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

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Abstract

The single photon annihilation contributions for the positronium ground state hyperfine splitting are calculated analytically to order $m_e \alpha^6$ using NRQED. Based on intuitive physical arguments the same result can also be determined by a trivial calculation using results from existing literature. Our result completes the hyperfine splitting calculation to order $m_e \alpha^6$. We compare the theoretical prediction with the most recent experimental measurement.
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. The existence of positronium was predicted in 1934 \(^1\) and experimentally verified at the beginning of the 1950s \(^2\). For the ground state hyperfine splitting (hfs), the mass difference between the \(^1\)S\(_1\) and \(^1\)S\(_0\) state, steadily improved experimental measurements have meanwhile reached a precision of 3.6 ppm \(^3\) which makes the calculation of all \(O(\alpha^2)\) corrections to the leading and next-to-leading order expression mandatory. So far only the order \(\alpha^2 \ln \alpha^{-1}\) corrections have been fully determined \(^4\). Including also the known \(O(\alpha^3 \ln^2 \alpha^{-1})\) corrections \(^3, 6\) the theoretical expression for the hfs reads

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

We have calculated the single photon annihilation \((1 - \gamma \text{ ann})\) contributions to the constant \(K\). All other contributions to \(K\) coming from the non-annihilation, and the two and three photon annihilation processes have been calculated before (see Table \(^5\)). Although our result completes the calculations to order \(m_e \alpha^6\) the theoretical situation remains unresolved due to a discrepancy in two older calculations for some of the non-annihilation contributions to order \(m_e \alpha^6\).

In this letter we report on two methods to determine \(W_{\text{NNLO}}^{1\gamma \text{ ann}}\). The first one is systematic using NRQED \(^7\), which is based on the concept of effective field theories and the separation of effects from non-relativistic and relativistic momenta, and the second one relies on physical intuition using two results from already existing literature. We also summarize the status of the theoretical calculation to the hfs in view of the most recent available experimental data. We would like to note that the presentation of our NRQED calculation is only meant to illustrate the basic steps of our calculation. A more detailed and explicit 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 \(^7\)

\[
\mathcal{L}_{\text{NRQED}} = -\frac{1}{2} (\mathbf{E}^2 - B^2) + \psi^\dagger \left[ i D_t + \frac{D^2}{2m_e} + c_1 \frac{D^4}{8m_e^2} \right] \psi + \ldots
\]

\[+ \psi^\dagger \left[ \frac{c_2}{2m_e} \mathbf{\sigma} \cdot \mathbf{B} + \frac{c_3}{8m_e^2} (D \cdot \mathbf{E} - E \cdot D) + \frac{c_4}{8m_e^2} i (D \times \mathbf{E} - E \times D) \right] \psi + \ldots\]

\[\quad - \frac{d_1}{4m_e^2} \mathbf{e}^2 (\psi^\dagger \mathbf{\sigma} \sigma_2 \mathbf{\chi}^*) (\mathbf{\chi}^T \sigma_2 \mathbf{\sigma} \psi) + \frac{d_2}{3m_e^2} \frac{1}{2} \left( \psi^\dagger \mathbf{\sigma} \sigma_2 \mathbf{\chi}^* \right) \mathbf{\chi}^T \sigma_2 \mathbf{\sigma} (-\frac{i}{2} D^2 \psi) + \text{H.c.} \right] + \ldots, \tag{2}
\]

where \(\psi\) and \(\chi\) are the electron and positron Pauli spinors and \(D_t\) and \(D\) the time and space components of the gauge covariant derivative \(D_\mu\). In Eq. (2) the straightforward bilinear positron terms are omitted and only those four fermion interaction relevant for the one photon annihilation contributions to the hfs are displayed. The renormalization constants \(c_1, \ldots, c_4, d_1, d_2\) are normalized to one at the Born level. For \(W_{\text{NNLO}}^{1\gamma \text{ ann}}\) only the radiative corrections to \(d_1\) have to be calculated. To order \(m_e \alpha^6\), 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 \(^8\) show that retardation corrections to the one photon annihilation diagrams would set in at order \(m_e \alpha^7\). In the instantaneous approximation, all NRQED interactions can be written as two-body potentials. In

\(^{1}\) We use natural units, in which \(\hbar = c = 1\).
Figure 1: Interaction potentials contributing to \( W_{\text{NNLO}}^{1-\gamma\text{ann}} \). \( V_{\text{kin}} \) denotes the relativistic kinetic energy correction coming from the \( D^4/8m_e^3 \) terms in the NRQED Lagrangian.

