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Positronium hyperfine splitting: analytical value at $\mathcal{O}(m\alpha^6)$

Andrzej Czarnecki*
Physics Department, Brookhaven National Laboratory,
Upton, NY 11973

Kirill Melnikov†
Institut für Theoretische Teilchenphysik,
Universität Karlsruhe, D–76128 Karlsruhe, Germany

Alexander Yelkhovsky‡
Budker Institute for Nuclear Physics,
Novosibirsk, 630090, Russia

Abstract

We present an analytic calculation of the $\mathcal{O}(m\alpha^6)$ recoil corrections to the hyperfine splitting (HFS) of the ground state energy levels in positronium. We find $\Delta E_{\rm rec} = m\alpha^6\left(-\frac{1}{6}\ln\alpha + \frac{331}{432} - \frac{\ln 2}{4} - \frac{17\zeta(3)}{8\pi^2} + \frac{5}{12\pi^2}\right) \approx m\alpha^6\left(-\frac{1}{6}\ln\alpha + 0.37632\right)$, confirming Pachucki's numerical result [1]. We present a complete analytic formula for the $\mathcal{O}(m\alpha^6)$ HFS of the positronium ground state and, including $\mathcal{O}(m\alpha^7\ln^2\alpha)$ effects, find $\left(E(1^3S_1) - E(1^1S_0)\right)_{\rm theory} = 203\ 392(1)$ MHz. This differs from the experimental results by about 3 standard deviations.

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*e-mail: czar@bnl.gov

†e-mail: melnikov@particle.physik.uni-karlsruhe.de

‡e-mail: yelkhovsky@inp.nsk.su

Spectroscopy of positronium, an atom consisting of an electron and a positron, provides a sensitive test of the Quantum Electrodynamics (QED) applied to bound state problems. Electron and positron are so much lighter than the lightest hadrons that the effects of strong interactions are negligible compared with the accuracy of present and any conceivable future experiments. For this reason positronium represents a unique system which can, in principle, be described with very high precision by means of the QED only. One should also mention that the measurements of positronium spectrum are performed with very high accuracy [2].

There are two main approaches used in the studies of bound states. The Bethe–Salpeter method is based on an exact two-body relativistic wave equation [3]. The other approach is the so–called Non-Relativistic Quantum Electrodynamics (NRQED) [4], which is an effective field theory based on the QED for small energies and momenta. Thus, by construction, the NRQED takes advantage of non–relativistic energy of the electron and positron in positronium.

We note in passing that similar techniques are used nowadays for describing heavy quark–antiquark bound states. From this perspective, positronium may serve as a testing ground for methods which can in the future be applied to the QCD.

The HFS of the positronium ground state (i.e. the difference between the energies of the ground state with total spin 1 and 0) belongs to one of the most accurately measured physical quantities. Two experimental values of the highest precision are:

$$\Delta\nu \equiv E(1^3S_1) - E(1^1S_0) = 203\;387.5(1.6)\text{ MHz}, \tag{1}$$

and

$$\Delta\nu = 203\;389.10(0.74)\text{ MHz}, \tag{2}$$

obtained respectively in [5,6]. The bulk of this effect is of the order $m\alpha^4$, where $m = 0.51099907(15)$ MeV (corresponding to $1.2355898(4) \times 10^{14}$ MHz) is the electron mass and $\alpha = 1/137.03599959(51)$ is the fine structure constant. Higher order corrections must be included to fully exploit the experimental accuracy. In particular, since $m\alpha^6 = 18.658$ MHz, a complete calculation at this order is required. With an exception of the leading logarithm, effects of order $m\alpha^7$ have not yet been studied. Clearly, the experimental precision warrants further studies of such corrections.

The history of theoretical calculations of various contributions to the HFS of positronium is quite long. They can be represented by a series in powers and logarithms of the fine structure constant,

$$\Delta\nu = m\alpha^4 \left(n_0 + \alpha n_1 + \alpha^2 n_2 + \ldots\right). \tag{3}$$

The leading order $\mathcal{O}(m\alpha^4)$ HFS was obtained in [7–9],

$$n_0 = \frac{7}{12}. \tag{4}$$

The first correction was calculated in [10],

$$n_1 = -\frac{1}{\pi}\left(\frac{8}{9} + \frac{\ln 2}{2}\right). \tag{5}$$

The second correction consists of the following contributions:

$$m\alpha^6 n_2 = \Delta E_{g-2} + \Delta E_{\rm annih} + \Delta E_{\rm rad\ rec} + \Delta E_{\rm rec}. \tag{6}$$

