

Single Photon Annihilation Contributions to the Positronium Hyperfine Splitting to Order $m_e\alpha^6$

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The single photon annihilation contributions for the positronium ground state hyperfine splitting are calculated analytically to order $m_e\alpha^6$ using nonrelativistic QED. Based on intuitive physical arguments the same result can also be determined using results from previous calculations. Our result completes the hyperfine splitting calculation to order $m_e\alpha^6$. We compare the theoretical prediction with the most recent experimental measurement. [S0031-9007(97)04336-6]

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Positronium, a two-body bound state consisting of an electron and a positron, belongs to the first systems studied within the relativistic quantum theory developed by Dirac [1]. The existence of positronium was predicted in 1934 [2] and experimentally verified at the beginning of the 1950s [3]. For the ground state hyperfine splitting (hfs), the mass difference between the 1^3S_1 and 1^1S_0 states, steadily improved experimental measurements have meanwhile reached a precision of 3.6 ppm [4] which makes the calculation of all $\mathcal{O}(\alpha^2)$ (NNLO) corrections to the leading and next-to-leading order expression mandatory. So far only the $\mathcal{O}(\alpha^2 \ln \alpha^{-1})$ corrections have been fully determined [5]. Including also the known $\mathcal{O}(\alpha^3 \ln^2 \alpha^{-1})$ corrections [6,7], the theoretical expression for the hfs reads (we use natural units, in which $\hbar = c = 1$)

$$W = m_e\alpha^4 \left[\frac{7}{12} - \frac{\alpha}{\pi} \left(\frac{8}{9} + \frac{1}{2} \ln 2 \right) + \alpha^2 \left(\frac{5}{24} \ln \alpha^{-1} + K \right) - \frac{7}{8\pi} \alpha^3 \ln^2 \alpha^{-1} \right]. \quad (1)$$

We have calculated the single photon annihilation ($1\text{-}\gamma$ ann) contributions to the constant K . All other contribu-

tions to K coming from the nonannihilation, and the two and three photon annihilation processes have been calculated before (see Table I below). Although our result completes the calculations to $\mathcal{O}(m_e\alpha^6)$ the theoretical situation remains unresolved due to a discrepancy in two older calculations for some of the nonannihilation contributions to $\mathcal{O}(m_e\alpha^6)$.

In this Letter we report on two methods to determine the single photon annihilation contributions to the $\mathcal{O}(m_e\alpha^6)$ hfs, $W_{\text{NNLO}}^{1\text{-}\gamma \text{ ann}}$. The first one is systematic using nonrelativistic QED (NRQED) [8], which is based on the concept of effective field theories and the separation of effects from nonrelativistic and relativistic momenta, and the second one relies on physical intuition using two older results. We also summarize the status of the theoretical calculation to the hfs in view of the most recent available experimental data. We note that the presentation of our NRQED calculation is only meant to illustrate the basic steps of our calculation. A more detailed work on the NRQED method is in preparation. Our second method, on the other hand, is almost trivial and represents a true “back of the envelope” calculation.

For the NRQED calculation we start from the NRQED Lagrangian [8]

$$\begin{aligned} \mathcal{L}_{\text{NRQED}} = & \frac{1}{2} (\mathbf{E}^2 - \mathbf{B}^2) + \psi^\dagger \left[iD_t + \frac{\mathbf{D}^2}{2m_e} + c_1 \frac{\mathbf{D}^4}{8m_e^3} \right] \psi + \dots \\ & + \psi^\dagger \left[\frac{c_1 e}{2m_e} \boldsymbol{\sigma} \cdot \mathbf{B} + \frac{c_3 e}{8m_e^2} (\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D}) + \frac{c_4 e}{8m_e^2} i(\mathbf{D} \times \mathbf{E} - \mathbf{E} \times \mathbf{D}) \right] \psi + \dots \\ & - \frac{d_1 e^2}{4m_e^2} (\psi^\dagger \boldsymbol{\sigma} \sigma_2 \chi^*) (\chi^T \sigma_2 \boldsymbol{\sigma} \psi) + \frac{d_2 e^2}{3m_e^4} \frac{1}{2} \{ (\psi^\dagger \boldsymbol{\sigma} \sigma_2 \chi^*) [\chi^T \sigma_2 \boldsymbol{\sigma} (-\frac{i}{2} \vec{\mathbf{D}})^2 \psi] + \text{H.c.} \} + \dots, \quad (2) \end{aligned}$$

where ψ and χ are, respectively, the electron and positron Pauli spinors and D_t and \mathbf{D} are, respectively, the time and space components of the gauge covariant derivative D_μ . In Eq. (2) the straightforward bilinear positron terms are omitted and only those four fermion interactions relevant for $W_{\text{NNLO}}^{1\text{-}\gamma \text{ ann}}$ are displayed. The renormalization constants $c_1, \dots, c_4, d_1, d_2$ are normalized to one at the Born level.