In momentum space representation all the potentials needed for the present calculation are given by (see Fig. 1)

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

\[
V_{\text{rel}}(p, q) = -\frac{e^2}{m_e^2} \left[ \frac{|p \times q|^2}{(|p - q|^2 + \lambda^2)^2} - \frac{(p - q) \times S_- \cdot (p - q) \times S_+}{|p - q|^2 + \lambda^2} \right. \\
\left. + \frac{3}{2} \frac{(p \times q) \cdot (S_- + S_+)}{|p - q|^2 + \lambda^2} - \frac{1}{4} \frac{|p - q|^2}{|p - q|^2 + \lambda^2} \right],
\]

\[
V_4(p, q) = \frac{e^2}{2m_e^2} \left[ \frac{3}{4} + S_- \cdot S_+ \right],
\]

\[
V_{\text{4der}}(p, q) = -\frac{e^2}{3m_e^4} (p^2 + q^2) \left[ \frac{3}{4} + S_- \cdot S_+ \right],
\]

where \( \lambda \) is a small fictitious photon mass to regularize IR divergences and \( S_\mp \) denotes the electron/positron spin operator. \( V_{\text{rel}} \) 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 \( V_{\text{4der}} \) 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.

1. **Matching calculation**: calculation of the \( \mathcal{O}(\alpha) \) and \( \mathcal{O}(\alpha^2) \) contributions to the constant \( d_1 \) 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, \( e^+e^- \rightarrow \gamma \rightarrow e^+e^- \), up to two loops and to NNLO in the velocity of the electrons and positrons in the c.m. frame.

2. **Bound state calculation**: calculation of \( W_{\text{NNLO}}^{1-\gamma\text{ann}} \) by solving the non-relativistic bound state problem in form of the Schrödinger equation (i.e. including the non-relativistic 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 \( e^+e^- \rightarrow \gamma \rightarrow e^+e^- \) for free and on-shell electrons and positrons up to two loops and NNLO in the velocity the diagrams displayed in Fig. 3.
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 annihilate into a single photon due to $C$ invariance. We have regularized all UV divergent integrations by using a momentum cut-off. 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 [6]. Therefore, to be consistent exactly the same way of routing has to be used in the bound state calculation. 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 [9] and the one and two-loop contributions to the vacuum polarization function [10] have been known for quite a long time, the two-loop vertex corrections have been calculated recently by one of the authors [11]. The QED amplitude is renormalized by the common on-shell renormalization scheme, where $\alpha$ is the fine structure constant and the wave function renormalization constant is fixed by the requirement that the residue of the fermion propagator is one. The $O(\alpha)$ and $O(\alpha^2)$ contributions of the renormalization constant $d_1$ are then determined by demanding equality of the NRQED and QED amplitude at the one- and the two-loop level. 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 $W_{NNLO}^{1+\gamma,\text{ann}}$ we start from the well known solution of the non-relativistic positronium problem (in form of the Schrödinger equation) and incorporate $V_4$, $V_{4\text{der}}$, $V_{\text{rel}}$ and $V_{\text{kin}}$ 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 again 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. 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 order $m_e\alpha^6$ one photon annihilation contributions to the hfs reads\(^2\)

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

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 vacuum polarization contributions calculated in [14] are in agreement with our result.

The second, more intuitive method to determine $W_{n}^{1-\gamma,\text{ann}}$ 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 T IPT\(^3\):

$$W_{n}^{1-\gamma,\text{ann}} = \langle n | V_4 + V_{4\text{der}} + V_4 \sum_{\ell \neq n} \frac{|l\rangle \langle l|}{E_n - E_\ell} V_4 + V_4 \sum_{k \neq n} \frac{|k\rangle \langle k|}{E_n - E_k} V_4 \sum_{m \neq n} \frac{|m\rangle \langle m|}{E_n - E_m} V_4 |n\rangle + \ldots$$

$$+ \left[ \langle n | V_4 \sum_{\ell \neq n} \frac{|l\rangle \langle l|}{E_n - E_\ell} (V_{\text{rel}} + V_{\text{kin}}) |n\rangle \right] + \text{H.c.}$$

$$+ \left[ \langle n | V_4 \sum_{k \neq n} \frac{|k\rangle \langle k|}{E_n - E_k} V_4 \sum_{m \neq n} \frac{|m\rangle \langle m|}{E_n - E_m} (V_{\text{rel}} + V_{\text{kin}}) |n\rangle \right] + \text{H.c.} + \ldots,$$  

where $| i\rangle$, $i = l, m, k$, represent normalized (bound state and continuum) eigenfunctions to the positronium Schrödinger equation with the eigenvalues $E_i$. 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 $A_n \equiv \langle \overrightarrow{0} | \sum_{\ell \neq n} \frac{|l\rangle \langle l|}{E_n - E_\ell} | \overrightarrow{0} \rangle$ (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, $P_n \equiv \langle n | V_4 | n\rangle + \langle n | V_4 \sum_{\ell \neq n} \frac{|l\rangle \langle l|}{E_n - E_\ell} (V_{\text{rel}} + V_{\text{kin}}) |n\rangle + \text{H.c.} + \langle n | V_{4\text{der}} | n\rangle$ (where the effects from $V_{\text{rel}}$ and $V_{\text{kin}}$ are included in 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 non-relativistic 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\(^3\). Both quantities have been determined recently in [14, 13]. From the results of [14, 13] it is straightforward to derive the renormalized versions of $A_n$ and $P_n$,

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

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

\(^2\) The contributions in $W_{n}^{1-\gamma,\text{NNLO}}$ coming from the vacuum polarization effects of the annihilation photon have been calculated before in [12, 14]. The result in [12] contains an error in the treatment of the one-loop vacuum polarization (see [14]). The vacuum polarization contributions calculated in [14] are in agreement with our result.

