk_3)'' F(k_1, k_2 = 2n - k_1 - k_3, k_3). \quad (25)$$

Expression (23) for  $\Delta E$  is equivalent to the expression found by CDFR after performing the  $\gamma$  matrix algebra.

The formulas for  $M_I$  and  $M_{II}$  can be transformed into a more useful form. The integration region in (23) is symmetric under the group  $S_3$  of permutations. Also,  $D_I$  is symmetric under  $1 \leftrightarrow 3$  and  $D_{II}$  is symmetric under  $2 \leftrightarrow 3$ , so, for instance, in  $M_I$  we can write  $(X_{11} + X_{33}) \rightarrow 2X_{11}$ . We use these symmetries, along with the identities

$$2 = X_1 + X_2 + X_3, \quad (26a)$$

$$X_{ii} = 4 - 4X_j - 4X_k + X_{jj} + X_{kk} + 2X_{jk}, \quad (26b)$$

$$X_{jk} = \frac{1}{2} [(X_{ii} - 2X_i) - (X_{jj} - 2X_j) - (X_{kk} - 2X_k)], \quad (26c)$$

where  $i, j$ , and  $k$  are distinct, to write

$$M_I \rightarrow N_I + (8 - 4X_3)(X_{33} - 2X_3), \quad (27a)$$

$$M_{II} \rightarrow N_{II} - (8 - 4X_3)(X_{22} - 2X_2), \quad (27b)$$

where

$$N_I = 12X_{11} + 6X_{22} + 4X_{22}X_3 + 13X_{11}X_{33} - 36X_{11}X_3 - 4X_{11}X_3^2 - 4X_{13} + 4X_{13}X_1X_3 + 2X_{13}^2 + 32X_1X_3, \quad (28a)$$

$$N_{II} = 12X_{11} - 24X_{22} - 4X_{22}X_3 - 44X_{11}X_2 + 14X_{11}X_{23} + 4X_1X_{12} - 32X_1X_{23} + 8X_2X_{13} - 8X_1^2X_{23} - 56X_{12} + 72X_1X_2 + 16X_1^2X_2. \quad (28b)$$

Since the extra terms in (27) cancel one against the other, we have for the energy shift

$$\Delta E = \frac{m\alpha^6}{12\pi^2} \int (dk_1)''(dk_3)'' \left[ \frac{N_I}{D_I} + \frac{N_{II}}{D_{II}} \right]. \quad (29)$$

The advantage of using the  $N$ 's over the  $M$ 's is that unusual terms, such as  $-i\pi \ln 2$ , which appear and eventually cancel when individual terms in the  $M$ 's are integrated, are never seen with the  $N$ 's.

### III. INFRARED REGULARIZATION

Although the complete energy shift of (29) is finite, individual terms in  $\Delta E$  are divergent in the infrared (ir). These divergences occur because  $D_I$  and  $D_{II}$  go to zero in some regions of the momentum integration. The regions

most likely to cause ir trouble are where  $k_1, k_3 \rightarrow 0$ ,  $k_1, k_2 \rightarrow 0$  or  $k_2, k_3 \rightarrow 0$ . In these regions the denominators behave like

$$D_I \rightarrow 2^6 k_1^2 (k_1 \cdot n)^2 k_3^2 (k_3 \cdot n)^2, \quad k_1, k_3 \rightarrow 0 \quad (30a)$$

$$\rightarrow 2^6 k_1^2 (k_1 \cdot n)^2 k_2^2 [(k_1 + k_2) \cdot n]^2, \quad k_1, k_2 \rightarrow 0 \quad (30b)$$

$$\rightarrow 2^6 k_3^2 (k_3 \cdot n)^2 k_2^2 [(k_2 + k_3) \cdot n]^2, \quad k_2, k_3 \rightarrow 0 \quad (30c)$$

