BNL-HET-98/44, TTP 99-03, hep-ph/9901394

Positronium S state spectrum: analytic results 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

(January 1999)

Abstract

We present an analytic calculation of the $\mathcal{O}(m\alpha^6)$ recoil and radiative recoil corrections to energy levels of positronium nS states and their hyperfine splitting. A complete analytic formula valid to $\mathcal{O}(m\alpha^6)$ is given for the spectrum of S states. Technical aspects of the calculation are discussed in detail. Theoretical predictions are given for various energy intervals and compared with experimental results.

PACS numbers: 36.10.Dr, 06.20.Jr, 12.20.Ds, 31.30.Jv

---

*e-mail: czar@quark.phy.bnl.gov

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

‡e-mail: yelkhovsky@inp.nsk.su

I. INTRODUCTION

Spectroscopy of positronium (Ps) provides a sensitive test of bound state theory based on the Quantum Electrodynamics (QED). Because of the small mass of electron and positron, the effects of strong and weak interactions are negligible compared with the accuracy of present 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. Tests of the QED predictions are made possible by the very high experimental accuracy of positronium spectroscopy [1].

The gross spectrum of positronium is well described by the Schrödinger equation with the Coulomb potential. Energy levels are

$$E(n) = -\frac{m\alpha^2}{4n^2}, \tag{1}$$

where n is the principal quantum number. For the purpose of interpreting modern experiments the precision of Eq. (1) is insufficient. Corrections to the energy levels can in part be described by the Quantum Mechanics; however, for a complete description one has to resort to the Quantum Field Theory (QFT). Unfortunately, an application of the QFT to the bound states is difficult and special methods have to be devised [2–5].

Various approaches to bound state calculations have been reviewed e.g. in [6]. Here we focus on a method close to the so–called Non-Relativistic Quantum Electrodynamics (NRQED) [5], which is an effective field theory based on the QED, for small energies and momenta. Eq. (1) implies that the characteristic velocity of the electron and positron in positronium is of the order of the fine structure constant $\alpha \ll 1$. It is appropriate to apply a non-relativistic approximation to this system.

Recently much progress has been achieved in the framework of non-relativistic effective theories, mainly by employing dimensional regularization. It has been shown [7] that this regularization procedure permits an exact separation of effects arising at various characteristic energy scales. Using that method, which we will call dimensionally regularized NRQED (NRQED_ϵ) the complete energy spectrum of Ps has been reproduced to order $m\alpha^5$ [8]. More recently, we have computed $m\alpha^6$ corrections to the hyperfine splitting (HFS) of the Ps ground state [9], confirming one of previously obtained numerical results [10]. In the present paper we generalize that result to all S states, confirming [11], and compute also their spin independent shift at $\mathcal{O}(m\alpha^6)$ (obtained numerically in [11]).

It is convenient to describe the energy of an nS state of Ps by dividing it up into the spin–averaged part and a part dependent on the total Ps spin (hyperfine splitting):

$$E(J,n) = E_{\text{aver}}(n) + \boldsymbol{s}_+\boldsymbol{s}_- E_{\text{hfs}}(n), \tag{2}$$

where J is the total spin value of the Ps and $\boldsymbol{s}_\pm$ are the spins of the electron and positron, respectively. One finds:

$$\begin{aligned} J=1 \quad &(\text{triplet state}): \qquad \boldsymbol{s}_+\boldsymbol{s}_- = +\frac{1}{4}, \\ J=0 \quad &(\text{singlet state}): \qquad \boldsymbol{s}_+\boldsymbol{s}_- = -\frac{3}{4}. \end{aligned} \tag{3}$$

Both the spin–averaged energy and the hyperfine splitting can be represented by series in powers and logarithms of the fine structure constant. In the lowest order $E_{\rm aver}(n) = E(n)$ is given by Eq. (1), and $E_{\rm hfs}(n) = \mathcal{O}(m\alpha^4)$.

To order $m\alpha^5$ the results for $E_{\rm aver}$ and $E_{\rm hfs}$ were found in [12–14]. Those corrections have several sources: electron and positron charge radii and anomalous magnetic moments, vacuum polarization, two-photon exchange, two-photon annihilation and one-loop correction to the single-photon annihilation.

Current accuracy of high precision experiments requires a complete calculation of the $\mathcal{O}(m\alpha^6)$ corrections $\Delta E_{\rm aver}$ and $\Delta E_{\rm hfs}$.

The most precisely measured property of positronium is the ground state HFS, i.e. the energy difference between the two lowest states with total spin 1 and 0. Two best experimental values are

$$\Delta\nu \equiv E(1^3S_1) - E(1^1S_0) = 203\ 387.5(1.6)\ \text{MHz}, \tag{4}$$

found in [15,16] and

$$\Delta\nu = 203\ 389.10(0.74)\ \text{MHz}, \tag{5}$$

obtained in [17]. Another quantity of the experimental interest is the energy difference of 2^3S_1 and 1^3S_1 states [18]:

$$E(2^3S_1) - E(1^1S_1) = 1\ 233\ 607\ 216.4(3.2)\ \text{MHz}. \tag{6}$$

The absolute accuracy of this measurement is clearly less impressive than that of the hyperfine splitting. However, since $m\alpha^6 = 18.658$ MHz, a complete calculation of the energy levels at this order is warranted.

At order $m\alpha^6$ both $\Delta E_{\rm aver}$ and $\Delta E_{\rm hfs}$ can be written as

$$\Delta E = \Delta E_{\rm rad} + \Delta E_{\rm annih} + \Delta E_{\rm rad\ rec} + \Delta E_{\rm rec}. \tag{7}$$

The logarithmic contributions at this order, $\mathcal{O}(m\alpha^6 \ln\alpha)$, present in the annihilation $\Delta E_{\rm annih}$ and recoil $\Delta E_{\rm rec}$ corrections, were found first [19,20]. $\Delta E_{\rm rad}$ arises from the radiative corrections to the Breit potential at $\mathcal{O}(\alpha, \alpha^2)$ [21,22]. The three, two, and one-photon annihilation contributions giving $\Delta E_{\rm annih}$ were found in [23], [24], and [25,26], respectively. The non-annihilation radiative recoil contributions $\Delta E_{\rm rad\ rec}$ were calculated in [27,28], while pure recoil corrections $\Delta E_{\rm rec}$ were obtained in [10,5,29] for the HFS and in [11] for $E_{\rm aver}$.

