Calculation of the two-photon-annihilation contribution to the positronium hyperfine interval at order $m\alpha^6$

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The two-photon-annihilation contribution to the positronium hyperfine interval is obtained in analytic form at order $m\alpha^6$ using the Fried-Yennie gauge. The contribution to the hyperfine interval is $-0.0325m\alpha^6=-0.606$ MHz. This differs from the result of an earlier Feynman gauge evaluation. The errors in the earlier calculation are identified. The corrected Feynman gauge result agrees with the Fried-Yennie gauge result.

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I. INTRODUCTION

The ground-state hyperfine interval of positronium has been measured to be [1,2]

$$\Delta E_{\rm hfs}=203\,389.10\pm0.74\ \text{MHz}\ . \tag{1}$$

The theoretical result for this interval is [3,4]

$$\Delta E_{\rm hfs}=m\alpha^4\left[\tfrac{7}{12}-\frac{\alpha}{\pi}\left(\tfrac{1}{2}\ln 2+\tfrac{8}{9}\right)+\tfrac{5}{24}\alpha^2\ln(\alpha^{-1})+K\alpha^2+\cdots\right]. \tag{2}$$

The theoretical value, including all contributions through order $m\alpha^6\ln(\alpha^{-1})$, is [5]

$$\Delta E_{\rm hfs}=203\,400.287(18)\ \text{MHz}\ . \tag{3}$$

The $m\alpha^6$ term, with a coefficient of 1, would contribute 18.658 MHz. Known contributions to the coefficient K and to $\Delta E_{\rm hfs}$ are shown in Table I. The theoretical value for the hyperfine interval, including all known contributions to K, is

$$\Delta E_{\rm hfs}=203\,402.7(6)\ \text{MHz}\ . \tag{4}$$

The error is dominated by the numerical uncertainty in the calculation of the recoil correction [16]. Other contributions to K, involving one-photon-annihilation graphs, remain uncalculated.

In this paper, we show that the largest contribution to K, coming from two-photon-annihilation graphs, is in fact not correct. The correct contribution from these graphs is $-0.0325m\alpha^6=-0.606$ MHz. The corrected theoretical value for the hyperfine interval is

$$\Delta E_{\rm hfs}=203\,389.0(6)\ \text{MHz}\ , \tag{5}$$

in agreement with the experimental result. We perform our calculation in the Fried-Yennie gauge [17] in order to eliminate spurious infrared divergences. The calculation of Cung, Devoto, Fulton, and Repko [9–11] (CDFR) for this term was performed in the Feynman gauge. We deal with the binding singularity in the ladder graph in the natural way, by letting the binding energy and nonzero relative momentum regulate the divergence. CDFR used a nonphysical photon mass to regulate the singularity. However, the method of CDFR is correct and should have led to the correct answer. We identify several mistakes in the calculation of CDFR. After correcting these mistakes, we find their (corrected) answer to be the same as ours.

The outline of this paper is as follows. In Sec. II, the two-photon-annihilation contribution at order $m\alpha^5$ is calculated. We do this in order to establish notation and introduce some techniques that will be useful in the $m\alpha^6$ calculation. In Sec. III, we show the details of the order-$m\alpha^6$ calculation in the Fried-Yennie gauge. In Sec. IV, we discuss the $m\alpha^6$ calculation in the Feynman gauge. In Sec. V, we present our conclusions. In the Appendix, we discuss the evaluation of some integrals that come up in the calculations.

TABLE I. Known order-$m\alpha^6$ contributions to the positronium hyperfine interval.

Origin of contribution	Contribution to K	Contribution to $\Delta E_{\rm hfs}$ (in Mhz)
Three-photon annihilation [6–8]	−0.0519	−0.969
Two-photon-annihilation [9–11]	0.7038	13.131
One-photon-annihilation with fourth- and higher-order vacuum polarization [12,13]	−0.1492	−2.783
Radiative-recoil [14,15]	−0.5394(13)	−10.064(25)
Recoil [16]	0.17(3)	3.1(6)
Total	0.13(3)	2.4(6)
Corrected two-photon-annihilation [this work]	−0.0325	−0.606
Corrected total	−0.60(3)	−11.3(6)

II. CALCULATION AT ORDER $m\alpha^5$

The contribution of the two-photon-annihilation graph (Fig. 1) to the positronium hyperfine interval at order $m\alpha^5$ was first calculated by Karplus and Klein [18] as part of their complete calculation of the hyperfine interval to that order. We will obtain their result using a bound-state formalism that can be easily used to obtain the order-$m\alpha^6$ contribution as well.

The energy shift due to an interaction kernel δK has the form [19]

$$\Delta E = i\bar{\Psi}^0(\delta K)\Psi^0 \ . \tag{6}$$

The reference wave functions Ψ^0 and $\bar{\Psi}^0$ in Eq. (6) are dependent on the exact bound-state formalism used. However, for calculations of order-α corrections to a lowest-order effect, it is sufficient to approximate the wave functions by

$$\Psi^0(p) = (2\pi)\delta(p^0)\frac{1}{\sqrt{2}}\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}\phi(\mathbf{p}) \ , \tag{7a}$$

$$\bar{\Psi}^0(p) = (2\pi)\delta(p^0)\frac{1}{\sqrt{2}}\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}^T\phi(\mathbf{p}) \ , \tag{7b}$$

where the δ functions represent the sharp peak of the wave functions near zero relative energy, the matrix factors (where each entry represents a 2×2 matrix) describe the combination of a spin-$\frac{1}{2}$ particle with its antiparticle to form a spin singlet, and $\phi(\mathbf{p})$ is the nonrelativistic Schrödinger-Coulomb wave function

$$\phi(\mathbf{p}) = \phi_0\frac{8\pi\gamma}{(\mathbf{p}^2+\gamma^2)^2} \ , \tag{8}$$

with

$$\phi_0 = \left[\frac{\gamma^3}{\pi}\right]^{1/2} \ , \quad \gamma = \frac{m\alpha}{2} \ . \tag{9}$$

The quantity δK in Eq. (6) is the irreducible interaction kernel K minus the reference kernel K_0. For the case at hand, K is given by the central part of the diagram of Fig. 1, which also (implicitly) includes a similar contribution with crossed photons. The dependence of δK on two relative momenta and two sets of two Dirac indices is implicit. (A detailed description of these conventions can be found in Ref. [19]).

The contribution to ΔE due to the graph in Fig. 1 is

$$\Delta E_{\rm LO} = i(-1)\int (dk)'(dp)'(dp')'\mathrm{tr}\left[\bar{\Psi}^{0T}(p)(-ie\gamma^{\mu_1})\frac{i}{\gamma(P/2+p'-k)-m}(-ie\gamma^{\mu_2})\right]\frac{-i}{k^2}Y_{\mu_1,\nu_1}(k)\frac{-i}{(P-k)^2}Y_{\mu_2,\nu_2}(P-k)$$
$$\times\sum_{\sigma\in S_2}\mathrm{tr}\left[(-ie\gamma^{\nu_{\sigma(2)}})\frac{i}{\gamma(P/2+p-k_{\sigma(1)})-m}(-ie\gamma^{\nu_{\sigma(1)}})\Psi^0(p)\right] \ , \tag{10}$$

where the i comes from Eq. (6), the (-1) is due to Fermi statistics, the integration measure is $(dk)'=d^4k/(2\pi)^4$, the sum is over the two permutations of the photons, $P\approx(2m,\mathbf{0})$ is the (rest-frame) positronium energy-momentum vector, $k_1=k$, $k_2=P-k$, and

$$Y_{\mu\nu}(k) = g_{\mu\nu}+2\frac{k_\mu k_\nu}{k^2} \tag{11}$$

is part of the Fried-Yennie gauge photon propagator. To order $m\alpha^5$, the relative momenta p' and p in the electron propagators can be neglected. Then the p' and p integrals can be performed using the δ functions and

$$\int\frac{d^3p}{(2\pi)^3}\frac{8\pi\gamma}{(\mathbf{p}^2+\gamma^2)^2} = 1 \ . \tag{12}$$