For $W_{\text{NNLO}}^{1\text{-}\gamma \text{ ann}}$ only the radiative corrections to d_1 have to be calculated. To $\mathcal{O}(m_e\alpha^6)$, and if we consider only the contributions from the one photon annihilation graphs, all retardation effects can be neglected. This means that the transverse photon propagators can be used in the instantaneous approximation, i.e., their energy dependence is dropped. Indeed, simple counting rules [9] show that

retardation corrections to the one photon annihilation diagrams would set in at $\mathcal{O}(m_e \alpha^7)$. In the instantaneous approximation, all NRQED interactions can be written as two-body potentials. In momentum space representation the potentials needed for the present calculation are given

$$V_{\text{rel}}(\mathbf{p}, \mathbf{q}) = -\frac{e^2}{m_e^2} \left[\frac{|\mathbf{p} \times \mathbf{q}|^2}{(|\mathbf{p} - \mathbf{q}|^2 + \lambda^2)^2} - \frac{(\mathbf{p} - \mathbf{q}) \times \mathbf{S}_- \cdot (\mathbf{p} - \mathbf{q}) \times \mathbf{S}_+}{|\mathbf{p} - \mathbf{q}|^2 + \lambda^2} + i \frac{3}{2} \frac{(\mathbf{p} \times \mathbf{q}) \cdot (\mathbf{S}_- + \mathbf{S}_+)}{|\mathbf{p} - \mathbf{q}|^2 + \lambda^2} - \frac{1}{4} \frac{|\mathbf{p} - \mathbf{q}|^2}{|\mathbf{p} - \mathbf{q}|^2 + \lambda^2} \right], \quad (4)$$

$$V_4(\mathbf{p}, \mathbf{q}) = \frac{e^2}{2m_e^2} \left[\frac{3}{4} + \mathbf{S}_- \cdot \mathbf{S}_+ \right], \quad (5)$$

$$V_{4\text{der}}(\mathbf{p}, \mathbf{q}) = -\frac{e^2}{3m_e^4} (\mathbf{p}^2 + \mathbf{q}^2) \left[\frac{3}{4} + \mathbf{S}_- \cdot \mathbf{S}_+ \right], \quad (6)$$

where λ is a small fictitious photon mass to regularize IR divergences and \mathbf{S}_\mp denotes the electron/positron spin operator. V_{rel} denotes the $1/m_e^2$ corrections to the Coulomb potential including longitudinal and transverse photon exchange. V_4 accounts for the leading order annihilation process $e^+e^- \rightarrow \gamma \rightarrow e^+e^-$ and $V_{4\text{der}}$ denotes relativistic corrections to V_4 from the energy dependence of the annihilation photon and from the $1/m_e^2$ contributions in the Dirac spinors. The calculation of $W_{\text{NNLO}}^{1-\gamma \text{ ann}}$ proceeds in two basic steps.

Step 1: Matching calculation.—Calculation of the $\mathcal{O}(\alpha)$ and $\mathcal{O}(\alpha^2)$ contributions to d_1 by matching the NRQED and QED amplitudes for the elastic s -channel scattering of free and on-shell electrons and positrons via a single photon, up to two loops and to NNLO in the velocity of the electrons and positrons in the c.m. frame.

Step 2: Bound state calculation.—Calculation of $W_{\text{NNLO}}^{1-\gamma \text{ ann}}$ by solving the nonrelativistic bound state problem in the form of the Schrödinger equation (i.e., including the nonrelativistic kinetic energy and the Coulomb interaction) exactly and by treating the relativistic effects using Rayleigh-Schrödinger time-independent perturbation theory (TIPT).