and

$$D_{II} \rightarrow 2^6 k_1^2 (k_1 \cdot n)^2 k_3^2 (k_3 \cdot n) [(k_1 + k_3) \cdot n], \quad k_1, k_3 \rightarrow 0 \quad (31a)$$

$$\rightarrow 2^6 k_1^2 (k_1 \cdot n)^2 k_2^2 (k_2 \cdot n) [(k_1 + k_2) \cdot n], \quad k_1, k_2 \rightarrow 0 \quad (31b)$$

$$\rightarrow 2^6 k_2^2 (k_2 \cdot n) k_3^2 (k_3 \cdot n) [(k_2 + k_3) \cdot n]^2, \quad k_2, k_3 \rightarrow 0. \quad (31c)$$

The differential element of momentum space looks like  $k_1^3 dk_1 k_3^3 dk_3$ , with equivalent forms  $k_1^3 dk_1 k_2^3 dk_2$  or  $k_2^3 dk_2 k_3^3 dk_3$  useful when  $k_1, k_2 \rightarrow 0$  or  $k_2, k_3 \rightarrow 0$  [since  $k_1, k_2$  or  $k_2, k_3$  could have been chosen as the independent variables of integration in (25) instead of  $k_1, k_3$ ]. With no numerators the integrals of  $(D_I)^{-1}$  and  $(D_{II})^{-1}$  would have log-squared divergences. The numerator factors in  $N_I$  and  $N_{II}$ , by vanishing in appropriate regions of momentum space, can reduce the degree of divergence to a single log or to a finite result. In order to eliminate the divergence in the  $D_I$  integral it is necessary to have at least one factor of  $k_1$  and one factor of  $k_3$  in the numerator. For the  $D_{II}$  integral it is necessary to have at least one factor of  $k_1$  and one factor of either  $k_2$  or  $k_3$  in the numerator.

Since we plan to deal with the terms in  $N_I$  and  $N_{II}$  one by one, it is necessary to regulate the ir divergences. Two regularization procedures are the "binding" method and the "photon mass" method. In the binding method of CDFR the substitutions

$$(k_i^2 - 2k_i \cdot n) \rightarrow (k_i^2 - 2k_i \cdot n - \epsilon) \quad (32)$$

are made in the electron propagation factors in  $D_I$  and  $D_{II}$ , where  $\epsilon$  is small and positive and will go to zero at the end of the calculation. The parameter  $\epsilon$  is related to the binding energy of positronium if that energy is taken

into account. In the photon mass method the substitutions

$$(k_i^2) \rightarrow (k_i^2 - \lambda^2) \quad (33)$$

are made in the photon propagation factors in  $D_I$  and  $D_{II}$ , where  $\lambda$  is small and will go to zero at the end. Either one of these methods serves to regulate the ir divergences.

In the binding regularization method it is crucial that the integrand be written as a single fraction with a common denominator before the regularization is made. CDFR regularized (23) directly, and were thus led to an incorrect result for  $\Delta E$ . A simple example contains the essence of this point. Consider the integral

$$I = \int_0^1 dx \left[ \frac{1+x}{x} - \frac{2}{(2x)} \right] = 1. \quad (34)$$

Done separately, the two terms in the integrand of  $I$  are divergent. If we regularize these terms individually, by adding a small quantity  $\varepsilon$  to the individual denominators, we get

$$\int_0^1 dx \left[ \frac{1+x}{x+\varepsilon} - \frac{2}{(2x)+\varepsilon} \right] = 1 - \ln 2 + O(\varepsilon \ln \varepsilon), \quad (35)$$

which is incorrect. A correct regularization procedure involves finding a common denominator and then regularizing,