The expression for the energy shift becomes

$$\Delta E_{\rm LO} = \frac{m\alpha^5}{\pi}\frac{1}{16}\int\frac{d^4k}{i\pi^2}\frac{1}{k^2(k-2N)^2(k^2-2kN)^2}\mathrm{tr}\left[\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}\gamma^{\mu_1}[\gamma(N-k)+1]\gamma^{\mu_2}\right]$$
$$\times Y_{\mu_1,\nu_1}(k)Y_{\mu_2,\nu_2}(2N-k)\sum_{\sigma\in S_2}\mathrm{tr}\left[\gamma^{\nu_{\sigma(2)}}[\gamma(N-k_{\sigma(1)})+1]\gamma^{\nu_{\sigma(1)}}\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}\right] \ , \tag{13}$$

where a factor of m has been scaled out of k, $N=(1,\mathbf{0})$, and now $k_1=k$, $k_2=2N-k$. The trace

$$T^{\nu_2\nu_1}(k) = \mathrm{tr}\left[\gamma^{\nu_2}[\gamma(N-k)+1]\gamma^{\nu_1}\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}\right]$$
$$= -2i\epsilon^{0\nu_2\nu_1\beta}k_\beta \ , \tag{14}$$

where $\epsilon^{0ijk}=-\epsilon^{ijk}$ [4], satisfies

$$T^{\nu_2\nu_1}(k) = T^{\nu_1\nu_2}(2N-k) \ , \tag{15}$$

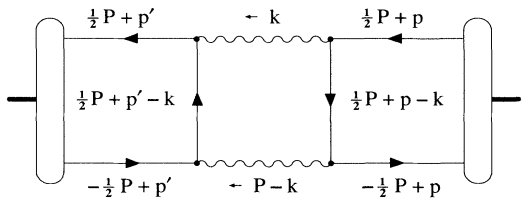

FIG. 1. Lowest-order two-photon-annihilation graph with momentum assignments.

so the two terms in the permutation sum are equal. Evidently the longitudinal terms in the Y factors do not contribute. One has that

$$\Delta E_{\rm LO}=\frac{m\alpha^5}{\pi}\frac{1}{16}\int\frac{d^4k}{i\pi^2}\frac{1}{k^2(k-2N)^2(k^2-2kN)^2}\times(2i\epsilon^{0\mu_1\mu_2\alpha}k_\alpha)\times g_{\mu_1\nu_1}g_{\mu_2\nu_2}(2)(-2i\epsilon^{0\nu_2\nu_1\beta}k_\beta)$$
$$=\frac{m\alpha^5}{\pi}I_{\rm LO}\ , \tag{16}$$

where

$$I_{\rm LO}=\int\frac{d^4k}{i\pi^2}\frac{-\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)^2}\ . \tag{17}$$

An infinitesimal imaginary part is implicit in each denominator factor ($k^2\to k^2+i\epsilon$, etc.) in order to define the positions of the poles. The $i\epsilon$ terms are necessary because the integral $I_{\rm LO}$ has an imaginary part [coming from the region in k space where both $k^2=0$ and $(k-2N)^2=0$]. The integral $I_{\rm LO}$ is most easily evaluated by use of the identity

$$-\mathbf{k}^2=\tfrac{1}{4}[k^2(k-2N)^2-(k^2-2kN)^2]\ . \tag{18}$$

The individual terms produced by Eq. (18) each have ultraviolet divergences, but these are easily regularized (e.g., by dimensional regularization). The result for $I_{\rm LO}$ is

$$I_{\rm LO}=\tfrac{1}{2}\ln 2-\tfrac{1}{2}-\frac{i\pi}{4}\ , \tag{19}$$

so the energy shift is

$$\Delta E_{\rm LO}=\frac{m\alpha^5}{\pi}\left[\frac{1}{2}\ln 2-\frac{1}{2}-\frac{i\pi}{4}\right]\ . \tag{20}$$

This is the shift of the parapositronium energy. The contribution to the hyperfine interval (orthopositronium minus parapositronium) is

$$\Delta E_{\rm hfs}=\frac{m\alpha^5}{\pi}(-\tfrac{1}{2}\ln 2+\tfrac{1}{2})\ . \tag{21}$$

The imaginary part gives the lowest-order parapositronium decay rate as

$$\Gamma_{\rm LO}=-2\,{\rm Im}(\Delta E_{\rm LO})=\tfrac{1}{2}m\alpha^5\ . \tag{22}$$

III. CALCULATION AT ORDER $m\alpha^6$ IN THE FRIED-YENNIE GAUGE

The two-photon-annihilation graphs that contribute to the parapositronium energy level at order $m\alpha^6$ are shown in Fig. 2. The most interesting graph is the ladder graph, Fig. 2(d). It is a difference graph, with the ladder photon shown representing the difference between a Fried-Yennie gauge ladder photon and the reference kernel.

A. The vacuum polarization graph

The vacuum polarization graph, Fig. 2(a), is the simplest to evaluate. The effect of the vacuum polarization insertion is to alter the photon propagator by

$$\frac{1}{k^2}\to-\frac{1}{k^2}\Pi_R(k^2)\ , \tag{23}$$

where $\Pi_R(k^2)$ is the renormalized vacuum polarization factor [20]

$$\Pi_R(k^2)=-\frac{2\alpha}{\pi}\int_0^1 dx\,x(1-x)\ln[1-x(1-x)k^2/m^2]$$
$$=-\frac{\alpha}{3\pi}\frac{k^2}{m^2}\int_0^1 dx\frac{x^2(3-8x+4x^2)}{[1-x(1-x)k^2/m^2]}\ . \tag{24}$$

The second form in Eq. (24) is the result of an integration by parts. The vacuum polarization (VP) contribution to the energy shift is

$$\Delta E_{\rm VP}=\frac{m\alpha^5}{\pi}(2)\int\frac{d^4k}{i\pi^2}\frac{-\mathbf{k}^2(-1)\Pi_R(m^2k^2)}{k^2(k-2N)^2(k^2-2kN)^2}$$
$$=\frac{m\alpha^6}{\pi^2}I_{\rm VP}\ . \tag{25}$$

The factor of 2 comes because the vacuum polarization bubble can occur on either photon line. The vacuum polarization factor $\Pi_R(k^2)$ is gauge invariant, so the energy shift due to this graph is also independent of gauge. Since $\Pi_R(k^2)$ vanishes when $k^2=0$, the vacuum polarization contribution is purely real. From the first form given in Eq. (24), it is clear that $-\Pi_R(k^2)$ is a positive factor (since $k^2<0$ after the Wick rotation done in the course of evaluating the integral). Consequently, $I_{\rm VP}$ has the same sign as the real part of $I_{\rm LO}$ in Eqs. (17) and (19). That is, $I_{\rm VP}$ is negative.