\(^3\) $S_0$ states do not contribute to $W_{n}^{1-\gamma,\text{ann}}$ 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 electron-positron distance.
where \( C_1 = \frac{1}{2\pi^2}(-3 + \frac{21}{2}\zeta_3) - \frac{11}{18} + \frac{3}{2}\ln 2 \) and \( C_2 = \frac{1}{\pi^2}(-\frac{527}{36} - \zeta_3) + \frac{4}{3}\ln 2 - \frac{43}{18} \). \( \gamma \) is the Euler constant and \( \Psi \) the digamma function. Inserting \( A_{\text{phys}}^n \) and \( P_{\text{phys}}^n \) back into expression (8) we arrive at

\[
W_{1-\gamma}^{\text{ann}} = P_{\text{phys}}^n \left[ 1 - \frac{2\alpha\pi}{m_e^2} A_{\text{phys}}^n + \left( \frac{2\alpha\pi}{m_e^2} A_{\text{phys}}^n \right)^2 \right].
\]

It is an easy task to check for the ground state \( n = 1 \) that in Eq. (11) the well known order \( m_e\alpha^4 \) \((W_{1-\gamma}^{\text{ann}} = \frac{1}{4}m_e\alpha^4)\) and \( m_e\alpha^5 \) \((W_{1-\gamma}^{\text{ann}} = -\frac{11}{36}m_e\alpha^5)\) one photon annihilation contributions to the hfs are correctly reproduced and that the \( m_e\alpha^6 \) contributions are equal to \( W_{1-\gamma}^{\text{ann}} \) of Eq. (7). This second, very simple intuitive method to determine \( W_{1-\gamma}^{\text{ann}} \) does not only represent a nice cross check for the systematic NRQED calculation but also illustrates that \( W_{1-\gamma}^{\text{ann}} \) is directly related to other physical quantities. Beyond order \( m_e\alpha^6 \) expression (11) is not valid because essential retardation effects are not taken into account.

| Order \( m_e\alpha^n \) | Specification | analytical/numerical | Contr. in Mhz | Refs. |
|------------------------|---------------|----------------------|---------------|-------|
| 1. \( m_e\alpha^4 \)    | a             | 204 386.7(1)         | \[16\]        |
| 2. \( m_e\alpha^5 \)    | a             | -1005.5              | \[17\]        |
| 3. \( m_e\alpha^6 \ln \alpha^{-1} \) | a             | 19.1                 | \[4\]         |
| 4. \( m_e\alpha^6 \)    | non-annihilation (C/L) | n | -7.2(6) | \[18\] + \[19\] + \[7\] |
| 5. \( m_e\alpha^6 \)    | non-annihilation (Pa) | n | -3.29(4) | \[18\] + \[19\] + \[20\] |
| 6. \( m_e\alpha^6 \)    | 1 photon annihilation | a | -2.34 | this work |
| 7. \( m_e\alpha^6 \)    | 2 photon annihilation | a | -0.61 | \[21\] |
| 8. \( m_e\alpha^6 \)    | 3 photon annihilation | a | -0.97 | \[22\] |
| 9. \( m_e\alpha^7 \ln^2 \alpha^{-1} \) | a             | -0.92 | \[4\] + \[3\] |

**Table 1:** Summary of the theoretical calculations to the hfs. Only the references with the first correct calculations are given.

In Table \[4\] we have summarized the status of the theoretical calculation to the hfs of the positronium ground state including our own result. To order \( m_e\alpha^6 \) the logarithmic in \( \alpha \) and constant contributions are given separately. The constant terms are further subdivided into non-annihilation, 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 \( \alpha \), \( \hbar \) and \( m_e \) and the errors in 4. and 5. are numerical. For all other contributions the errors are negligible. As indicated, there are two contradictory calculations for some of non-annihilation contributions based on results from Caswell and Lepage (C/L) \[7\] and Pachucki (Pa) \[20\]. The result containing the Caswell-Lepage calculation leads to perfect agreement between theory and experiment \((W_{\text{th}} - W_{\text{ex}} = -0.8(1.0) \text{ Mhz})\), whereas the hfs prediction based on the result by Pachucki leads to a discrepancy of more than four standard deviations \((W_{\text{th}} - W_{\text{ex}} = 3.1(0.7) \text{ Mhz})\). 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 using the Bethe-Salpeter formalism and numerical methods. Their result agrees with ours representing an independent cross check. We thank G. Adkins and his group for reporting their result to us prior to publication. We also thank G.P. Lepage for useful discussions. This work is supported in part by the Department of Energy under contract DOE DE-FG03-90ER40546 and by the Natural Sciences and Engineering Research Council of Canada.

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