The logarithmic contributions at this order, $\mathcal{O}(m\alpha^6 \ln\alpha)$, present in the annihilation $\Delta E_{\rm annih}$ and recoil corrections $\Delta E_{\rm rec}$, were found first [11,12]. ΔE_{g-2} arises from the anomalous magnetic moment of the electron at $\mathcal{O}(\alpha, \alpha^2)$. The three-, two- and one-photon annihilation contributions giving $\Delta E_{\rm annih}$ were found in [13–15], respectively. The non-annihilation radiative recoil contributions $\Delta E_{\rm rad\ rec}$ were studied in [16,17], while pure recoil corrections $\Delta E_{\rm rec}$ were discussed in [1,4,18].

For most of these contributions, several independent calculations were performed and an agreement was achieved. Moreover, the results for all contributions to HFS are known in the analytic form, with the exception of the pure recoil corrections $\Delta E_{\rm rec}$. By pure recoil corrections one understands those induced by diagrams where each virtual photon is created by electron and absorbed by positron, as shown in Fig. 1. For these effects, three independent calculations arrived at three different results [1,4,18]. The discrepancy has not been clarified so far and the resulting uncertainty in the theoretical prediction for the HFS of the ground state is much larger than the experimental error. The importance of clarifying this theoretical point has been emphasized by several authors. In this Letter we present an analytic calculation of these corrections. Numerically our result coincides with Ref. [1].

We start with a short description of the framework of our calculation, leaving the details to a separate publication. First, we calculate the on–shell scattering amplitude for non–relativistic ($v \ll 1$) particles to the necessary order. Along with the leading amplitude of a single Coulomb exchange, it includes the relative order $\mathcal{O}(v^2)$ Breit corrections and also higher order $\mathcal{O}(v^4, \alpha v^3)$ terms. By construction, it is gauge–invariant. Taken with a minus sign, this amplitude provides the effective potential for non–relativistic particles.

Further, we solve the Schrödinger equation incorporating corrections to the Coulomb potential using ordinary quantum mechanical perturbation theory. According to standard rules, we get the $\mathcal{O}(m\alpha^6)$ correction to the ground–state energy as a sum of the relativistic corrections to the tree level and one–loop scattering amplitude, and of the second order correction due to the Breit potential. Previously, this scheme was used for the calculation of the $\mathcal{O}(m\alpha^6 \ln\alpha)$ corrections to the levels of S-states [19] and of the $\mathcal{O}(m\alpha^6)$ corrections to the levels of P-states [20].

An implementation of this program leads to a divergent result. The reason for this divergence is well known – it is the application of the non–relativistic expansion in the relativistic momentum region, where it is not appropriate. The divergence is canceled if one includes additional short-distance or hard–scale contributions to the scattering amplitude, which cannot be obtained from the non–relativistic expansion.

To deal with the divergences in both the non–relativistic region and in the short–distance corrections we employ dimensional regularization. In the context of bound state calculations in QED this regularization scheme was used in Ref. [21], where the known results for $\mathcal{O}(m\alpha^5)$ corrections to positronium energy levels were successfully reproduced. The advantage of the dimensional regularization is that it makes the matching calculation of the low-scale effective theory and the complete QED extremely simple. To obtain the contribution of a given Feynman diagram to the Wilson coefficient of the $\delta(\vec{r})$-like effective operator, we only need to calculate that diagram for zero incoming momenta of all particles. We stress that this is only correct if one uses dimensional regularization for both infrared and ultraviolet divergences. With any other regularization scheme an additional calculation is required.

We find that in the sum of the short- and long–distance contributions the singularities $1/\epsilon = 2/(4-D)$ disappear and one arrives at a finite result.

Since the dimensional regularization is used throughout the Letter, we mention how the spinor algebra was treated. To calculate the shift in the ground state energy due to some operator $\mathcal{O}_i$ one has to calculate the trace of the form $\mathrm{Tr}\left[\Psi^\dagger \mathcal{O}_i \Psi\right]$, where Ψ is an appropriate wave function. The spinor parts of the relevant wave functions are:

$$\Psi_{\mathrm{P}} = \frac{1+\gamma_0}{2\sqrt{2}}\gamma_5, \qquad \Psi_{\mathrm{O}} = \frac{1+\gamma_0}{2\sqrt{2}}\boldsymbol{\gamma\xi},$$

for para- and orthopositronium states, respectively. In the latter case $\boldsymbol{\xi}$ is the polarization vector. The traces are calculated in the D-dimensional space. Since we always encounter an even number of γ_5's, we treat them as anticommuting. We also average over directions of the vector $\boldsymbol{\xi}$. In order to obtain corrections to the HFS we first calculate separately the traces for ortho- and parapositronium states and then take the difference of the two.