For the actual calculation of $I_{\rm VP}$, we let $k\to 2N-k$ in Eq. (25) (or equivalently, we let the bubble be on the photon carrying momentum $2N-k$), and use the second form of Π_R in Eq. (24). We find that [21]

$$I_{\rm VP}=2\int\frac{d^4k}{i\pi^2}\frac{-\mathbf{k}^2}{k^2(k^2-2kN)^2}\frac{1}{3}\int_0^1 dx\frac{x^2(3-8x+4x^2)}{[1-x(1-x)(2N-k)^2]}$$
$$=\frac{2}{3}\int_0^1 dx\frac{x(3-8x+4x^2)}{(1-x)}\int\frac{d^4k}{i\pi^2}\frac{\mathbf{k}^2}{k^2(k^2-2kN)^2\left[k^2-4kN+4-\dfrac{1}{x(1-x)}\right]}$$
$$=\int dx\,dz\,ds\,x^2(3-8x+4x^2)\frac{z(1-s)}{s(1-2x)^2+zx(1-x)(1+s)^2}$$
$$=-\tfrac{1}{6}\zeta(2)\ , \tag{26}$$

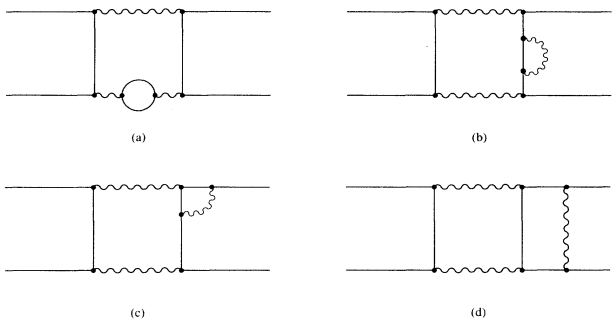

FIG. 2. Two-photon-annihilation graphs with one-loop corrections: (a) is the vacuum polarization graph, (b) is the self-energy graph, (c) is the vertex graph, and (d) is the ladder graph. The wave-function factors are implicit here.

where $\zeta(n)$ is the Riemann zeta function [$\zeta(2)=\pi^2/6$, $\zeta(3)=1.202\,056\,90\ldots$, etc.]. Our result is negative, as expected. It differs from the corresponding result of CDFR by a minus sign.

B. The self-energy graph

The self-energy graph, Fig. 2(b), is also easy to evaluate. The renormalized Fried-Yennie gauge self-energy function is [22]

$$\Sigma_R(p)=(\gamma p-m)^2\gamma p C(p^2)\ , \tag{27}$$

where [23]

$$C(p^2)=-\frac{3\alpha}{2\pi}\int dx\,dz\frac{x(1-x)}{[m^2x+(m^2-p^2)(1-x)z]}\ . \tag{28}$$

The electron propagator has the expansion

$$\begin{aligned}\frac{1}{\gamma p-m-\Sigma_R(p)}&=\frac{1}{\gamma p-m}\\&\quad+\frac{1}{\gamma p-m}\Sigma_R(p)\frac{1}{\gamma p-m}+\cdots\\&=\frac{1}{\gamma p-m}+\gamma p C(p^2)+\cdots\ ,\end{aligned} \tag{29}$$

so to compute the self-energy (SE) contribution, one simply makes the replacement

$$\frac{1}{\gamma p-m}=\frac{\gamma p+m}{p^2-m^2}\to\gamma p C(p^2) \tag{30}$$

in one trace of $\Delta E_{\rm LO}$ and multiplies by 2. This replacement is equivalent to

$$\frac{1}{p^2-m^2}\to C(p^2)\ , \tag{31}$$

since only the γp term in $\gamma p+m$ contributes in the trace. After extracting all factors of the electron mass, we can use $p=N-k$ and write

$$\Delta E_{\rm SE}=\frac{m\alpha^6}{\pi^2}I_{\rm SE}\ , \tag{32}$$

with

$$\begin{aligned}I_{\rm SE}&=2\int\frac{d^4k}{i\pi^2}\frac{-\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)}\\&\quad\times\frac{3}{2}\int dx\,dz\frac{x}{z}\frac{1}{k^2-2kN-\dfrac{x}{(1-x)z}}\\&=[-\tfrac{3}{4}\zeta(2)+\tfrac{3}{2}\ln^2 2-\tfrac{3}{2}\ln 2+\tfrac{3}{4}]\\&\quad+i\pi(-\tfrac{3}{2}\ln 2+\tfrac{3}{4})\ .\end{aligned} \tag{33}$$

In this case, we found it convenient to use

$$-\mathbf{k}^2=\tfrac{1}{2}[(2-k^0)k^2+k^0(k^2-2kN)] \tag{34}$$

to split $I_{\rm SE}$ into two terms, each simpler than $I_{\rm SE}$ itself.

C. The vertex graph

The vertex graph is shown in Fig. 2(c). The vertex contribution is obtained from the lowest-order graph by the replacement

$$\gamma^\nu\to\Lambda_R^\nu \tag{35}$$

and multiplication by 4, where Λ_R^ν is the renormalized Fried-Yennie gauge vertex correction factor. By analogy with Eqs. (13) and (16), one has

$$\begin{aligned}\Delta E_V=\frac{m\alpha^5}{\pi}\frac{1}{16}\int\frac{d^4k}{i\pi^2}&\frac{1}{k^2(k-2N)^2(k^2-2kN)^2}\\&\times(2i\epsilon^{0\mu_1\mu_2\alpha}k_\alpha)g_{\mu_1\nu_1}g_{\mu_2\nu_2}\\&\times(2)(4)\mathrm{tr}\left[\gamma^{\nu_2}[\gamma(N-k)+1]\right.\\&\left.\times\Lambda_R^{\nu_1}(N-k,N)\begin{bmatrix}0&1\\0&0\end{bmatrix}\right],\end{aligned} \tag{36}$$

where the factor of 4 reflects the fact that the vertex correction can act on any of the four vertices. Again, all factors of the electron mass have been extracted from Λ_R^ν. Now any factor of N^ν or k^ν in Λ_R^ν gives zero because of the other trace, any factor of $\gamma N-1$ on the right in Λ_R^ν gives zero because of the spin-matrix part of the wave function, and any factor of $[\gamma(N-k)-1]\gamma^\nu$ in Λ_R^ν gives zero because the corresponding trace vanishes. With these simplifications, the effective vertex correction is [21,22]

$$\begin{aligned}&\Lambda_R^\nu(N-k,N)\\&\quad\to-\frac{\alpha}{4\pi}\int dx\,du\,dt\left[\frac{-4x(1-x)S^\nu}{H^2}+\frac{2R^\nu}{H}\right.\\&\qquad+\frac{2\gamma^\nu x^2(H-x)}{\bar{H}^2}\\&\qquad\left.+\frac{6\gamma^\nu x(H-x)}{\bar{H}}\right],\end{aligned} \tag{37}$$

where

$$H=-ur\left[k^2-2kN\left[\frac{1-x}{r}\right]-\left[\frac{x}{ur}\right]\right], \tag{38a}$$

$$H-x=-xu(1-u)k^2-(1-x)u(k^2-2kN)\ , \tag{38b}$$

$$\overline{H}=-urt\left[k^2-2kN\left[\frac{1-x}{r}\right]-\left[\frac{x}{urt}\right]\right]\ , \tag{38c}$$

$$S^\nu=\gamma^\nu k^2[u(1-u)(2+k^0)-1] +\gamma^\nu(k^2-2kN)[-u(1+k^0)+1]\ , \tag{38d}$$

$$R^\nu=\gamma^\nu k^2[-2+3x-x^2u(1-u)] +\gamma^\nu(k^2-2kN)[2-3x-x(1-x)u] +i\sigma^{\nu\beta}k_\beta x(1-x)\ , \tag{38e}$$

with $r=1-xu$ [24]. Because of the trace relation

$$\begin{aligned}\mathrm{tr}\left[\gamma^{\nu_2}[\gamma(N-k)+1]i\sigma^{\nu_1\beta}k_\beta\begin{bmatrix}0&1\\0&0\end{bmatrix}\right] &=4i\epsilon^{0\nu_2\nu_1\beta}k_\beta\\ &=-2\,\mathrm{tr}\left[\gamma^{\nu_2}[\gamma(N-k)+1]\gamma^{\nu_1}\begin{bmatrix}0&1\\0&0\end{bmatrix}\right]\ ,\end{aligned} \tag{39}$$

one has that effectively

$$\Lambda_R^{\nu_1}\to\Lambda\gamma^{\nu_1}\ , \tag{40}$$

where

$$\begin{aligned}\Lambda=-\frac{\alpha}{4\pi}\int dx\,du\,dt\Bigg[&\frac{-4x(1-x)}{H^2}\{k^2[u(1-u)(2+k^0)-1]+(k^2-2kN)[-u(1+k^0)+1]\}\\ &+\frac{2}{H}\{k^2[-2+3x-x^2u(1-u)]+(k^2-2kN)[2-3x-x(1-x)u]-2x(1-x)\}\\ &+\frac{2x^2(H-x)}{\overline{H}^2}+\frac{6x(H-x)}{\overline{H}}\Bigg]\ .\end{aligned} \tag{41}$$