In this paper we present an analytic calculation of the recoil and radiative recoil corrections, $\Delta E_{\rm rad}$ and $\Delta E_{\rm rad\ rec}$, to energy levels of arbitrary nS positronium states. The rest of this paper is organized as follows: in Section II we discuss our method in general terms. Section III is devoted to the calculation of the HFS. Many technical details of this calculation are discussed there. In Section IV we present a calculation of the average energy $E_{\rm aver}$. It is very similar to HFS, except that some additional operators contribute. Also the $\mathcal{O}(m\alpha^6)$ radiative recoil corrections are discussed. Our results are summarized in Section VI, where also an overview of the theoretical and experimental situation is given and a complete analytic formula for the nS energy levels to order $m\alpha^6$ is presented.

II. FRAMEWORK OF THE CALCULATION

Before getting into details, let us describe the general framework of our calculation of the $\mathcal{O}(m\alpha^6)$ corrections to energy levels.

First, we calculate an on–shell scattering amplitude for non-relativistic ($v \ll 1$) particles to the needed order (the fact that $v \sim \alpha$ in Ps serves as a counting rule for contributions of various operators). In addition to the leading, single Coulomb exchange, this includes the relative $\mathcal{O}(v^2)$ Breit corrections and also higher order $\mathcal{O}(v^4, \alpha v^3)$ terms. This non-relativistic amplitude is gauge invariant, and taken with a minus sign provides the potential for non–relativistic particles.

Next, we use the ordinary quantum mechanical perturbation theory to find the corrections due to that potential; as unperturbed states we use the solutions of the Schrödinger equation with the Coulomb potential. We get the $\mathcal{O}(m\alpha^6)$ correction to energy levels as the sum of the first order correction due to $\mathcal{O}(v^4, \alpha v^3)$ perturbation and of the second order correction due to the Breit Hamiltonian. Previously, this scheme was used for the calculation of the $\mathcal{O}(m\alpha^6 \ln \alpha)$ corrections to the levels of S-states [30] and of the $\mathcal{O}(m\alpha^6)$ corrections to the levels of P-states [31,32].

In the present calculation the result of the non-relativistic calculation is divergent. This is because also the short-distance ("hard") corrections contribute. They arise from virtual momenta regions of the order of electron mass and cannot be obtained from the non–relativistic expansion.

Our calculation is performed in the spirit of NRQED. We apply dimensional regularization, which offers technical advantages over more common techniques, based on the introduction of an intermediate cut-off to separate the relativistic and non–relativistic momentum regions. Dimensional regularization makes the matching of the low-scale effective theory and the complete QED extremely simple. We find that in the sum of the short and long–distance contributions the singularities in the parameter[1] ϵ disappear and one arrives at a finite result.

The spinor algebra in dimensional regularization requires some comments. In order to obtain the energy shift due to an 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

$$\Psi_P = \frac{1+\gamma_0}{2\sqrt{2}}\gamma_5, \qquad \Psi_O = \frac{1+\gamma_0}{2\sqrt{2}}\boldsymbol{\gamma}\boldsymbol{\xi},$$

for para and orthopositronium states, respectively. In the latter case, $\boldsymbol{\xi}$ is the polarization vector (we average over its directions). The traces are calculated in a standard way in the D-dimensional space. One encounters only even numbers of γ_5 matrices, and we treat them as anticommuting.

Since the matrix elements involve the positronium wave function, it is easiest to calculate for the ground state ($n = 1$). However, once the corrections to the ground state have been found, there is a convenient way of finding them for excited states, with an arbitrary value

---

[1]Throughout the paper, we use the following notations: $D = 4 - 2\epsilon$ and $d = 3 - 2\epsilon$.

of the principal quantum number n. Only the non-relativistic contributions have a non-trivial dependence on n. Their computation in dimensional regularization would be difficult. However, this task is simplified using other regularizations. Finally, we eliminate the cut-off dependence by requiring that for $n = 1$ the result matches the formula we found for $n = 1$. The freedom of choosing the regularization scheme simplifies considerably this part of the calculation.

III. HFS OF THE POSITRONIUM GROUND STATE

In this Section we present a calculation of the recoil corrections to the Ps ground state, $\Delta_{\rm rec} E_{\rm hfs}$. It is given as a sum of soft (non-relativistic) Eq. (11) and hard Eq. (70) scales:

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

Those two groups of contributions are computed, respectively, in Sections III A and III B. Further, in Section III C, we find a generalization of this result for radially excited states (arbitrary n):

$$\Delta_{\rm rec} E_{\rm hfs}(n) = \frac{m\alpha^6}{n^3} \left[-\frac{1}{6} \left(\ln \frac{\alpha}{n} + \Psi(n) + \gamma_E \right) + \frac{7}{12n} - \frac{1}{2n^2} + \frac{295}{432} - \frac{\ln 2}{4} - \frac{17\zeta(3)}{8\pi^2} + \frac{5}{12\pi^2} \right], \quad (9)$$

where $\Psi(n)$ is the logarithmic derivative of the Γ-function and $\gamma_E \simeq 0.577216$ is the Euler constant. The n dependence of this result and its numerical value at $n = 1$ are in agreement with [10].