$$\begin{aligned} I &= \int_0^1 dx \frac{(1+x)(2x) - (2)(x)}{(x)(2x)} \rightarrow \int_0^1 dx \frac{(1+x)(2x) - (2)(x)}{(x+\varepsilon)(2x+\varepsilon)} \\ &= \int_0^1 dx \left[ \frac{1+x}{x+\varepsilon} - \frac{2}{2x+\varepsilon} \right] + \varepsilon \int_0^1 dx \frac{(1-x)}{(x+\varepsilon)(2x+\varepsilon)} \\ &= [1 - \ln 2 + O(\varepsilon \ln \varepsilon)] + \varepsilon \left[ \frac{1}{\varepsilon} \ln 2 + O(\ln \varepsilon) \right] = 1 + O(\varepsilon \ln \varepsilon), \end{aligned} \quad (36)$$

which has the correct limit as  $\varepsilon \rightarrow 0$ . A characteristic feature is the appearance of a term which is nominally of  $O(\varepsilon)$ , but which is multiplied by a divergent integral and gives a finite final contribution.

We now discuss the actual regularization of  $\Delta E$ . The energy shift with a common denominator looks like

$$\Delta E = \frac{m\alpha^6}{12\pi^2} \int (dk_1)'' (dk_3)'' \frac{N}{D}, \quad (37)$$

where

$$N = N_I (Y_2)^2 + N_{II} Y_2 Y_3, \quad (38)$$

$$D = k_1^2 k_2^2 k_3^2 (Y_1)^2 (Y_2)^2 (Y_3)^2, \quad (39)$$

with

$$Y_i = k_i^2 - 2k_1 \cdot n = X_{ii} - 2X_i. \quad (40)$$

In the binding regularization method one has

$$D \rightarrow D_\varepsilon = k_1^2 k_2^2 k_3^2 (Y_1 - \varepsilon)^2 (Y_2 - \varepsilon)^2 (Y_3 - \varepsilon)^2. \quad (41)$$

The numerator can be written in terms of the  $(Y - \varepsilon)$ 's as

$$\begin{aligned} N &= N_I [(Y_2 - \varepsilon) + \varepsilon]^2 + N_{II} [(Y_2 - \varepsilon) + \varepsilon] [(Y_3 - \varepsilon) + \varepsilon] \\ &= [N_I (Y_2 - \varepsilon)^2 + N_{II} (Y_2 - \varepsilon)(Y_3 - \varepsilon)] \\ &\quad + \varepsilon \{ 2N_I (Y_2 - \varepsilon) + N_{II} [(Y_2 - \varepsilon) + (Y_3 - \varepsilon)] \} \\ &\quad + \varepsilon^2 (N_I + N_{II}). \end{aligned} \quad (42)$$

With the definitions

$$(D_I)_\varepsilon = k_1^2 k_2^2 k_3^2 (Y_1 - \varepsilon)^2 (Y_3 - \varepsilon)^2, \quad (43a)$$

$$(D_{II})_\varepsilon = k_1^2 k_2^2 k_3^2 (Y_1 - \varepsilon)^2 (Y_2 - \varepsilon)(Y_3 - \varepsilon), \quad (43b)$$

for the regularized denominators  $D_I$  and  $D_{II}$ , we have for the energy shift,

$$\Delta E = \frac{m\alpha^6}{12\pi^2} \int (dk_1)'' (dk_3)'' \left[ \left( \frac{N_I}{(D_I)_\varepsilon} + \frac{N_{II}}{(D_{II})_\varepsilon} \right) + \varepsilon \left( \frac{2N_I (Y_2 - \varepsilon) + N_{II} [(Y_2 - \varepsilon) + (Y_3 - \varepsilon)]}{(D)_\varepsilon} \right) + \varepsilon^2 \left( \frac{N_I + N_{II}}{(D)_\varepsilon} \right) \right]. \quad (44)$$

The first term is the one evaluated (correctly) by CDFR. The last two are finite corrections to the result of CDFR.