The vertex contribution to the energy shift is

$$\Delta E_V=\frac{m\alpha^5}{\pi}(4)\int\frac{d^4k}{i\pi^2}\frac{-\mathbf{k}^2\Lambda}{k^2(k-2N)^2(k^2-2kN)^2}=\frac{m\alpha^6}{\pi^2}I_V\ . \tag{42}$$

The result of a lengthy calculation is that

$$I_V=[\tfrac{21}{16}\zeta(3)-\tfrac{3}{2}\zeta(2)\ln 2+\tfrac{1}{4}\zeta(2)-2\ln^2 2+2\ln 2+\tfrac{5}{2}]+i\pi[-\tfrac{3}{8}\zeta(2)+2\ln 2-1]\ . \tag{43}$$

D. The ladder graph

The ladder graph is shown in Fig. 2(d), and with momentum labeling in Fig. 3. The ladder graph requires more care than the others because of the infrared sensitivity in the l integral due to the "binding singularity." We will not be able to set $|\mathbf{p}|\to 0$ and $P^0\to 2m$ in the part of the ladder graph containing the l integral.

The ladder contribution to the energy shift, by analogy with Eqs. (13) and (16), is

$$\begin{aligned}\Delta E_L=\frac{m\alpha^5}{\pi}\frac{1}{16}\int\frac{d^4k}{i\pi^2}\frac{1}{k^2(k-2N)^2(k^2-2kN)}&(2i\epsilon^{0\mu_1\mu_2\alpha}k_\alpha)g_{\mu_1\nu_1}g_{\mu_2\nu_2}(2)(2)\\ \times\int(dp)'\frac{1}{\phi_0}\Bigg[&\frac{\alpha}{4\pi}\int\frac{d^4l}{i\pi^2}\frac{1}{[(l-WN)^2-1][(l+WN)^2-1]}\\ &\times\frac{Y_{\lambda\kappa}(l-p)}{(l-p)^2}\frac{A^{\lambda\nu_2\nu_1\kappa}(l)}{[(l+WN-k)^2-1]}(2\pi)\delta(p^0)\phi(\mathbf{p})\\ &-\frac{1}{[(p+WN-k)^2-1]}\mathrm{tr}\{\gamma^{\nu_2}[\gamma(p+WN-k)+1]\gamma^{\nu_1}\sqrt{2}\Psi^0(p)\}\Bigg]\ ,\end{aligned} \tag{44}$$

where one factor of 2 comes from the two permutations of the annihilation photons, and the other from the two places for the ladder photon to appear. Equation (44) represents the difference between a graph with a Fried-Yennie gauge ladder photon and one with the reference kernel K_0. In the first term, we made use of the approximation Eq. (7a) for the wave function. In the second term, the reference bound-state equation

$$SK_0\Psi_0=\Psi_0\ , \tag{45}$$

where S equals (or approximately equals) the propagation factor for a free electron and a positron was used to eliminate the integral over l. The quantity W that appears in Eq. (44) is half of the positronium energy

$$W=m\left[1-\frac{\alpha^2}{8}+O(\alpha^4)\right]\ , \tag{46}$$

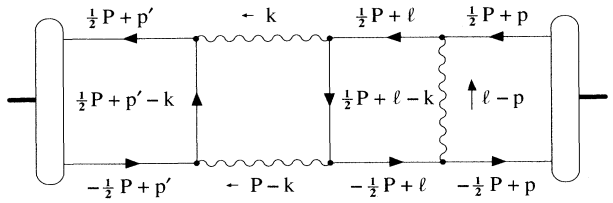

FIG. 3. Ladder graph with momentum assignments.

and $P=(2W,\mathbf{0})$. The trace term is

$$A^{\lambda\nu_2\nu_1\kappa}(l)=\mathrm{tr}\left[\gamma^{\lambda}[\gamma(l-WN)+1]\gamma^{\nu_2}\times[\gamma(l+WN-k)+1]\gamma^{\nu_1}\times[\gamma(l+WN)+1]\gamma^{\kappa}\begin{bmatrix}0&1\\0&0\end{bmatrix}\right] . \quad (47)$$

The binding singularity occurs in the l integral

$$B_{\lambda\kappa}(\mathbf{p})\equiv\int\frac{d^4l}{i\pi^2}\frac{-Y_{\lambda\kappa}(l-p)}{[(l-WN)^2-1][(l+WN)^2-1](l-p)^2} . \quad (48)$$

In the limit $\mathbf{p}\to 0$ and $W\to 1$, this integral is singular in the infrared. If the l^0 integral is done by poles, closing the l^0 contour, say, in the lower half-plane, the infrared singularities are associated with poles at positions $l^0=|\mathbf{l}|$ from the photon propagator and $l^0=(\mathbf{l}^2+1)^{1/2}-1$ from a fermion propagator. The first singularity is cured by the Fried-Yennie gauge factor $Y_{\lambda\kappa}$. The second (binding) singularity remains.

The first term in Eq. (44) has a naive order of $m\alpha^6$. However, because of the binding singularity this is reduced to order $m\alpha^5$. The $m\alpha^5$ part of the first term can be separated out by writing

$$\frac{A^{\lambda\nu_2\nu_1\kappa}(l)}{[(l+WN-k)^2-1]}=\frac{A^{\lambda\nu_2\nu_1\kappa}(0)}{[(WN-k)^2-1]}+\left[\frac{A^{\lambda\nu_2\nu_1\kappa}(l)}{[(l+WN-k)^2-1]}-\frac{A^{\lambda\nu_2\nu_1\kappa}(0)}{[(WN-k)^2-1]}\right] . \quad (49)$$

The order-$m\alpha^5$ contribution is contained in the first term of Eq. (49), since the binding singularity is associated with small l. We designate the difference between the contributions of the first term of Eq. (49) and the second term of Eq. (44) the binding part of ΔE_L. We designate the contribution of the second term of Eq. (49) the free part of ΔE_L. Both the binding and free parts of ΔE_L have order $m\alpha^6$.

We consider first the binding part of ΔE_L. It is

$$\Delta E_L^{\text{binding}}=\frac{m\alpha^5}{\pi}\frac{1}{16}\int\frac{d^4k}{i\pi^2}\frac{1}{k^2(k-2N)^2(k^2-2kN)}(2i\epsilon^{0\mu_1\mu_2\alpha}k_{\alpha})g_{\mu_1\nu_1}g_{\mu_2\nu_2}(2)(2)$$
$$\times\int(dp)'\frac{1}{\phi_0}\left[\frac{\alpha}{4\pi}\int\frac{d^4l}{i\pi^2}\frac{1}{[(l-WN)^2-1][(l+WN)^2-1]}\times\frac{Y_{\lambda\kappa}(l-p)}{(l-p)^2}\frac{A^{\lambda\nu_2\nu_1\kappa}(0)}{[(WN-k)^2-1]}(2\pi)\delta(p^0)\phi(\mathbf{p})\right.$$
$$\left.-\frac{1}{[(p+WN-k)^2-1]}\mathrm{tr}\{\gamma^{\nu_2}[\gamma(p+WN-k)+1]\gamma^{\nu_1}\sqrt{2}\Psi^0(p)\}\right] . \quad (50)$$