The problem is naturally divided up into the calculation of the matrix elements of the effective operators (soft contributions) and the Wilson coefficients of the effective $\delta(\vec{r})$-like operators (hard contributions) in the effective Hamiltonian:

$$\Delta E_{\mathrm{rec}} = \Delta_{\mathrm{soft}} E_{\mathrm{rec}} + \Delta_{\mathrm{hard}} E_{\mathrm{rec}}. \tag{7}$$

The calculation of Wilson coefficients is always done for the incoming and outgoing particles at rest. Both technically and conceptually, this is close to the calculation of the matching coefficient of the vector quark-antiquark current in QCD and its NRQCD counterpart, described e.g. in [22,23].

This technique is remarkably useful for the so–called radiative recoil corrections to the HFS, where one of the three exchanged photons is created and absorbed by the same particle, as shown in Fig. 2. It is sufficient to calculate the corresponding integrals exactly at the threshold in dimensional regularization, since there are no non–relativistic contributions to the radiative recoil corrections and no matching is required. Performing this calculation we obtain:

$$\Delta E_{\mathrm{rad\ rec}} = m\alpha^6 \left(\frac{\zeta(3)}{2\pi^2} + \frac{4}{3}\ln 2 - \frac{79}{48} + \frac{41}{36\pi^2} \right). \tag{8}$$

This result is in complete agreement with the analytic result published previously [17].

Applying the same technique to obtain the hard–scale contribution to the recoil corrections ΔE_{rec} we obtain:[1]

$$\Delta_{\mathrm{hard}} E_{\mathrm{rec}} = \frac{\pi\alpha^3}{3m^2}|\psi_d(0)|^2 \left(-\frac{1}{\epsilon} + 4\ln m - \frac{51\zeta(3)}{\pi^2} + \frac{10}{\pi^2} - 6\ln 2 \right). \tag{9}$$

[1]We neglect factors $\Gamma^2(1+\epsilon)$ and $(4\pi)^{2\epsilon}$ which do not contribute to the final, finite result.

In the above equation $\psi_d(0)$ stands for the value at the origin of the ground state solution of the d–dimensional Schrödinger equation.

The calculation of the soft scale contributions requires the treatment of the relativistic corrections to the tree level and one-loop scattering amplitudes, as well as the second iteration of the Breit potential. The main difficulty associated with this calculation is that it should be done in $d = 3 - 2\epsilon$ dimensions, thus necessarily spoiling some simplifying features of the Coulomb problem in three dimensions. Still, the calculation is feasible. Since the non–relativistic Hamiltonian is only singular for $r \to 0$, it turns out possible to extract this divergence in the form $|\psi_d(0)|^2/\epsilon$, without solving the Schrödinger equation in d-dimensions. Our final result for all non–relativistic contributions reads

$$\Delta_{\rm soft} E_{\rm rec} = \frac{\pi\alpha^3}{3m^2} |\psi_d(0)|^2 \left(\frac{1}{\epsilon} - 4\ln(m\alpha) + \frac{331}{18} \right). \tag{10}$$

In the sum of the hard and non-relativistic contributions, Eqs. (9,10), the $1/\epsilon$ divergences disappear and we can take the limit $\epsilon \to 0$ in the sum. We thus arrive at the final result for the recoil corrections to the HFS of the positronium ground state:

$$\Delta E_{\rm rec} = \Delta_{\rm hard} E_{\rm rec} + \Delta_{\rm soft} E_{\rm rec} = m\alpha^6 \left(-\frac{1}{6}\ln\alpha + \frac{331}{432} - \frac{\ln 2}{4} - \frac{17\zeta(3)}{8\pi^2} + \frac{5}{12\pi^2} \right). \tag{11}$$

Numerically this is $\Delta E_{\rm rec} = m\alpha^6 \left(-\frac{1}{6}\ln\alpha + 0.37632\right)$ which is in excellent agreement with Ref. [1], where for the non-logarithmic part of the correction a number 0.3767(17) was obtained. In view of the fact that in Ref. [1] a different regularization was used, this agreement gives us confidence in the correctness of the result[2].