A. Soft scale contributions

We divide up the non-relativistic contributions to HFS into 6 parts: tree level Coulomb and magnetic photon exchanges, retardation, one-loop operators, and second iteration of Breit Hamiltonian which includes intermediate S and D wave states:

$$\Delta_{\rm nonrel} E_{\rm hfs} = \Delta_{\rm C} E_{\rm hfs} + \Delta_{\rm M} E_{\rm hfs} + \Delta_{\rm ret} E_{\rm hfs} + \Delta_{\rm 1-loop} E_{\rm hfs} + \Delta_{\rm S} E_{\rm hfs} + \Delta_{\rm D} E_{\rm hfs}. \quad (10)$$

These partial results, given in Eqs. (21, 26, 33, 35, 51, 67) add up to [9]

$$\Delta_{\rm nonrel} E_{\rm hfs} = \frac{\pi\alpha^3}{3m^2} \psi^2(0) \left(\frac{1}{\epsilon} - 4 \ln(m\alpha) + \frac{331}{18} \right). \quad (11)$$

In the remainder of this Section we discuss in detail how these contributions are calculated.

According to standard procedure [33] we identify the on–shell scattering amplitude, taken with the minus sign, with the matrix element of an interaction operator in the momentum representation. The soft scale contributions are calculated using the time-independent "old-fashioned" perturbation theory and the Coulomb gauge. Since this technique is not very common, let us recall its basic ingredients. Exchange of a Coulomb or magnetic photon is described, respectively, by $-4\pi\alpha/\boldsymbol{q}^2$ or $-4\pi\alpha\alpha_i \otimes \alpha_j(\delta_{ij} - q_i q_j/\boldsymbol{q}^2)/2|\boldsymbol{q}|$. In the latter case, the denominator $2|\boldsymbol{q}|$ arises from the magnetic photon's phase space element.

An intermediate state introduces the factor $(E - E_{\rm int} + i0)^{-1}$, where $E_{\rm int}$ is the energy of the intermediate state and E is the total energy of the process.

Dirac spinors are

$$u(\boldsymbol{p}) = \sqrt{\frac{2\omega_p}{\omega_p + m}}\Lambda_+(\boldsymbol{p})w, \tag{12}$$

where w denotes the four-spinor of a particle at rest; projectors on the positive and negative electron energy states are given by

$$\Lambda_\pm(\boldsymbol{p}) = \frac{1}{2}\left(1 \pm \frac{\boldsymbol{\alpha p} + \beta m}{\omega_p}\right), \qquad \omega_p = \sqrt{\boldsymbol{p}^2 + m^2}.$$

In an expression for the potential the projector Λ_- contributes an additional minus sign.

We begin with the contributions of the tree level effective operators, describing an exchange of the Coulomb or magnetic quanta. The tree level operators, relevant for the $\mathcal{O}(m\alpha^6)$ calculation of the HFS, arise as $\mathcal{O}(v^2)$ corrections to the Breit potential.

1. Tree-level Coulomb photon exchange

For the HFS we need the spin-dependent part of the $\mathcal{O}(v^4)$ correction to the Coulomb exchange (see Eq. (A2)):

$$V_C(\boldsymbol{p}', \boldsymbol{p}) = -\frac{\pi\alpha}{16m^4}\frac{[\boldsymbol{\sigma p}, \boldsymbol{\sigma p}'][\boldsymbol{\sigma}'\boldsymbol{p}, \boldsymbol{\sigma}'\boldsymbol{p}']}{\boldsymbol{q}^2}. \tag{13}$$

To calculate the spin part of the matrix element, we take the trace with d-dimensional sigma–matrices and find (the factor $1/d$ in Eq. (14) arises from the average over directions of the o-Ps polarization vector)

$$\frac{1}{2d}\mathrm{Tr}\left(\sigma_i[\boldsymbol{\sigma p}, \boldsymbol{\sigma p}']\sigma_i[\boldsymbol{\sigma}'\boldsymbol{p}', \boldsymbol{\sigma}'\boldsymbol{p}]\right) = 4\frac{d-4}{d}\left[\boldsymbol{p}'^2\boldsymbol{p}^2 - (\boldsymbol{p}'\boldsymbol{p})^2\right], \tag{14}$$

$$\frac{1}{2}\mathrm{Tr}\left([\boldsymbol{\sigma p}, \boldsymbol{\sigma p}'][\boldsymbol{\sigma}'\boldsymbol{p}', \boldsymbol{\sigma}'\boldsymbol{p}]\right) = 4\left[\boldsymbol{p}'^2\boldsymbol{p}^2 - (\boldsymbol{p}'\boldsymbol{p})^2\right], \tag{15}$$

respectively for ortho and parapositronium. Using

$$\boldsymbol{p}'^2\boldsymbol{p}^2 - (\boldsymbol{p}'\boldsymbol{p})^2 = (\boldsymbol{p}'\boldsymbol{p})\,\boldsymbol{q}^2 - (\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p}), \tag{16}$$

and noting that the average value of $\boldsymbol{p}'\boldsymbol{p}$ in an S–state vanishes, we obtain the contribution of $V_C(\boldsymbol{p}, \boldsymbol{p}')$ to the ground state HFS:

$$\Delta_C E_{\rm hfs} = \langle V_C(\boldsymbol{p}', \boldsymbol{p})\rangle\Big|^{S=1}_{S=0} = -\frac{\pi\alpha}{dm^4}\left\langle\frac{(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{\boldsymbol{q}^2}\right\rangle. \tag{17}$$

In Eq. (17) the matrix element is to be calculated over the ground state wave function in d dimensions:

$$\langle f(\boldsymbol{p},\boldsymbol{p}')\rangle \equiv \int \frac{\mathrm{d}^d p}{(2\pi)^d}\frac{\mathrm{d}^d p'}{(2\pi)^d}\phi(p)\phi(p')f(\boldsymbol{p},\boldsymbol{p}').$$

Let us briefly explain how the integral in Eq. (17) is calculated. Although the integrand does not look complicated, the difficulty is that the exact form of the wave function $\psi(r)$ in d dimensions is not known. Fortunately, it turns out to be unnecessary.