In the first term, since we are only calculating order-α corrections to the lowest-order energy shift, we can set $W\to 1$ in the trace factor $A^{\lambda\nu_2\nu_1\kappa}(0)$ and in the denominator $[(WN-k)^2-1]$. In the second term, we can ignore the $\mathbf{p}$ dependence in the electron propagator, set $W\to 1$, and use the approximation Eq. (7a) for the wave function. These approximations for the second term are safe for nonrelativistic $|\mathbf{p}|$. However, for relativistic $|\mathbf{p}|$, we are leaving out contributions of order $m\alpha^6$. Fortunately, these contributions are identical, but opposite in sign, to the order-$m\alpha^6$ contributions that were neglected in going from Eq. (10) to Eq. (13) for ΔE_{LO} [25]. We did not calculate these (bound-state, formalism-dependent) contributions, but in order to keep things straight we will give them a name. With the approximations mentioned, we have

$$\Delta E_L^{\text{binding}}=\frac{m\alpha^6}{\pi^2}I_L^{\text{binding}} , \quad (51)$$

with

$$I_L^{\text{binding}}=\frac{1}{16}\int\frac{d^4k}{i\pi^2}\frac{1}{k^2(k-2N)^2(k^2-2kN)^2}(2i\epsilon^{0\mu_1\mu_2\alpha}k_\alpha)g_{\mu_1\nu_1}g_{\mu_2\nu_2}(2)(2)$$
$$\times\int\frac{d^3p}{(2\pi)^3}\frac{8\pi\gamma}{(\mathbf{p}^2+\gamma^2)^2}\left\{\frac{1}{4}\int\frac{d^4l}{i\pi^2}\frac{1}{[(l-WN)^2-1][(l+WN)^2-1]}\right.$$
$$\left.\times\frac{Y_{\lambda\kappa}(l-p)}{(l-p)^2}A^{\lambda\nu_2\nu_1\kappa}(0)-\frac{\pi}{\alpha}T^{\nu_2\nu_1}(k)\right\}-I^{\text{rel}}\,, \tag{52}$$

where I^{rel} is the uncalculated relativistic contribution mentioned above. We can make the replacements

$$(\gamma N+1)\gamma^\kappa\to 2N^\kappa\,, \tag{53a}$$

$$\gamma^\lambda(-\gamma N+1)\to -2N^\lambda\,, \tag{53b}$$

in $A^{\lambda\nu_2\nu_1\kappa}(0)$ because of the spin-matrix part of the wave function. One has

$$A^{\lambda\nu_2\nu_1\kappa}(0)\to -4N^\lambda N^\kappa T^{\nu_2\nu_1}(k)\,, \tag{54}$$

so that

$$I_L^{\text{binding}}=2I_{\text{LO}}\int\frac{d^3p}{(2\pi)^3}\frac{8\pi\gamma}{(\mathbf{p}^2+\gamma^2)^2}\left[B(\mathbf{p})-\frac{\pi}{\alpha}\right]-I^{\text{rel}}\,, \tag{55}$$

where

$$B(\mathbf{p})\equiv B_{00}(\mathbf{p})$$
$$=\int\frac{d^4l}{i\pi^2}\frac{-1}{[(l-WN)^2-1][(l+WN)^2-1](l-p)^2}$$
$$\times\left[1+2\frac{l_0l_0}{(l-p)^2}\right]. \tag{56}$$

Now $B(\mathbf{p})$ was evaluated in the Appendix to [26], with the result

$$B(\mathbf{p})\approx\frac{\pi}{|\mathbf{p}|}\arctan\left[\frac{\mathbf{p}}{\gamma}\right]-3\,. \tag{57}$$

The $\mathbf{p}$ integral in Eq. (55) can be done using Eq. (12) and

$$\int\frac{d^3p}{(2\pi)^3}\frac{8\pi\gamma}{(\mathbf{p}^2+\gamma^2)^2}\frac{\pi}{|\mathbf{p}|}\arctan\left[\frac{|\mathbf{p}|}{\gamma}\right]=\frac{\pi}{\alpha}\,. \tag{58}$$

One finds that

$$I_L^{\text{binding}}=-6I_{\text{LO}}-I^{\text{rel}}\,. \tag{59}$$

The free part of ΔE_L, from Eqs. (44) and (49), is

$$\Delta E_L^{\text{free}}=\frac{m\alpha^5}{\pi}\frac{1}{16}\int\frac{d^4k}{i\pi^2}\frac{1}{k^2(k-2N)^2(k^2-2kN)}(2i\epsilon^{0\mu_1\mu_2\alpha}k_\alpha)g_{\mu_1\nu_1}g_{\mu_2\nu_2}(2)(2)$$
$$\times\frac{\alpha}{4\pi}\int\frac{d^4l}{i\pi^2}\frac{1}{(l^2-2lN)(l^2+2lN)l^2}Y_{\lambda\kappa}(l)\left[\frac{A^{\lambda\nu_2\nu_1\kappa}(l)}{[(l+N-k)^2-1]}-\frac{A^{\lambda\nu_2\nu_1\kappa}(0)}{(k^2-2kN)}\right], \tag{60}$$

where we have set $W\to 1$ and $\mathbf{p}\to 0$ (outside of the wave function), and have done the $\mathbf{p}$ integral using Eq. (12). The term containing the traces can be written as

$$\left[\frac{A^{\lambda\nu_2\nu_1\kappa}(l)}{[(l+N-k)^2-1]}-\frac{A^{\lambda\nu_2\nu_1\kappa}(0)}{(k^2-2kN)}\right]=\frac{1}{[(l+N-k)^2-1]}\left[[A^{\lambda\nu_2\nu_1\kappa}(l)-A^{\lambda\nu_2\nu_1\kappa}(0)]-\frac{l^2+2l(N-k)}{(k^2-2kN)}A^{\lambda\nu_2\nu_1\kappa}(0)\right]. \tag{61}$$

Now the traces (with $W\to 1$ in $A^{\lambda\nu_2\nu_1\kappa}$) are

$$Y_{\lambda\kappa}(l)(A^{\lambda\nu_2\nu_1\kappa}(l)-A^{\lambda\nu_2\nu_1\kappa}(0))$$
$$=-4i\epsilon^{\tau\nu_2\nu_1\beta}\left[-\frac{1}{l^2}(l^2-2lN)(l^2+2lN)N_\tau l_\beta+(l^2-2lN)(N_\tau k_\beta+\tfrac{1}{2}l_\tau k_\beta)+(l^2+2lN)(N_\tau k_\beta-N_\tau l_\beta-\tfrac{1}{2}l_\tau k_\beta)\right], \tag{62a}$$

and

$$Y_{\lambda\kappa}(l)A^{\lambda\nu_2\nu_1\kappa}(0)=-4i\epsilon^{\tau\nu_2\nu_1\beta}(-2)\left[1+\frac{2l_0^2}{l^2}\right]N_\tau k_\beta\,. \tag{62b}$$

So with

$$\Delta E_L^{\text{free}}=\frac{m\alpha^6}{\pi^2}I_L^{\text{free}}\ , \tag{63}$$

one has

$$I_L^{\text{free}}=\int\frac{d^4k}{i\pi^2}\frac{(N^\tau k^\beta-N^\beta k^\tau)}{k^2(k-2N)^2(k^2-2kN)}\int\frac{d^4l}{i\pi^2}\frac{1}{l^2(l^2-2lN)(l^2+2lN)[l^2+2l(N-k)+k^2-2kN]}$$
$$\times\left[\frac{(l^2-2lN)(l^2+2lN)}{l^2}\left[-N_\tau l_\beta-\frac{2l(N-k)}{(k^2-2kN)}N_\tau k_\beta\right]\right.$$
$$+(l^2-2lN)\left[N_\tau k_\beta+\tfrac{1}{2}l_\tau k_\beta-\frac{lk}{(k^2-2kN)}N_\tau k_\beta\right]$$
$$+(l^2+2lN)\left[N_\tau k_\beta-N_\tau l_\beta-\tfrac{1}{2}l_\tau k_\beta+\frac{2+l(2N-k)}{(k^2-2kN)}N_\tau k_\beta\right]$$
$$\left.-\frac{4lk}{(k^2-2kN)}N_\tau k_\beta\right]\ , \tag{64}$$

where we have used

$$\tfrac{1}{16}(2i\epsilon^{0\mu_1\mu_2\alpha}k_\alpha)g_{\mu_1\nu_1}g_{\mu_2\nu_2}(2)(2)\tfrac{1}{4}(-4i\epsilon^{\tau\nu_2\nu_1\beta})$$
$$=(N^\tau k^\beta-N^\beta k^\tau) \tag{65}$$

and

$$(-2)\left[1+\frac{2l_0^2}{l^2}\right]=2lN\frac{(l^2-2lN)}{l^2}-(2+2lN)$$
$$=\frac{(l^2-2lN)(l^2+2lN)}{l^2}-\tfrac{1}{2}(l^2-2lN)$$
$$-\tfrac{1}{2}(l^2+2lN)-2\ . \tag{66}$$