Matching calculation: To determine the NRQED amplitude for $e^+e^- \rightarrow \gamma \rightarrow e^+e^-$ for free and on-shell electrons and positrons up to two loops and NNLO in the velocity the diagrams displayed in Fig. 2 have to be calculated. It is sufficient to consider only scattering of the e^+e^- pair in a 3S_1 state because a 1S_0 state cannot an-

by (see Fig. 1)

$$V_c(\mathbf{p}, \mathbf{q}) = -\frac{e^2}{|\mathbf{p} - \mathbf{q}|^2 + \lambda^2}, \quad (\text{Coulomb interaction}), \quad (3)$$

nihilate into a single photon due to C invariance. We have regularized all UV divergent integrations by using a momentum cutoff. As a consequence the finite terms in the NRQED amplitude (and also in the constant d_1) depend on the routing of the loop momenta through the diagrams [7]. We come back to this point later. The corresponding QED amplitude for the scattering process has to be determined by using conventional covariant multi-loop perturbation theory. Whereas the one-loop results for the vertex corrections [10] and the one- and two-loop contributions to the vacuum polarization function [11] have been known for quite a long time, the two-loop vertex corrections have been calculated recently by one of the authors [12]. (The two-loop vertex diagram, in which one of the loops is the vacuum polarization, has been calculated before in [13,14].) The QED amplitude is renormalized within the common on-shell renormalization scheme. The $\mathcal{O}(\alpha)$ and $\mathcal{O}(\alpha^2)$ contributions to d_1 are then determined by demanding equality of the NRQED and QED amplitude at the one- and two-loop levels. Because all IR divergent and velocity dependent contributions are equal in NRQED and QED, d_1 contains only UV divergent and constant contributions.

Bound state calculation: To finally determine $W_{\text{NNLO}}^{1-\gamma \text{ ann}}$ we start from the well known solution of the nonrelativistic positronium problem and incorporate V_4 , $V_{4\text{der}}$, V_{rel} , and V_{kin} via first and second order TIPT. For each insertion of V_4 , the contributions from d_1 have also to be taken into account. The divergences in d_1 automatically remove the UV divergences which arise in the bound state calculation. At this point we want to emphasize that, to be consistent, the routing of the momenta in the bound state calculation has to be exactly the same as the routing in the NRQED scattering diagrams. Also the finite terms in the bound state integrals depend on the routing.

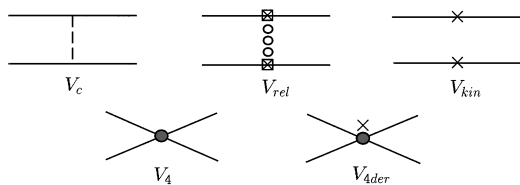


FIG. 1. Interaction potentials contributing to $W_{\text{NNLO}}^{1-\gamma \text{ ann}}$. V_{kin} denotes the relativistic kinetic energy correction coming from the $\mathbf{D}^4/8m_e^3$ terms in the NRQED Lagrangian.

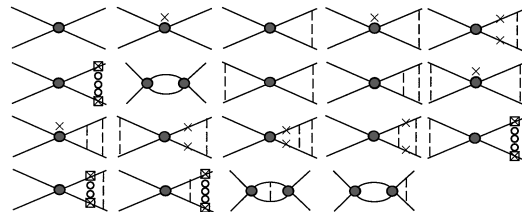


FIG. 2. NRQED diagrams for the matching calculation. Permutations are not displayed.

Combining the result of the bound state integrals with the contributions in d_1 leads to the cancellation of the routing-dependent terms. We have checked this fact by choosing different routings in our calculation.

The final result for the $\mathcal{O}(m_e \alpha^6)$ one photon annihilation contributions to the hfs reads

$$W_{\text{NNLO}}^{1-\gamma \text{ ann}} = \frac{m_e \alpha^6}{4} \left[\frac{1}{\pi^2} \left(\frac{1477}{81} + \frac{13}{8} \zeta_3 \right) - \frac{1183}{288} + \frac{9}{4} \ln 2 + \frac{1}{6} \ln \alpha^{-1} \right]. \quad (7)$$

The $\ln \alpha^{-1}$ term was already known and is included in the $\ln \alpha^{-1}$ contribution quoted in Eq. (1). The one photon

annihilation contribution to the constant K corresponds to a contribution of -2.34 Mhz to the theoretical prediction of the hfs (see Table I). (The contributions in $W_{\text{NNLO}}^{1-\gamma \text{ ann}}$ coming from the vacuum polarization effects of the annihilation photon have been calculated before in [13,15,16]. The result in [15] contains an error in the treatment of the one-loop vacuum polarization (see [16]). The vacuum polarization contributions calculated in [13,16] are in agreement with our result.)