The recoil correction was the last correction to positronium bound state HFS not known analytically. Having obtained its value (Eq. (11)), we are now in position to present the final analytic result for the HFS of the positronium ground state including $\mathcal{O}(m\alpha^6)$ terms:

$$\begin{aligned} E(1^3S_1) - E(1^1S_0) = m\alpha^4 \Bigg\{ & \frac{7}{12} - \frac{\alpha}{\pi}\left(\frac{8}{9} + \frac{1}{2}\ln 2\right) \\ & + \frac{\alpha^2}{\pi^2}\left[-\frac{5}{24}\pi^2 \ln\alpha + \frac{1367}{648} - \frac{5197}{3456}\pi^2 + \left(\frac{221}{144}\pi^2 + \frac{1}{2}\right)\ln 2 - \frac{53}{32}\zeta(3) \right] \Bigg\}. \end{aligned} \tag{12}$$

Numerically this corresponds to $\Delta\nu = 203\ 392.899$ MHz, if we use the central values for m and α, given after Eq.(2).

To arrive at the final prediction for the HFS splitting of the positronium ground state, one should try to quantify the theoretical error. The errors caused by the uncertainties in the fine structure constant and the electron mass are ~ 0.003 and 0.07 MHz, respectively. The main uncertainty comes from the unknown higher order effects. Though formally $m\alpha^7 \sim 0.1$ MHz, the leading $\mathcal{O}(m\alpha^7 \ln^2\alpha)$ terms contribute -0.92 MHz to the HFS [25]. Therefore, it remains

[2]When this work was completed, we were informed [24] about an independent numerical calculation of the recoil corrections. Though that work is still in progress, its preliminary results seem to coincide with the results of Ref. [1] and of the present work with rather good accuracy.

very important to calculate the remaining, non-leading terms in $\mathcal{O}(m\alpha^7)$. In this context we note that the complete $\mathcal{O}(m\alpha^6)$ correction, including the $m\alpha^6 \ln\alpha$ term, gives a shift of 11.79 MHz, whereas the term $m\alpha^6 \ln\alpha$ alone contributes 19.12 MHz. We see that an estimate of the complete correction based on the $m\alpha^6 \ln(\alpha)$ approximation would not be accurate.

At the moment the best we can do is to take the leading log contribution $\mathcal{O}(m\alpha^7 \ln^2\alpha)$ as an estimate of the higher orders corrections to HFS and thus attribute ~ 1 MHz uncertainty to the theoretical prediction. Combining this theoretical uncertainty with Eq. (12), we obtain the theoretical estimate for the HFS of the ground state of the positronium:

$$\Delta\nu_{\mathrm{theory}} = 203\;392(1)\ \mathrm{MHz}. \tag{13}$$

Compared to the experimental results Eq. (1,2) we observe a significant deviation of the order of $3-4$ experimental errors. We look forward to future improved measurements of positronium HFS and their confrontation with QED.

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FIGURES

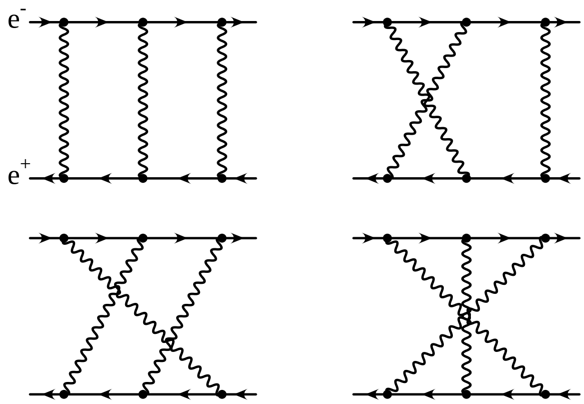

FIG. 1. Feynman diagrams representing pure recoil corrections to positronium HFS.

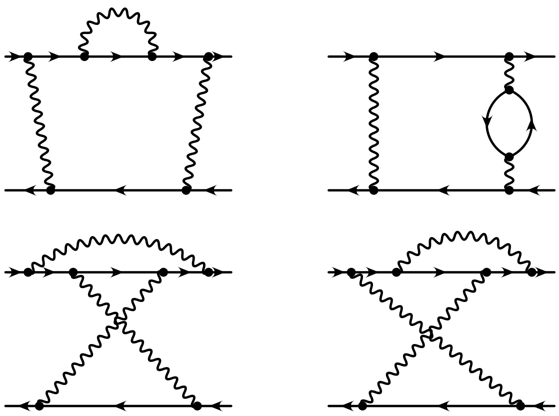

FIG. 2. Examples of radiative recoil corrections to positronium HFS.