There are two alternative ways to calculate this integral. One is to transform it to the coordinate space. A divergence arises at $r = 0$ and in the final result is proportional to the d-dimensional $\psi(0)$; the remaining, finite part can be easily calculated in $d = 3$.[2]

In the alternative approach we use the fact that the wave function in Eq. (17) satisfies the d-dimensional Schrödinger equation, which in the momentum space reads[3]

$$\phi(p) = \frac{4\pi\alpha m}{\boldsymbol{p}^2 - mE}\int \frac{\mathrm{d}^d k}{(2\pi)^d}\frac{\phi(k)}{(\boldsymbol{p}-\boldsymbol{k})^2}. \tag{18}$$

Using this equation we rewrite the integral in Eq. (17) as

$$\left\langle \frac{(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{\boldsymbol{q}^2}\right\rangle_{\boldsymbol{p},\boldsymbol{p}'} = \left\langle \frac{(4\pi\alpha m)^2(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{(\boldsymbol{p}^2-mE)(\boldsymbol{p}-\boldsymbol{k})^2\boldsymbol{q}^2(\boldsymbol{p}'^2-mE)(\boldsymbol{p}'-\boldsymbol{k}')^2}\right\rangle_{\boldsymbol{k},\boldsymbol{k}'}, \tag{19}$$

where the integration over $\boldsymbol{p}$, $\boldsymbol{p}'$, as well as $\boldsymbol{k}$, $\boldsymbol{k}'$, in the last expression is understood. The integral over $\boldsymbol{p}$ and $\boldsymbol{p}'$ receives a divergent contribution only from the region where $\boldsymbol{p}$ and $\boldsymbol{p}'$ simultaneously become infinite. Therefore, a single subtraction is sufficient to make this integral finite. It is convenient to subtract from (19) the following expression:

$$\left\langle \frac{(4\pi\alpha m)^2(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{(\boldsymbol{p}^2-mE)^2\boldsymbol{q}^2(\boldsymbol{p}'^2-mE)^2}\right\rangle_{\boldsymbol{k},\boldsymbol{k}'}. \tag{20}$$

After the subtraction is done, two nice features emerge. In Eq. (20) the integration over $\boldsymbol{k}, \boldsymbol{k}'$ factorizes and leads to $\psi^2(0)$ times a two-loop integral, which can be easily calculated for arbitrary d. On the other hand, the difference between the last integral in Eq. (19) and the integral in Eq. (20) is finite and can be calculated for $d = 3$ using the explicit form of the wave function,

$$\phi(p) = \sqrt{\frac{\pi\alpha m}{2}}\frac{2m^2\alpha^2}{(\boldsymbol{p}^2-mE)^2}, \qquad E = -\frac{m\alpha^2}{4}.$$

We note that the counterterm (20) is constructed in such a way that the above mentioned difference vanishes for the ground state. This can be easily seen by integrating over $\boldsymbol{k}, \boldsymbol{k}'$ in

---

[2]In general, also the derivative of the wave function at the origin, $\mathrm{d}\psi(r)/\mathrm{d}r$ at $r = 0$, can appear in the divergent part of the integral. However, the Schrödinger equation relates it to $\psi(0)$.

[3]This equation corresponds to a summation of an infinite number of ladder diagrams in the Coulomb gauge. For consistency it is essential to use here dimensional regularization in the same way as in the other loop integrations.

Eq. (20) and using the fact that the $\boldsymbol{p}, \boldsymbol{p}'$-dependent terms in the denominator of Eq. (20) coincide (up to a normalization factor) with the three-dimensional ground state wave functions in the momentum representation.

Both methods described above lead to the same result. For $d = 3 - 2\epsilon$ we obtain:[4]

$$\Delta_C E_{\rm hfs} = \frac{\pi\alpha^3}{24m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) - \frac{1}{3}\right), \tag{21}$$

where $\psi(0)$ is the value of the d-dimensional ground state wave function at the origin.

2. Tree-level exchange of a magnetic photon

We now consider the correction caused by the tree level exchange of a magnetic photon, Fig. 1(b). We neglect the energy dependence in the photon propagator; it will be restored in the following Section, where we discuss retardation effects. The relevant potential is obtained from Eq. (A4):

$$V_M(\boldsymbol{p}', \boldsymbol{p}) = \frac{\pi\alpha}{16m^4}\frac{[\boldsymbol{\sigma}'\boldsymbol{q}, \sigma'^i]}{\boldsymbol{q}^2}\left\{\left[\boldsymbol{\sigma}\frac{\boldsymbol{p}'+\boldsymbol{p}}{2}, \sigma^i\right]\left(\boldsymbol{p}'^2 - \boldsymbol{p}^2\right) + [\boldsymbol{\sigma q}, \sigma^i]\left(\boldsymbol{p}^2 + \boldsymbol{p}'^2\right)\right\} + (\boldsymbol{\sigma} \leftrightarrow \boldsymbol{\sigma}'). \tag{22}$$

Contribution of this interaction to the ground state HFS is

$$\Delta_M E_{\rm hfs} = \langle V_M(\boldsymbol{p}', \boldsymbol{p})\rangle\Big|_{S=0}^{S=1} = -2\frac{d-1}{d}\frac{\pi\alpha}{m^4}\left\langle \boldsymbol{p}^2 + \boldsymbol{p}'^2 + \frac{\left(\boldsymbol{p}^2 - \boldsymbol{p}'^2\right)^2}{2\boldsymbol{q}^2}\right\rangle. \tag{23}$$

In $d = 3$ this matrix element is linearly divergent. To demonstrate how we treat linear divergences let us consider the $\boldsymbol{p}^2$ term on the RHS of the above equation:

$$\left\langle \boldsymbol{p}^2 \right\rangle = \psi(0)\int\frac{{\rm d}^d p}{(2\pi)^d}\boldsymbol{p}^2\phi(p) = m\psi(0)\int\frac{{\rm d}^d p}{(2\pi)^d}\left(E\phi(p) + \int\frac{{\rm d}^d k}{(2\pi)^d}\frac{4\pi\alpha}{(\mathbf{p}-\mathbf{k})^2}\phi(k)\right). \tag{24}$$