In the photon-mass regularization scheme the common denominator subtlety does not arise, and one has

$$\Delta E = \frac{m\alpha^6}{12\pi^2} \int (dk_1)'' (dk_3)'' \left[ \frac{N_I}{(D_I)_\lambda} + \frac{N_{II}}{(D_{II})_\lambda} \right], \quad (45)$$

where

$$(D_I)_\lambda = (k_1^2 - \lambda^2)(k_2^2 - \lambda^2)(k_3^2 - \lambda^2)(Y_1)^2 (Y_3)^2, \quad (46a)$$

$$(D_{II})_\lambda = (k_1^2 - \lambda^2)(k_2^2 - \lambda^2)(k_3^2 - \lambda^2)(Y_1)^2 Y_2 Y_3. \quad (46b)$$

IV. EVALUATION OF THE INTEGRAL FOR  $\Delta E$ 

The infrared finite terms (which are all but the first three terms of  $N_I$  and  $N_{II}$ ) are easy to integrate using Feynman parameters. The definition of the momentum space element  $(dk)'' = d^4k / (i\pi^2)$  includes the factors of  $i$  and  $\pi$  that arise in the momentum-space integral. One has, for example,

$$\int (dk)'' (k^2 - 2k \cdot p - M^2)^{-\alpha} = \frac{(-1)^\alpha \Gamma(\alpha-2)}{\Gamma(\alpha) \Delta^{\alpha-2}}, \quad (47a)$$

$$\Delta = p^2 + M^2. \quad (47b)$$

Other integration formulas are given in Ref. 22.

Some of the infrared finite terms have imaginary parts. The imaginary parts appear when the argument of a log produced by a parametric integration takes a negative value. With the usual prescription that electron and photon masses have small negative imaginary parts, i.e., that

$$k^2 \rightarrow k^2 + i\eta, \quad (48a)$$

$$k^2 - 2k \cdot n \rightarrow k^2 - 2k \cdot n + i\eta, \quad (48b)$$

the phases of the complex logs are well defined. As pointed out by CDFR, the integrals with nonvanishing imaginary parts are those which do not vanish when all photon propagators are replaced by factors of  $\delta(k^2)$ . Hence integrals with a factor of  $X_{ii}$  in the numerator are real, and all others are complex. We have arranged the calculation so that none of the individual integrals that need to be evaluated has both an infrared divergence and an imaginary part.

The results for the infrared finite integrals are displayed in Table I. The integrals, defined by

TABLE I. Infrared finite integrals defined by Eq. (49). The value of a particular integral is found by summing the products of the coefficients shown with the terms in the top row. For example,  $\langle X_{11} X_3 \rangle_I = \zeta(2) - \frac{1}{2}$ .

	$\zeta(3)$	$\zeta(2)\ln 2$	$\zeta(2)$	$\ln 2$	1	$(-i\pi)\zeta(2)$	$-i\pi$
$\langle X_{11} X_{33} \rangle_I$					-1		
$\langle X_{11} X_3 \rangle_I$			1		$-\frac{1}{2}$		
$\langle X_{11} X_3^2 \rangle_I$			$\frac{1}{2}$		$-\frac{3}{4}$		
$\langle X_{13} \rangle_I$				1			$\frac{1}{2}$
$\langle X_{13} X_1 X_3 \rangle_I$	$-\frac{3}{4}$	2	$-\frac{3}{2}$	2	$-\frac{1}{4}$	$-\frac{1}{2}$	1
$\langle X_{13}^2 \rangle_I$	3	-8	5	-6	1	2	-3
$\langle X_1 X_3 \rangle_I$	$\frac{3}{8}$	-1	1		$-\frac{1}{4}$	$\frac{1}{4}$	
$\langle X_{11} X_2 \rangle_{II}$			$\frac{1}{2}$				
$\langle X_{11} X_{23} \rangle_{II}$	$\frac{3}{4}$	-3	2				
$\langle X_1 X_{12} \rangle_{II}$		$\frac{1}{2}$				$\frac{1}{4}$	
$\langle X_1 X_{23} \rangle_{II}$	$\frac{3}{4}$	$-\frac{5}{2}$	1			$\frac{1}{4}$	
$\langle X_2 X_{13} \rangle_{II}$	$\frac{3}{8}$	$-\frac{1}{2}$	$\frac{1}{2}$	-1		$\frac{1}{2}$	$-\frac{1}{2}$
$\langle X_1^2 X_{23} \rangle_{II}$		-1		2	$-\frac{1}{4}$	$-\frac{1}{2}$	1
$\langle X_{12} \rangle_{II}$		$\frac{3}{4}$				$\frac{3}{8}$	
$\langle X_1 X_2 \rangle_{II}$		$\frac{1}{2}$	$\frac{1}{4}$			$\frac{1}{4}$	
$\langle X_1^2 X_2 \rangle_{II}$			$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$		$\frac{1}{4}$