Now the $(N^\tau k^\beta-N^\beta k^\tau)$ factor kills all $N_\tau N_\beta$ and $k_\tau k_\beta$ terms in the large square brackets of Eq. (64). So, after the l integral is done, only $N_\tau k_\beta$ terms survive, and

$$(N^\tau k^\beta-N^\beta k^\tau)N_\tau k_\beta=-\mathbf{k}^2\ . \tag{67}$$

After performing the l integral, the contribution of the first term in the large square brackets of Eq. (64) is

$$I_{L1}^{\text{free}}=\int\frac{d^4k}{i\pi^2}\frac{-\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)^2}$$
$$\times\int du\frac{k^2-2kN+2}{k^2-2kN-(1-u)/u}$$
$$=\tfrac{1}{2}\zeta(2)-\tfrac{5}{4}\ . \tag{68}$$

The second and third terms in the large square brackets of Eq. (64) can be combined by use of the change of variables

$$k\to 2N-k\ ,\quad l\to -l \tag{69}$$

in the third term. For this change of variables, one finds that $k^2(k-2N)^2$, (k^2-2kN), and $[l^2+2l(N-k)+k^2-2kN]$ are unchanged, while $(N^\tau k^\beta-N^\beta k^\tau)$ gets a minus sign. The contribution of the second and third terms is

$$I_{L23}^{\text{free}}=\int\frac{d^4k}{i\pi^2}\frac{(N^\tau k^\beta-N^\beta k^\tau)}{k^2(k-2N)^2(k^2-2kN)}\int\frac{d^4l}{i\pi^2}\frac{1}{l^2(l^2+2lN)(l^2+2l(N-k)+k^2-2kN)}$$
$$\times\left[2N_\tau k_\beta+l_\tau k_\beta+\frac{2-2lk}{(k^2-2kN)}N_\tau k_\beta\right]$$
$$=\int\frac{d^4k}{i\pi^2}\frac{-\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)}\int dx\,du\frac{-1}{H}\left[2-x+\frac{2-2x(k^2u-kN)}{(k^2-2kN)}\right]$$
$$=[-\tfrac{21}{16}\zeta(3)+\tfrac{3}{2}\zeta(2)\ln 2-\tfrac{7}{4}\zeta(2)+\ln^2 2+\tfrac{1}{4}]+i\pi[\tfrac{3}{8}\zeta(2)-\ln 2]\ . \tag{70}$$

Note that the denominator factor H that results from the l integral also occurred in the vertex correction function [see Eq. (38a)]. The contribution of the fourth term in Eq. (64) is

$$I_{L4}^{\text{free}}=\int\frac{d^4k}{i\pi^2}\frac{-\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)^2}\int\frac{d^4l}{i\pi^2}\frac{-4lk}{l^2(l^2-2lN)(l^2+2lN)[l^2+2l(N-k)+k^2-2kN]}$$
$$=[\tfrac{21}{16}\zeta(3)-\tfrac{3}{2}\zeta(2)\ln 2-\tfrac{1}{4}\zeta(2)-\tfrac{1}{2}\ln^2 2+\tfrac{1}{2}]+i\pi[-\tfrac{3}{8}\zeta(2)+\tfrac{1}{2}\ln 2]\ . \tag{71}$$

This is the most difficult integral in this calculation. The evaluation of $I_{L4}^{\rm free}$ is discussed in the Appendix.

The total result for $I_L^{\rm free}$ is obtained from Eqs. (68), (70), and (71). It is

$$I_L^{\rm free}=[-\tfrac{3}{2}\zeta(2)+\tfrac{1}{2}\ln^2 2-\tfrac{1}{2}]+i\pi(-\tfrac{1}{2}\ln 2)\ . \tag{72}$$

And finally, combining the results of Eqs. (59) and (72), we obtain the total contribution of the ladder graph:

$$I_L=[-\tfrac{3}{2}\zeta(2)+\tfrac{1}{2}\ln^2 2-3\ln 2+\tfrac{5}{2}] +i\pi(-\tfrac{1}{2}\ln 2+\tfrac{3}{2})-I^{\rm rel}\ . \tag{73}$$

E. Results

It is now a simple matter to tabulate the results. The total energy shift to order $m\alpha^6$ is

$$\Delta E_{\rm tot}=\frac{m\alpha^6}{\pi^2}I_{\rm tot}\ , \tag{74}$$

where

$$I_{\rm tot}=I_{\rm VP}+I_{\rm SE}+I_V+I_L+I^{\rm rel}\ . \tag{75}$$

The $I^{\rm rel}$ term is the relativistic contribution of the lowest-order graph. Performing the sum, we find

$$I_{\rm tot}=[\tfrac{21}{16}\zeta(3)-\tfrac{3}{2}\zeta(2)\ln 2-\tfrac{13}{6}\zeta(2)-\tfrac{5}{2}\ln 2+\tfrac{23}{4}] +i\pi[-\tfrac{3}{8}\zeta(2)+\tfrac{5}{4}]\ . \tag{76}$$

The contribution to the hyperfine interval is $-0.0325m\alpha^6=-0.606$ MHz. This result differs by -13.74 MHz from the result of CDFR [9–11].

As a partial check of our result, we can use it to obtain the order-α correction to the parapositronium decay rate:

$$\begin{aligned}\Gamma&=-2\,{\rm Im}(\Delta E)\\ &=\tfrac{1}{2}m\alpha^5-2\frac{m\alpha^6}{\pi}[-\tfrac{3}{8}\zeta(2)+\tfrac{5}{4}]\\ &=\frac{m\alpha^5}{2}\left[1-\frac{\alpha}{\pi}\left[5-\frac{\pi^2}{4}\right]\right]\ .\end{aligned} \tag{77}$$

This agrees with the result of Harris and Brown [27]. As a more detailed check, we have verified that the partial decay rates due to each of the contributing diagrams agree with the Fried-Yennie gauge results for the partial decay rates previously obtained by Adkins [28].

IV. CALCULATION AT ORDER $m\alpha^6$ IN THE FEYNMAN GAUGE

Because of the discrepancy between our Fried-Yennie gauge result and the old Feynman gauge result of CDFR, we recalculated the correction using the Feynman gauge. In the process, we uncovered several mistakes in the work of CDFR. After correcting these mistakes, the two calculations agreed.

The vacuum polarization contribution is gauge independent. We found the CDFR result for this graph to be missing an overall minus sign. The correct result is given in Eq. (26).

We agree with the CDFR result for the self-energy contribution. It is

$$I_{\rm SE}({\rm Feynman})=[-\tfrac{1}{2}\zeta(2)+\ln^2 2+\tfrac{1}{2}\ln 2-\tfrac{1}{4}] +i\pi(-\ln 2-\tfrac{1}{4})+2I_{\rm LO}\ln\lambda\ , \tag{78}$$

where $m\lambda$ is a fictitious photon mass added to the theory in order to allow the usual mass-shell renormalization scheme to be implemented.