Shifting the integration variable $\boldsymbol{p} \to \boldsymbol{p} + \boldsymbol{k}$ we find that the $\boldsymbol{p}$-integral in the last term is scale-less. In dimensional regularization such integrals vanish. The first term in Eq. (24) is finite in three dimensions. We obtain

$$\left\langle \boldsymbol{p}^2 \right\rangle = mE\psi^2(0). \tag{25}$$

Applying a similar procedure to the last term in Eq. (23) we find the contribution of $V_M(\boldsymbol{p}', \boldsymbol{p})$ to the ground state HFS:

$$\Delta_M E_{\rm hfs} = \frac{\pi\alpha}{m^4}\left[m^2\alpha^2\psi^2(0) - 4\frac{d-1}{d}\left\langle\frac{(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{\boldsymbol{q}^2}\right\rangle\right] = \frac{\pi\alpha^3}{3m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) + \frac{5}{3}\right). \tag{26}$$

---

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

3. Retardation effects

Let us now consider the retardation effects, which mean that the magnetic photon emitted by the electron propagates for a finite amount of time before being absorbed by the positron. During this time, the electron and positron can interact by several Coulomb exchanges (Fig. 1(c,d,e)). To calculate the influence of these effects on the HFS, it is sufficient to take the spin-dependent parts of the current $\boldsymbol{j}(\boldsymbol{p}',\boldsymbol{p}) = u^+(\boldsymbol{p}')\boldsymbol{\alpha} u(\boldsymbol{p})$ in the leading nonrelativistic approximation:

$$\boldsymbol{j}(\boldsymbol{p}',\boldsymbol{p}) \to \frac{[\boldsymbol{\sigma q},\boldsymbol{\sigma}]}{4m}. \tag{27}$$

The scattering operator describing the retardation effects is nonlocal both in space and time:

$$-A_{\rm ret} = -\alpha \int \frac{\mathrm{d}^d k}{(2\pi)^d} \exp\left(-i\boldsymbol{k r}_p\right) \frac{[\boldsymbol{\sigma' k},\sigma_i']}{4m} \frac{4\pi}{2k} \frac{\delta_{ij} - \frac{k_i k_j}{\boldsymbol{k}^2}}{k + H - E} \frac{[\boldsymbol{\sigma k},\sigma_j]}{4m} \exp\left(i\boldsymbol{k r}_e\right) + \mathrm{H.c.} \tag{28}$$

Here we assume that the magnetic photon with the momentum $\boldsymbol{k}$ is emitted by the electron at a point $\boldsymbol{r}_e$ and absorbed by the positron at a point $\boldsymbol{r}_p$. Between those moments, the evolution of the system "positronium + photon" is governed by the propagator $4\pi(\delta_{ij} - k_i k_j/k^2)/(2k)(k + H - E)^{-1}$, H being the Hamiltonian of the nonrelativistic positronium slowly moving due to recoil. In the region of interest $k \gg E$ and one can expand the amplitude (28) over the powers of $(H - E)/k \sim \alpha$. The zeroth term of this expansion is the spin–dependent part of the Breit potential,

$$-A_{\rm ret}^{(0)}(\boldsymbol{q}) = -\frac{\pi\alpha}{4m^2} \frac{[\boldsymbol{\sigma' q},\sigma'^i][\boldsymbol{\sigma q},\sigma^i]}{\boldsymbol{q}^2}. \tag{29}$$

We need the second order term:

$$V_{\rm ret} = \alpha \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{4\pi}{2\boldsymbol{k}^4} \frac{[\boldsymbol{\sigma' k},\sigma'^i]}{4m} [H, \exp\left(-i\boldsymbol{k r}_p\right)][H, \exp\left(i\boldsymbol{k r}_e\right)] \frac{[\boldsymbol{\sigma k},\sigma^i]}{4m} + \mathrm{H.c.} \tag{30}$$

Only kinetic part of the Hamiltonian,

$$H_{\rm kin} = \frac{\boldsymbol{p}_e^2}{2m} + \frac{\boldsymbol{p}_p^2}{2m}, \tag{31}$$

has to be retained in the commutators. We find

$$V_{\rm ret} = \alpha \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{4\pi}{2\boldsymbol{k}^4} \frac{[\boldsymbol{\sigma' k},\sigma'^i]}{8m^2} (\boldsymbol{k}^2 + 2\boldsymbol{k p}_p) \exp\left(i\boldsymbol{k}(\boldsymbol{r}_e - \boldsymbol{r}_p)\right) (\boldsymbol{k}^2 + 2\boldsymbol{k p}_e) \frac{[\boldsymbol{\sigma k},\sigma^i]}{8m^2} + \mathrm{H.c.} \tag{32}$$

Transforming back to the relative coordinate $\boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_p$ and the relative momentum $\boldsymbol{p} = \boldsymbol{p}_e = -\boldsymbol{p}_p$, we get for the ground state HFS:

$$\Delta_{\rm ret} E_{\rm hfs} = \frac{\pi\alpha}{m^4} \left(\frac{m^2\alpha^2}{3}\psi^2(0) - 4\frac{d-1}{d} \left\langle \frac{(\boldsymbol{p'q})(\boldsymbol{qp})}{\boldsymbol{q}^2} \right\rangle \right) = \frac{\pi\alpha^3}{3m^2}\psi^2(0) \left(\frac{1}{\epsilon} - 4\ln(m\alpha) - \frac{1}{3} \right). \tag{33}$$

4. One-loop operators

Now we turn to the operators generated by one-loop diagrams. For the HFS the only contribution comes from the graph in Fig. 1(f), which describes the mixed Coulomb-magnetic exchange with a transition of one of the particles to a negative energy state. In other words, this corresponds to a creation of an additional electron-positron pair by the electric or magnetic field of the electron or positron.