TABLE II. Infrared divergent integrals. These integrals are defined as in Eq. (49) except that the denominator in (49) is regularized. The first set of results is for binding regularization (where  $\mu \rightarrow \varepsilon$ ), and the second set is for photon mass regularization (where  $\mu \rightarrow \lambda$ ). For example,  $\langle X_{22} \rangle_I = \ln^2 \varepsilon$  in binding regularization and  $\langle X_{11} \rangle_{II} = -\ln \lambda - 3\zeta(2)/2 + \frac{3}{2}$  in photon mass regularization.

	$\ln^2 \mu$	$\ln \mu$	$\zeta(2)$	1
$\langle X_{11} \rangle_I$	$\frac{1}{2}$	1	$2, \frac{9}{4}$	0, -1
$\langle X_{22} \rangle_I$	1	0	0	0
$\langle X_{22} X_3 \rangle_I$	0	-1	0	0
$\langle X_{11} \rangle_{II}$	0	-1	$-\frac{7}{4}, -\frac{3}{2}$	$2, \frac{3}{2}$
$\langle X_{22} \rangle_{II}$	$\frac{1}{2}$	0	$\frac{5}{4}, \frac{3}{4}$	$-1, -\frac{1}{2}$
$\langle X_{22} X_3 \rangle_{II}$	0	-1	$-\frac{3}{2}$	1

$$\langle Z \rangle_A = \int (dk_1)'' (dk_3)'' \frac{Z}{D_A}, \quad (49)$$

are expressed as linear combinations of the Riemann  $\zeta$  functions  $\zeta(3) = 1.202056903$  and  $\zeta(2) = \pi^2/6$ , along with  $\zeta(2)\ln 2$ ,  $\ln 2$ ,  $1$ ,  $-i\pi$ , and  $-i\pi\zeta(2)$ . The integration formulas given in the Appendix of CDFR and in Lewin<sup>23</sup> are useful in the evaluation of these integrals.

The results for the infrared divergent integrals are displayed in Table II. Table II contains the results for both binding regularization (with  $\mu = \varepsilon$ ) and photon mass regularization (with  $\mu = \lambda$ ). Results for the two regularization schemes differ only in the finite parts, which are given for both schemes.

The "extra" terms in the binding regularized  $\Delta E$  of

(44) get contributions only from the most singular (i.e., the first three) terms in  $N_I$  and  $N_{II}$ . These contributions are  $m\alpha^6/(12\pi^2)$  times

$$\varepsilon \langle -12X_{22}(Y_2 - \varepsilon) + 24X_{22}(Y_3 - \varepsilon) + 4X_{22}X_3(Y_2 - \varepsilon) - 4X_{22}X_3(Y_3 - \varepsilon) \rangle + \varepsilon^2 \langle 6X_{22} \rangle, \quad (50)$$

where

$$\langle Z \rangle = \int (dk_1)^{\prime\prime} (dk_3)^{\prime\prime} \frac{Z}{(D)_\varepsilon}. \quad (51)$$