CDFR combined the vertex and ladder contributions together. However, in their analysis of the vertex correction, they wrote down a vertex "integrand" [their Eq. (17) in Ref. [10]]. This formula has a sign error before the integral on the second line. The sign should be plus. This sign error also appears in Devoto's dissertation [11], Eq. (3.77), but not in his previous Eq. (3.71). This error is evidently simply a misprint, since the combined expression for the vertex and ladder contributions [Eq. (22) in Ref. [10]] is correct. Another misprint appears in Eq. (21) of Ref. [10]; the $(p-k)_\lambda$ in the numerator of the first term of the integral I_λ should be $(p-kx)_\lambda$. This factor is correct in the dissertation [Eq. (3.87)]. There are two mistakes in the table of integrals "Table I" of Ref. [10]. The first integral there should have the value

$$I_1({\rm CDFR})=\left[\frac{21}{4}\zeta(3)-6\frac{\pi^2}{6}\ln 2-\frac{\pi^2}{6}-2\ln^2 2+2\right] +i\pi\left[-\frac{3}{2}\frac{\pi^2}{6}+2\ln 2\right]\ . \tag{79}$$

This integral is just four times our $I_{L4}^{\rm free}$ of Eq. (71). The sixth integral in "Table I" is also incorrect. It should be

$$I_6({\rm CDFR})=-9\frac{\pi^2}{6}+\frac{21}{2}\ . \tag{80}$$

The evaluation of these two integrals is discussed in the Appendix. Using the corrected values of I_1(CDFR) and I_6(CDFR), we obtain

$$I_{V+L}({\rm Feynman})=[\tfrac{21}{16}\zeta(3)-\tfrac{3}{2}\zeta(2)\ln 2-\tfrac{3}{2}\zeta(2) -\ln^2 2-3\ln 2+6] +i\pi[-\tfrac{3}{8}\zeta(2)+\ln 2+\tfrac{3}{2}]-2I_{\rm LO}\ln\lambda\ . \tag{81}$$

The sum of the correct vacuum polarization contribution, the Feynman gauge self-energy contribution of Eq. (78), and the correct Feynman gauge vertex and ladder contribution of Eq. (81) is the same as the Fried-Yennie gauge result of Eq. (76).

For the record, the Feynman gauge vertex and ladder contributions individually are

$$I_V({\rm Feynman})=[\tfrac{21}{16}\zeta(3)-\tfrac{3}{2}\zeta(2)\ln 2-\tfrac{1}{4}\zeta(2) -\ln^2 2-2\ln 2+\tfrac{9}{2}] +i\pi[-\tfrac{3}{8}\zeta(2)+\ln 2+1]-4I_{\rm LO}\ln\lambda \tag{82}$$

and

$$I_L(\text{Feynman})=[-\tfrac{5}{4}\zeta(2)-\ln 2+\tfrac{3}{2}]+i\pi(\tfrac{1}{2})+2I_{\rm LO}\ln\lambda\ . \tag{83}$$

V. CONCLUSION

We have obtained the analytic result for the two-photon annihilation contribution to the positronium hyperfine interval at order $m\alpha^6$. Our result, given in Eqs. (74) and (76), is a contribution $-0.0325m\alpha^6=-0.606$ MHz to the hyperfine interval. A previous calculation of this quantity contained several errors. Once these errors are corrected, the two calculations agree. This result is now quite secure, since it has been obtained in two different gauges.

Our experience with these corrections confirms the general principle that QED calculations, and other calculations of importance, should be done by at least two independent groups. The work of CDFR has great value in providing the basis for one calculation of these corrections.

The corrected theoretical result for the hyperfine interval, given in Eq. (5), is in agreement with the experimental value. This leads us to expect that the remaining order-$m\alpha^6$ corrections will be small. What remains to be done at this order is to evaluate the one-photon-annihilation contributions and to check results that have not yet been confirmed. Also, the numerical error on the recoil corrections [16] should be reduced.

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APPENDIX: EVALUATION OF SELECTED INTEGRALS

In this appendix, we describe the evaluation of some momentum space integrals. We choose the integrals I_1(CDFR) and I_6(CDFR), since they are representative of the integrals that occur in the calculation, and they are the ones that were evaluated incorrectly by CDFR. We read these integrals off of Eq. (22) of CDFR [10], and make the alterations necessary to convert to our notation. Their parameters x and y we call u and x. Their p is our mN. They use a dimensional k vector while ours is dimensionless (a factor of the electron mass has been extracted). They use a spacelike metric while ours is timelike. Consequently, their factor

$$A=(k^2-2kp)x-(kx-p)^2y \tag{A1}$$

translates to our

$$H=-ur\left[k^2-2kN\left[\frac{1-x}{r}\right]-\left[\frac{x}{ur}\right]\right]\equiv -urR \tag{A2}$$

[see Eq. (38a)], where $r=1-xu$, as before.

The first integral we look at is

$$\begin{aligned} I_6(\text{CDFR})&=\int\frac{d^4k}{i\pi^2}\frac{4\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)^2}\\ &\quad\times\int dx\,du\frac{-(k-2N)^2(\frac{2}{3}-2x)}{urR}\\ &=\int dx\,du(\tfrac{3}{2}-2x)\frac{1}{ur}\\ &\quad\times\int\frac{d^4k}{i\pi^2}\frac{-4\mathbf{k}^2}{k^2(k^2-2kN)^2R}\ . \end{aligned} \tag{A3}$$

This integral is real because the numerator [of the first form of Eq. (A3)] vanishes when $(k-2N)^2=0$. We use the identity

$$-4\mathbf{k}^2=k^2(k^2-2kN)-(k^2-2kN)^2+2(2-k^0)k^2 \tag{A4}$$

to break this integral into simpler parts. The breakup generates ultraviolet divergences in the first two terms. We use dimensional regularization, with $n=4-2\epsilon$ dimensions of space-time, to deal with these. We find

$$\begin{aligned} I_6(\text{CDFR})&=\int dx\,du(\tfrac{3}{2}-2x)\frac{1}{ur}\\ &\quad\times\int\frac{d^nk}{i\pi^{n/2}}\left\{\frac{1}{(k^2-2kN)R}-\frac{1}{k^2R}\right.\\ &\quad\left.+\frac{2(2-k^0)}{(k^2-2kN)^2R}\right\}. \end{aligned} \tag{A5}$$

The k integral is done using a Feynman parameter s, always associating s with R and $(1-s)$ with the other denominator factor. One obtains

$$\begin{aligned} I_6(\text{CDFR})&=\int dx\,du(\tfrac{3}{2}-2x)\frac{1}{ur}\left\{\int ds\left[\Gamma(\epsilon)-\ln\left[\frac{T}{ur^2}\right]\right]-\int ds\left[\Gamma(\epsilon)-\ln\left[\frac{sT'}{ur^2}\right]\right]\right.\\ &\quad\left.-\int ds(1-s)2\left[2-\frac{\omega}{r}\right]\frac{ur^2}{T}\right\}\\ &=\int dx\,du(\tfrac{3}{2}-2x)\int ds\left\{\frac{1}{ur}\ln\left[\frac{sT'}{T}\right]+2\frac{(1-s)(\omega-2r)}{T}\right\}, \end{aligned} \tag{A6}$$

where

$$\omega = r - sx(1-u) , \tag{A7a}$$

$$T = u\omega^2 + xsr , \tag{A7b}$$

$$T' = xr + su(1-x)^2 . \tag{A7c}$$

The ultraviolet divergences cancel, as they must. At this stage, we evaluate the integral numerically using the adaptive Monte Carlo multidimensional integration routine VEGAS [29]. It is essential to get a numerical evaluation of an integral as soon as possible in order to minimize the chance of making mistakes. We obtain

$$I_6(\text{CDFR}) \approx -4.304\,411(11) , \tag{A8}$$

using approximately 100 million function evaluations. Continuing with the analytic evaluation, we perform the s integral, saving the x and u integrals until the end. Keeping the two terms in the curly brackets separate, we find

$$I_6(\text{CDFR}) = \int dx\, du \left(\tfrac{3}{2}-2x\right) \left\{ \left[\frac{x}{u^2(1-x)^2} \ln\left[\frac{e}{xr}\right] - \frac{1}{x(1-u)^2} \ln\left[\frac{e}{ur}\right] + \frac{1}{xu^2} \ln r \right] + 2\left[-\frac{e}{x^2(1-u)^3} \ln\left[\frac{e}{ur}\right] + \frac{1}{x^2u^2} \ln r + \frac{1}{xu(1-u)} \right] \right\}$$

$$= [\zeta(2)-4] + [-10\zeta(2) + \tfrac{29}{2}] = -9\zeta(2) + \tfrac{21}{2} , \tag{A9}$$

where

$$e = x + u - 2xu . \tag{A10}$$

The second integral that we will consider here is

$$I_1(\text{CDFR}) = \int \frac{d^4k}{i\pi^2} \frac{4\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)^2} \int \frac{d^4l}{i\pi^2} \frac{4lk}{l^2(l^2-2lN)(l^2+2lN)[l^2+2l(N-k)+k^2-2kN]} . \tag{A11}$$