The second, more intuitive method to determine $W_{\text{NNLO}}^{1-\gamma \text{ ann}}$ starts from the formal result for the energy shift due to one photon annihilation for S -wave triplet bound states with radial quantum numbers n using first to third order TIPT,

$$W_n^{1-\gamma \text{ ann}} = \langle n | V_4 + V_{4\text{der}} + V_4 \sum_{l \neq n}^f \frac{|l\rangle\langle l|}{E_n - E_l} V_4 + V_4 \sum_{k \neq n}^f \frac{|k\rangle\langle k|}{E_n - E_k} V_4 \sum_{m \neq n}^f \frac{|m\rangle\langle m|}{E_n - E_m} V_4 |n\rangle + \dots + \left[\langle n | V_4 \sum_{l \neq n}^f \frac{|l\rangle\langle l|}{E_n - E_l} (V_{\text{rel}} + V_{\text{kin}}) |n\rangle + \text{H.c.} \right] + \left[\langle n | V_4 \sum_{k \neq n}^f \frac{|k\rangle\langle k|}{E_n - E_k} V_4 \sum_{m \neq n}^f \frac{|m\rangle\langle m|}{E_n - E_m} (V_{\text{rel}} + V_{\text{kin}}) |n\rangle + \text{H.c.} \right] + \dots, \quad (8)$$

where $|i\rangle$, $i = l, m, k$, represent normalized (bound state and continuum) eigenfunctions to the positronium Schrödinger equation with the eigenvalues E_i . (1S_0 states do not contribute because they cannot annihilate into a single photon. States with higher orbital angular momentum, on the other hand, are irrelevant because their wave functions vanish for zero distances.) It is evident from the form of the operator V_4 that $W_n^{1-\gamma \text{ ann}}$ depends only on the zero-distance Coulomb-Green function $A_n \equiv \langle \vec{0} | \sum_{l \neq n} \frac{|l\rangle\langle l|}{E_l - E_n} | \vec{0} \rangle$ (where the n^3S_1 bound state pole is subtracted) and on the rate for annihilation of a n^3S_1 bound state into a single photon, $P_n \equiv \langle n | V_4 | n \rangle + [\langle n | V_4 \sum_{l \neq n} \frac{|l\rangle\langle l|}{E_n - E_l} (V_{\text{rel}} + V_{\text{kin}}) | n \rangle + \text{H.c.}] + \langle n | V_{4\text{der}} | n \rangle$ (where the effects from V_{rel} and V_{kin} are included in the form of corrections to the wave

function). Because A_n and P_n are UV divergent from the integration over the high energy modes, they have to be renormalized. In the NRQED approach this was achieved by the renormalization constant d_1 . Here, renormalization will be carried out by relating A_n and P_n to physical (and finite) quantities which incorporate the proper short-distance physics from the one photon annihilation process. For A_n this physical quantity is just the QED vacuum polarization function in the nonrelativistic limit and for P_n the Abelian contribution of the NNLO expression for the leptonic decay width of a superheavy quark-antiquark n^3S_1 bound state [17]. Both quantities have been determined recently in [16,18]. From the results of [16,18] it is straightforward to derive the renormalized versions of A_n and P_n ,

$$A_n^{\text{phys}} = \frac{m_e^2}{2\pi} \left\{ \frac{8}{9\pi} - \frac{\alpha}{2} \left(C_1 + \left[\ln\left(\frac{\alpha}{2n}\right) - \frac{1}{n} + \gamma + \Psi(n) \right] \right) \right\}, \quad (9)$$

$$P_n^{\text{phys}} = \frac{2\alpha\pi}{m_e^2} \left(\frac{m_e^3 \alpha^3}{8\pi n^3} \right) \left\{ 1 - 4\frac{\alpha}{\pi} + \alpha^2 \left(C_2 - \frac{37}{24n^2} - \frac{2}{3} \left[\ln\left(\frac{\alpha}{2n}\right) - \frac{1}{n} + \gamma + \Psi(n) \right] \right) \right\}, \quad (10)$$