Using Feynman rules for the time-independent perturbation theory, given at the beginning of this Section, we derive the corresponding potential:

$$V_{1-\text{loop}}(\boldsymbol{q}) = \frac{2\pi^2\alpha^2}{m^3}\int \frac{d^dk}{(2\pi)^d}\frac{[\boldsymbol{\sigma}(\boldsymbol{q}-\boldsymbol{k}),\sigma^i]}{(\boldsymbol{q}-\boldsymbol{k})^2}\frac{[\boldsymbol{\sigma'}\boldsymbol{k},\sigma'^i]}{\boldsymbol{k}^2}. \tag{34}$$

It induces the following correction to the ground state HFS (d-dimensional integration over $\boldsymbol{k}$ is implicitly assumed below)

$$\begin{aligned}
\Delta_{1-\text{loop}}E_{\text{hfs}} &= -2\frac{d-1}{d}\frac{\alpha^2}{m^3}\left\langle\frac{4\pi(\boldsymbol{p}'-\boldsymbol{k})}{(\boldsymbol{p}'-\boldsymbol{k})^2}\frac{4\pi(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p})^2}\right\rangle \\
&= -2\frac{d-1}{d}\frac{\alpha^2}{m^3}\left\langle\frac{\boldsymbol{p}'^2+\boldsymbol{p}^2}{2}\frac{4\pi}{(\boldsymbol{p}'-\boldsymbol{k})^2}\frac{4\pi}{(\boldsymbol{k}-\boldsymbol{p})^2}-\frac{4\pi p'^i}{(\boldsymbol{p}'-\boldsymbol{k})^2}\frac{4\pi p^i}{(\boldsymbol{k}-\boldsymbol{p})^2}\right\rangle \\
&= \frac{\pi\alpha}{m^4}\left\{\frac{m^2\alpha^2}{3}\psi^2(0)-8\frac{d-1}{d}\left\langle\frac{\boldsymbol{p}'^2\boldsymbol{p}^2}{\boldsymbol{q}^2}\right\rangle\right\} \\
&= -\frac{4\pi\alpha^3}{3m^2}\psi^2(0)\left(\frac{1}{\epsilon}-4\ln(m\alpha)-\frac{1}{3}\right).
\end{aligned} \tag{35}$$

5. Breit Hamiltonian

To complete the calculation of the soft scale contributions to the HFS we have to consider the second iteration of the Breit Hamiltonian. It is obtained by including the effects of tree level Coulomb and magnetic photon exchanges, as well as a correction to the kinetic energy. Using Eqs. (A2) and (A4) we find

$$U(\boldsymbol{p}',\boldsymbol{p}) = -\frac{\boldsymbol{p}^4}{4m^3}\delta(\boldsymbol{p}'-\boldsymbol{p})+\frac{\pi\alpha}{m^2}+\frac{4\pi\alpha}{m^2}\frac{(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})-(\boldsymbol{p}'\boldsymbol{p})\boldsymbol{q}^2}{\boldsymbol{q}^4}-\frac{\pi\alpha}{4m^2}\frac{[\boldsymbol{\sigma}\boldsymbol{q},\sigma^i][\boldsymbol{\sigma}'\boldsymbol{q},\sigma'^i]}{\boldsymbol{q}^2}. \tag{36}$$

In the position representation this Hamiltonian becomes

$$U(\boldsymbol{r},\boldsymbol{p}) = -\frac{\boldsymbol{p}^4}{4m^3}+\frac{d-1}{4m}\left\{\frac{\boldsymbol{p}^2}{m},C(r)\right\}+\frac{d\pi\alpha}{m^2}\delta(\boldsymbol{r})-\frac{1}{16m^2}\Big[[\boldsymbol{\sigma}\nabla,\sigma^i][\boldsymbol{\sigma}'\nabla,\sigma'^i],C(r)\Big], \tag{37}$$

where

$$C(r) \equiv -\frac{\alpha\Gamma(d/2-1)}{\pi^{d/2-1}r^{d-2}} \tag{38}$$

is the d–dimensional Coulomb potential.

6. Second iteration of the Breit Hamiltonian: S-wave

We consider first the contribution of the intermediate S–states. The S–wave part of the Breit Hamiltonian (37) reads

$$U_S(\boldsymbol{r},\boldsymbol{p}) = -\frac{\boldsymbol{p}^4}{4m^3} + \frac{d-1}{4m}\left\{\frac{\boldsymbol{p}^2}{m}, C(r)\right\} + \frac{d\pi\alpha}{m^2}\delta(\boldsymbol{r}) - \frac{\pi\alpha}{4dm^2}[\sigma_i,\sigma_j][\sigma_i',\sigma_j']\delta(\boldsymbol{r}). \tag{39}$$

It is convenient to divide up the calculation of the U_S contribution to the HFS into two parts and consider the first and the last two terms in Eq. (39) separately. We begin with the latter, which we denote by $\Delta_{S1}E_{\rm hfs}$:

$$\begin{aligned}\Delta_{S1}E_{\rm hfs} &= 8\frac{(d-1)(3d-2)}{d^2}\left(\frac{\pi\alpha}{m^2}\right)^2\left\langle\delta(\boldsymbol{r}')\sum_m{}'\frac{|m(\boldsymbol{r}')\rangle\langle m(\boldsymbol{r})|}{E-E_m}\delta(\boldsymbol{r})\right\rangle\\ &= 8\frac{(d-1)(3d-2)}{d^2}\left(\frac{\pi\alpha}{m^2}\right)^2\psi^2(0)\sum_m{}'\frac{|m(0)|^2}{E-E_m}.\end{aligned} \tag{40}$$

In three dimensions the last sum is ill-defined due to ultraviolet divergences in the zeroth and first terms of its expansion in α. We denote these singular terms by $G_0(0,0)$ and $G_1(0,0)$, respectively, and obtain

$$\Delta_{S1}E_{\rm hfs} = 8\frac{(d-1)(3d-2)}{d^2}\left(\frac{\pi\alpha}{m^2}\right)^2\psi^2(0)\left[-\frac{3m^2\alpha}{8\pi} + G_0(0,0) + G_1(0,0)\right]. \tag{41}$$