The individual terms here are

$$\varepsilon \langle X_{22}(Y_2 - \varepsilon) \rangle = -\zeta(2) + 1, \quad (52a)$$

$$\varepsilon \langle X_{22}(Y_3 - \varepsilon) \rangle = \zeta(2) - 2, \quad (52b)$$

$$\varepsilon \langle X_{22}X_3(Y_2 - \varepsilon) \rangle = 0, \quad (52c)$$

$$\varepsilon \langle X_{22}X_3(Y_3 - \varepsilon) \rangle = 0, \quad (52d)$$

$$\varepsilon^2 \langle X_{22} \rangle = -3\zeta(2) + 5. \quad (52e)$$

So the extra contribution is

$$\frac{m\alpha^6}{2\pi^2} [3\zeta(2) - 5]. \quad (53)$$

The contribution of the first term in the binding regularized  $\Delta E$  of (44) is shown in (3). This is the incomplete result of CDFR. Adding on the extra contribution we obtain the complete expression for the energy shift, which is

$$\Delta E = \frac{m\alpha^6}{2\pi^2} \left\{ \frac{3}{4}\zeta(3) - \frac{1}{3}\zeta(2)\ln 2 - \frac{1}{6}\zeta(2) - 4\ln 2 + \frac{3}{2} + (-i\pi) \left[ \frac{4}{3}\zeta(2) - 2 \right] \right\}. \quad (54)$$

This same result for  $\Delta E$  is obtained in the photon mass regularization scheme by evaluating (45).

## V. CONCLUSION

We have obtained the analytic result for the contribution of three-photon annihilation to the positronium hyperfine interval at order  $m\alpha^6$ . Our result is  $\Delta E = -0.969$  MHz. This effect is small compared to other known contributions at order  $m\alpha^6$ ,<sup>24</sup> not all contributions of this order have yet been obtained. We have shown that a previous result for  $\Delta E$  is incomplete, and we have traced the discrepancy to a subtlety in the regularization of infrared divergences. As a check of our analysis we performed our calculation twice, with two independent infrared regularization schemes, and obtained the same result each time.

## ACKNOWLEDGMENTS

This work was supported in part by the National Science Foundation under Grant No. PHY-87-04324 and by Franklin and Marshall College. One of the authors (G.S.A.) would like to thank the Aspen Center for Physics for hospitality while part of this work was completed.

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<sup>1</sup>The ground-state hyperfine interval is defined as the difference between the  $n=1$  triplet-S-state energy  $E(1^3S_1)$  and the  $n=1$  singlet-S-state energy  $E(1^1S_0)$ . Triplet states are called orthopositronium, and singlet states parapositronium.

<sup>2</sup>M. Deutsch and E. Dulit, Phys. Rev. **84**, 601 (1951).

<sup>3</sup>M. W. Ritter, P. O. Egan, V. W. Hughes, and K. A. Woodle, Phys. Rev. A **30**, 1331 (1984).

<sup>4</sup>The conventions and natural units [ $\hbar=c=1$ ,  $\alpha=e^2/4\pi \cong (137)^{-1}$ ] of J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964) are used throughout. The symbol  $m$  represents the electron mass  $m \cong 0.511$  MeV.

<sup>5</sup>The  $m\alpha^4$  contribution was obtained by J. Pirenne, Arch. Sci. Phys. Nat. **28**, 233 (1946); **29**, 121 (1947); **29**, 207 (1947); **29**, 265 (1947); V. B. Berestetski, Zh. Eksp. Teor. Fiz. **19**, 1130 (1949); V. B. Berestetski and L. D. Landau, *ibid.* **19**, 673 (1949); R. A. Ferrell, Phys. Rev. **84**, 858 (1951).

<sup>6</sup>The  $m\alpha^5$  contribution was obtained by R. Karplus and A. Klein, Phys. Rev. **87**, 848 (1952).