This integral is four times I_{L4}^{free} of Eq. (71). It has an imaginary part, so the implicit $i\epsilon$ factors in the denominators have to be maintained. We use the identity [Eq. (D.3) in Devoto [11]]

$$\frac{1}{(l^2-2lN)(l^2+2lN)} = \frac{1}{2l^2} \left\{ \frac{1}{l^2+2lN} + \frac{1}{l^2-2lN} \right\} \tag{A12}$$

to reduce the number of denominator factors. One has

$$I_1(\text{CDFR}) = \int \frac{d^4k}{i\pi^2} \frac{4\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)^2} \int \frac{d^4l}{i\pi^2} \frac{1}{l^4} \left[\frac{1}{l^2+2lN} + \frac{1}{l^2-2lN} \right] \frac{2lk}{[l^2+2l(N-k)+k^2-2kN]}$$

$$= \int \frac{d^4k}{i\pi^2} \frac{4\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)^2} (2) \int dx\, du (1-x) \left\{ \frac{(ku-N)k}{H^2} + \frac{[ku+N(1-2u)]k}{H'^2} \right\} , \tag{A13}$$

where the l integral has been done using the Feynman parameters x and u [associating factors of $1-x$, $x(1-u)$, and xu with the three denominators], H is given in Eq. (A2), and

$$H' = -ur \left[k^2 - 2kN \left[\frac{g}{r}\right] - \left[\frac{xa^2}{ur}\right] \right] , \tag{A14}$$

with

$$a = 1-2u , \tag{A15a}$$

$$g = 1+xa . \tag{A15b}$$

In this form, it is clear that I_1(CDFR) is in fact the first integral of Table I of CDFR [10].

In order to evaluate I_1(CDFR), we take $k \to 2N-k$ in the second term of Eq. (A13). Under this transformation, $H' \to H$, so

$$I_1(\text{CDFR}) = 4 \int \frac{d^4k}{i\pi^2} \frac{4\mathbf{k}^2}{k^2(k-2N)^2(k^2-2kN)^2} \int dx\, du (1-x) \frac{(ku-N)(k-N)}{H^2}$$

$$= 4 \int dx\, du \frac{(1-x)}{(ur)^2} \int \frac{d^4k}{i\pi^2} \left\{ \frac{-1}{(k^2-2kN)^2} + \frac{1}{k^2(k-2N)^2} \right\} \frac{(ku-N)(k-N)}{R^2} . \tag{A16}$$

The integral corresponding to the first term (term "A") in the curly brackets is real, and is evaluated using the same parameters as for I_6(CDFR). Writing $(ku-N)(k-N)$ as $(k^2-2kN)u+[1-(1-u)k^0]$, one has

$$I_{1A}(\text{CDFR})=4\int dx\,du(1-x)\int ds\left[\frac{s}{T}+\frac{r[(1-u)\omega-r]s(1-s)}{T^2}\right]$$
$$=4\int dx\,du\frac{(1-x)}{x^3}\left[-\frac{1}{(1-u)^2a}\ln\left[\frac{e}{ur}\right]-\frac{1}{u^2a}\ln r+\frac{1}{a^2}\ln\left[\frac{e}{u}\right]-\frac{x}{ua}\right]$$
$$=2\ . \tag{A17}$$

[Actually, a simpler way to evaluate I_{1A}(CDFR) is to do the k integral before the l integral. This alternate evaluation serves as a check.] The integral corresponding to the second term (term B) in the curly brackets of Eq. (A16) is complex. It is

$$I_{1B}(\text{CDFR})=4\int dx\,du\frac{(1-x)}{(ur)^2}\int\frac{d^4k}{i\pi^2}\frac{k^2u+[1-(1+u)k^0]}{k^2(k-2N)^2R^2}\ . \tag{A18}$$

The integral corresponding to the first term (term "$B1$") in the numerator here is relatively simple to evaluate. It is

$$I_{1B1}(\text{CDFR})=-4\int dx\,du\,ds\frac{1-x}{Y}$$
$$=-4\int dx\,du\frac{1-x}{ug^2}\ln\left[\frac{e}{xra^2}\right]$$
$$=-2\zeta(3)+24\zeta(2)\ln 2-24\zeta(2)\ , \tag{A19}$$

where

$$Y=xra^2+usg^2\ . \tag{A20}$$

The integral corresponding to the second term (term "$B2$") in the numerator of Eq. (A18) is

$$I_{1B2}(\text{CDFR})=4\int dx\,du\frac{(1-x)}{(ur)^2}\times\int\frac{d^4k}{i\pi^2}\frac{[1-(1+u)k^0]}{k^2(k-2N)^2R^2}\ . \tag{A21}$$

We do the k integral using Feynman parameters z and s [associating factors of $1-z$, $z(1-s)$, and zs with the three denominators], and obtain

$$I_{1B2}(\text{CDFR})=4\int dx\,du\,dz\,ds(1-x)rs[r-q(1+u)z]\frac{1}{W^2}\ , \tag{A22}$$

where

$$q=2r-sg\ , \tag{A23a}$$
$$W=uq^2z+D\ , \tag{A23b}$$
$$D=xrs-4ur^2(1-s)-i\epsilon\ . \tag{A23c}$$

We cannot perform a numerical evaluation at this point, since the integral is complex. We do the z integral, and obtain

$$I_{1B2}(\text{CDFR})=4\int dx\,du\,ds(1-x)r\left\{\frac{r}{YD}+(1+u)\left[\frac{1}{uqY}-\frac{s}{u^2q^3}\ln\left[\frac{sY}{D}\right]\right]\right\}\ . \tag{A24}$$

Both $1/D$ and the logarithm give rise to complex contributions. The real and imaginary parts of Eq. (A24) can be separated, but the resulting integrals are numerically ill-behaved. Consequently, we were not able to obtain a numerical value for this integral before reducing it to two-dimensional form. Continuing with the analytical evaluation, we perform the s integral, and obtain

$$I_{1B2}(\text{CDFR})=\int dx\,du(1-x)\left\{-\frac{1+u}{u^2(1-x)^2}\ln\left[\frac{e}{xr}\right]+\frac{1+u}{u^2g^2}\ln\left[\frac{e}{xra^2}\right]+\frac{4u}{h^2}\ln\left[\frac{4ue}{x^2a^2}\right]-i\pi\frac{4u}{h^2}\right\}$$
$$=\left[\tfrac{29}{4}\zeta(3)-30\zeta(2)\ln 2+23\zeta(2)-2\ln^2 2\right]+i\pi\left[-\tfrac{3}{2}\zeta(2)+2\ln 2\right]\ , \tag{A25}$$

where $h=2u+xa$. On summing Eqs. (A17), (A19), and (A25), we obtain the final result

$$I_1(\text{CDFR})=\left[\tfrac{21}{4}\zeta(3)-6\zeta(2)\ln 2-\zeta(2)-2\ln^2 2+2\right]+i\pi\left[-\tfrac{3}{2}\zeta(2)+2\ln 2\right]\ . \tag{A26}$$

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[1] 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 $E(1\,^1S_0)$. The triplet state is called orthopositronium and the singlet state is called parapositronium.

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