$G_0(0,0)$ and $G_1(0,0)$ are calculated in d dimensions,

$$\begin{aligned}G_0(0,0) &= -\int\frac{\mathrm{d}^dp}{(2\pi)^d}\frac{m}{\boldsymbol{p}^2-mE} = \frac{m^2\alpha}{8\pi},\\ G_1(0,0) &= -\int\frac{\mathrm{d}^dp'}{(2\pi)^d}\int\frac{\mathrm{d}^dp}{(2\pi)^d}\frac{m}{\boldsymbol{p}'^2-mE}\frac{4\pi\alpha}{\boldsymbol{q}^2}\frac{m}{\boldsymbol{p}^2-mE} = -\frac{m^2\alpha}{16\pi}\left(\frac{1}{\epsilon} - 4\ln(m\alpha) + 2\right),\end{aligned} \tag{42}$$

and one finds

$$\Delta_{S1}E_{\rm hfs} = -\frac{7\pi\alpha^3}{9m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) + \frac{115}{21}\right). \tag{43}$$

The contribution of the first two terms in Eq. (39) is calculated in the following way. We first write them as

$$-\frac{\boldsymbol{p}^4}{4m^3} + \frac{d-1}{4m}\left\{\frac{\boldsymbol{p}^2}{m}, C(r)\right\} = -\frac{1}{4m}\left[H^2 - d\{H, C(r)\} + (2d-1)C^2(r)\right], \tag{44}$$

where $H = \boldsymbol{p}^2/m + C(r)$ is the leading order Hamiltonian. Correction to the HFS induced by Eq. (44) reads

$$\Delta_{S2}E_{\rm hfs} = \frac{d-1}{d}\frac{\pi\alpha}{m^3}\left\langle\left[d\{H, C(r)\} - (2d-1)C^2(r)\right]G(\boldsymbol{r},\boldsymbol{r}')\delta(\boldsymbol{r}') + \mathrm{H.c.}\right\rangle. \tag{45}$$

We introduced here the reduced Green function

$$G(\boldsymbol{r},\boldsymbol{r}') = \sum_m{}' \frac{|m(\boldsymbol{r})\rangle\langle m(\boldsymbol{r}')|}{E-E_m}, \tag{46}$$

which satisfies the equation $(H-E)G(\boldsymbol{r},\boldsymbol{r}') = \psi(r)\psi(r') - \delta(\boldsymbol{r}-\boldsymbol{r}')$. Using obvious short-hand notations one can rewrite Eq. (45) as follows:

$$\begin{aligned}\Delta_{S2}E_{\rm hfs} = -\frac{2\pi\alpha}{3m^3}\Bigg\langle\Bigg(&6\alpha E\frac{1}{r}G + 3\frac{\alpha}{r}\psi(r)\psi(r') + 5\frac{\alpha^2}{r^2}(G-G_0)\\ &+\frac{3}{2}\frac{(d-1)(2d-1)}{d}C^2(r)G_0\Bigg)\delta(\boldsymbol{r}') + \text{H.c.}\Bigg\rangle,\end{aligned} \tag{47}$$

We dropped massless tadpoles and separated the contribution of G_0, which is the only one we have to calculate keeping $d\neq 3$. We find

$$\begin{aligned}\left\langle C^2 G_0\delta(\boldsymbol{r}') + \text{H.c.}\right\rangle &= \frac{8\pi\alpha}{m}\psi^2(0)G_1(0,0),\\ \left\langle\frac{\alpha}{r}G\delta(\boldsymbol{r}') + \text{H.c.}\right\rangle &= -\alpha\partial_\alpha\left\langle\delta(\boldsymbol{r})\right\rangle = -3\psi^2(0),\\ \left\langle\frac{\alpha}{r}\right\rangle &= -2E,\\ \left\langle\frac{1}{r^2}(G-G_0)\delta(\boldsymbol{r}') + \text{H.c.}\right\rangle &= -4m\psi^2(0).\end{aligned} \tag{48}$$

To obtain the last line we used the following equation:

$$G(r,0) - G_0(r,0) = \frac{m^2\alpha}{4\pi}e^{-\gamma r}\left(\ln(2\gamma r) + \gamma_E - \frac{5}{2} + \gamma r\right), \tag{49}$$

where $\gamma = m\alpha/2$. From Eq. (47) we now find

$$\Delta_{S2}E_{\rm hfs} = \frac{5\pi\alpha^3}{3m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) + \frac{88}{15}\right). \tag{50}$$

The sum of $\Delta_{S1}E_{\rm hfs}$ and $\Delta_{S2}E_{\rm hfs}$ gives the final result for the correction to the ground state HFS induced by the second iteration of the S-wave Breit Hamiltonian:

$$\Delta_S E_{\rm hfs} = \frac{8\pi\alpha^3}{9m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) + \frac{149}{24}\right). \tag{51}$$

7. Second iteration of the Breit Hamiltonian: D-wave

Because of the last term in Eq. (36) Breit Hamiltonian has non-vanishing matrix elements with $|\Delta L| = 2$. In our case this causes virtual transitions from the triplet S–state into D–states (transitions from the singlet state are forbidden by the total angular momentum conservation). Again, power counting shows that only the zeroth and the first order terms in the Green function expansion in α diverge in three dimensions. We first compute the remaining, higher order terms, which are finite for $d=3$.

The sum of those higher order terms can be written as

$$\Delta_D^{\text{h-o}} E_{\text{hfs}} = \langle U_D G_0 C G C G_0 U_D \rangle \,, \tag{52}$$

where

$$U_D = \frac{\alpha}{4m^2} \frac{3(\boldsymbol{\sigma n})(\boldsymbol{\sigma' n}) - \boldsymbol{\sigma\sigma'}}{r^3} \tag{53}$$

is the $|\Delta L| = 2$ part of the Breit Hamiltonian in three dimensions, G and G_0 are defined in the previous Section, and $C = -\alpha/r$ is the Coulomb potential.