where $C_1 = \frac{1}{2\pi^2} (-3 + \frac{21}{2} \zeta_3) - \frac{11}{16} + \frac{3}{2} \ln 2$ and $C_2 = \frac{1}{\pi^2} (\frac{527}{36} - \zeta_3) + \frac{4}{3} \ln 2 - \frac{43}{18}$. γ is the Euler constant and Ψ the digamma function. Inserting A_n^{phys} and P_n^{phys} back into expression (8) we arrive at

$$W_n^{1-\gamma \text{ ann}} = P_n^{\text{phys}} \left[1 - \frac{2\alpha\pi}{m_e^2} A_n^{\text{phys}} + \left(\frac{2\alpha\pi}{m_e^2} A_n^{\text{phys}} \right)^2 \right]. \quad (11)$$

It is an easy task to check for the ground state $n = 1$ that in Eq. (11) the well known order $m_e \alpha^4$ ($W_{\text{LO}}^{1-\gamma \text{ ann}} = \frac{1}{4} m_e \alpha^4$)

and $m_e \alpha^5$ ($W_{\text{NNLO}}^{1-\gamma \text{ ann}} = -\frac{11}{9\pi} m_e \alpha^5$) one photon annihilation contributions to the hfs are correctly reproduced and that the $m_e \alpha^6$ contributions are equal to $W_{\text{NNLO}}^{1-\gamma \text{ ann}}$ [Eq. (7)]. This second, very simple intuitive method does not only represent a cross check for the systematic NRQED calculation but also illustrates that $W^{1-\gamma \text{ ann}}$ is directly related to other physical quantities. Beyond $\mathcal{O}(m_e \alpha^6)$ expression (11) is not valid because essential retardation effects are not taken into account.

In Table I we have summarized the status of the theoretical calculation to the hfs including our own result. To

TABLE I. Summary of the theoretical calculations to the hfs. Only the references with the first correct calculations are given.

	Order	Specification	analytical/numerical	Contr. in Mhz	Refs.
1	$m_e \alpha^4$		a	204 386.7(1)	[19]
2	$m_e \alpha^5$		a	-1 005.5	[20]
3	$m_e \alpha^6 \ln \alpha^{-1}$		a	19.1	[5]
4	$m_e \alpha^6$	Nonannihilation (CL)	n	-7.2(6)	[8,21,22]
5		Nonannihilation (Pa)	n	-3.29(4)	[21-23]
6		1 Photon annihilation	a	-2.34	This work
7		2 Photon annihilation	a	-0.61	[24]
8		3 Photon annihilation	a	-0.97	[25]
9	$m_e \alpha^7 \ln^2 \alpha^{-1}$		a	-0.92	[6,7]
Sum (Caswell-Lepage)				203 388.3(6)	
Sum (Pachucki)				203 392.2(1)	
Experiment				203 389.1(7)	[4]

$\mathcal{O}(m_e \alpha^6)$ the logarithmic in α and constant contributions are given separately. The constant terms are further subdivided into nonannihilation, and one, two, and three photon annihilation contributions. The error in the order $m_e \alpha^4$ result 1 comes from the uncertainties in the input parameters α , \hbar , and m_e and the errors in 4 and 5 are numerical. For all other contributions the errors are negligible. The uncertainties due to the ignorance of the remaining $m_e \alpha^7 \ln \alpha^{-1}$ and $m_e \alpha^7$ contributions are not taken into account. There are two contradictory calculations for some of nonannihilation contributions based on results from Caswell and Lepage (CL) [8] and Pachucki (Pa) [23]. The result containing the Caswell-Lepage calculation leads to perfect agreement between theory and experiment [$W_{\text{th}} - W_{\text{ex}} = -0.8(1.0)$ Mhz], whereas the hfs prediction based on the result by Pachucki leads to a discrepancy of more than four standard deviations [$W_{\text{th}} - W_{\text{ex}} = 3.1(0.7)$ Mhz]. It remains the task of future examinations to finally resolve the theoretical situation.

During completion of this work we were informed of work on the same subject by Adkins, Fell, and Mitrikov [26] using the Bethe-Salpeter formalism and numerical methods. Their result agrees with ours representing an independent cross check.

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