<sup>7</sup>The  $m\alpha^6 \ln(1/\alpha)$  contributions were obtained by G. P. Lepage, Phys. Rev. A **16**, 863 (1977); G. T. Bodwin and D. R. Yennie, Phys. Rep. **43C**, 267 (1978); W. E. Caswell and G. P. Lepage, Phys. Rev. A **20**, 36 (1979).

<sup>8</sup>A. P. Mills, Jr., and G. H. Bearman, Phys. Rev. Lett. **34**, 246 (1975); P. O. Egan, W. E. Frieze, V. W. Hughes, and M. H. Yam, Phys. Lett. **54A**, 412 (1975).

<sup>9</sup>V. K. Cung, A. Devoto, T. Fulton, and W. W. Repko, Phys. Lett. **68B**, 474 (1977); Nuovo Cimento **43A**, 643 (1978).

<sup>10</sup>A. Ore and J. L. Powell, Phys. Rev. **75**, 1696 (1949).

<sup>11</sup>M. Gell-Mann and F. Low, Phys. Rev. **84**, 350 (1951).

<sup>12</sup>S. Mandelstam, Proc. R. Soc. London, Ser. A **233**, 248 (1955).

<sup>13</sup>D. Lurié, A. J. Macfarlane, and Y. Takahashi, Phys. Rev. **140**, B1091 (1965).

<sup>14</sup>E. E. Salpeter and H. A. Bethe, Phys. Rev. **84**, 1232 (1951).

<sup>15</sup>J. Schwinger, Proc. Natl. Acad. Sci. USA **37**, 452 (1951); **37**, 455 (1951).

<sup>16</sup>A matrix notation will be used when convenient to suppress relative momentum variables:  $G(P;p,q) = \langle p | G | q \rangle$ ,  $(2\pi)^4 \delta(p-q) = \langle p | 1 | q \rangle$ ,  $\psi(p) = \langle p | \psi \rangle$ , etc. The product  $AB$  implies integration over the intermediate relative momentum  $\langle p | AB | q \rangle = \int (dl)' \langle p | A | l \rangle \langle l | B | q \rangle$ , where  $(dl)' = d^4l/(2\pi)^4$ . A sum over Dirac indices is implicit.

<sup>17</sup>G. P. Lepage, Phys. Rev. A **16**, 863 (1977).

<sup>18</sup>G. S. Adkins, Ann. Phys. (N.Y.) **146**, 78 (1983).

<sup>19</sup>J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964), Sec. 5.2.

<sup>20</sup>A. C. Hearn (unpublished).

<sup>21</sup>muMATH is an interactive symbolic math system and muSIMP is the programming language in which muMATH is written. muMATH and muSIMP are available from Microsoft Corporation.

<sup>22</sup>See the Appendix of G. S. Adkins, Phys. Rev. D **27**, 1814 (1983).

<sup>23</sup>L. Lewin, *Polylogarithms and Associated Functions* (North-Holland, New York, 1981).

- <sup>24</sup>R. Barbieri, P. Christillin, and E. Remiddi, *Phys. Rev. A* **8**, 2266 (1973); M. A. Samuel, *ibid.* **10**, 1450 (1974); M. Douglas, *ibid.* **11**, 1527 (1975); V. K. Cung, T. Fulton, W. W. Repko, and D. Schnitzler, *Ann. Phys. (N.Y.)* **96**, 261 (1976); V. K. Cung, A. Devoto, T. Fulton, and W. W. Repko, *Nuovo Cimento* **43A**, 643 (1978); *Phys. Rev. A* **19**, 1886 (1979); W. E. Caswell and G. P. Lepage, *ibid.* **18**, 810 (1978); *Phys. Lett.* **167B**, 437 (1986); W. Buchmüller and E. Remiddi (unpublished); J. R. Sapirstein, E. A. Terray, and D. R. Yennie, *Phys. Rev. D* **29**, 2290 (1984).