The correction to the ground–state wave function,

$$\delta_0\psi(r) = G_0 U_D \psi(r), \tag{54}$$

which appears in Eq. (52), satisfies an inhomogeneous Schrödinger equation:

$$\left(E - \frac{\boldsymbol{p}^2}{m}\right) \delta_0\psi(r) = U_D\psi(r). \tag{55}$$

Solving this equation for $\delta_0\psi(r)$ we obtain

$$\Delta_D^{\text{h-o}} E_{\text{hfs}} = 8\delta_{S1} \left(\frac{\alpha^2}{24}\right)^2 \left\langle \frac{1}{mr^2} G_D(r, r_1) \frac{1}{mr_1^2} \right\rangle, \tag{56}$$

where $G_D(r, r_1)$ is the D-wave part of the Green function G, and the factor $8\delta_{S1}$ arises from

$$\left\langle \left[\boldsymbol{\sigma\sigma'} - 3(\boldsymbol{\sigma n})(\boldsymbol{\sigma' n})\right]^2 \right\rangle = \left\langle 3 + 4\boldsymbol{\sigma\sigma'} + (\boldsymbol{\sigma\sigma'})^2 \right\rangle = 8\delta_{S1}. \tag{57}$$

To calculate the matrix element in Eq. (56) we note that

$$\frac{1}{mr^2} = \frac{1}{6}\left(H_D - H\right), \tag{58}$$

where $H_D(H)$ is the radial Hamiltonian for $D(S)$-states. Using equations of motion for both the Green function and the wave function in Eq. (56) one finds

$$\Delta_D^{\text{h-o}} E_{\text{hfs}} = 8\left(\frac{\alpha^2}{24}\right)^2 \left\langle -\frac{1}{6mr^2} \right\rangle = -\frac{\pi\alpha^3\psi^2(0)}{108m^2}, \tag{59}$$

in agreement with [19].

To complete the calculation of the D-wave contribution we have to consider the zeroth and first order terms in the α expansion of the Green function,

$$\Delta_{D0} E_{\text{hfs}} = \langle U_D G_0 U_D \rangle \,, \tag{60}$$
$$\Delta_{D1} E_{\text{hfs}} = \langle U_D G_1 U_D \rangle \,. \tag{61}$$

The perturbation $U_D(\boldsymbol{p}', \boldsymbol{p})$ is extracted from Breit Hamiltonian, Eq. (36), and reads

$$U_D(\boldsymbol{p}',\boldsymbol{p}) = \frac{\pi\alpha}{4m^2}\left(\frac{[\sigma_i,\sigma_j][\sigma_i',\sigma_j']}{d} - \frac{[\boldsymbol{\sigma q},\sigma_i][\boldsymbol{\sigma' q},\sigma_i']}{\boldsymbol{q}^2}\right). \tag{62}$$

The average is taken over the d–dimensional wave function. Calculating the trace using the triplet wave function we obtain

$$\left\langle \left(\frac{[\sigma_i,\sigma_j][\sigma_i',\sigma_j']}{d} - \frac{[\boldsymbol{\sigma q}',\sigma^i][\boldsymbol{\sigma' q}',\sigma'^i]}{\boldsymbol{q}'^2}\right)\left(\frac{[\sigma_k,\sigma_l][\sigma_k',\sigma_l']}{d} - \frac{[\boldsymbol{\sigma q},\sigma^k][\boldsymbol{\sigma' q},\sigma'^k]}{\boldsymbol{q}^2}\right)\right\rangle$$
$$= \frac{4(d-2)^2}{d}\left\langle B_{ij}(\boldsymbol{q}')B_{ij}(\boldsymbol{q})\right\rangle, \qquad B_{ij}(\boldsymbol{q}) \equiv 4\pi\left(\frac{q_iq_j}{\boldsymbol{q}^2} - \frac{\delta_{ij}}{d}\right). \tag{63}$$

Therefore

$$\Delta_{D0}E_{\rm hfs} = -\frac{\alpha(d-2)^2}{4m^4d}\left\langle B_{ij}(\boldsymbol{p}'-\boldsymbol{k})g(k)B_{ij}(\boldsymbol{k}-\boldsymbol{p})\right\rangle, \tag{64}$$
$$\Delta_{D1}E_{\rm hfs} = -\frac{\alpha(d-2)^2}{4m^4d}\left\langle B_{ij}(\boldsymbol{p}'-\boldsymbol{k}')g(k')\frac{4\pi}{(\boldsymbol{k}'-\boldsymbol{k})^2}g(k)B_{ij}(\boldsymbol{k}-\boldsymbol{p})\right\rangle, \tag{65}$$

where

$$g(k) = \frac{2\gamma}{\boldsymbol{k}^2+\gamma^2}, \tag{66}$$

and d–dimensional integrations over $\boldsymbol{k}$ in (64) and over $\boldsymbol{k},\boldsymbol{k}'$ in (65) are understood. Some details of the integrations in Eqs. (64,65) are given in Appendix B. Adding the higher-order effects found in Eq. (59) we obtain the complete D-wave contributions to HFS

$$\Delta_D E_{\rm hfs} = \Delta_{D0}E_{\rm hfs} + \Delta_{D1}E_{\rm hfs} + \Delta_D^{\rm h-o}E_{\rm hfs}$$
$$= \frac{5\pi\alpha^3}{72m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) - \frac{19}{5}\right). \tag{67}$$

B. Hard scale contribution

Another contribution to the HFS arises from virtual momenta scales of the order of the electron mass. It can be calculated by considering the on–shell e^+e^- scattering amplitude with an exchange of three photons in the t-channel (see Fig. 2) exactly at the threshold, i.e. for zero relative velocity of the incoming electron and positron, in dimensional regularization. The use of the dimensional regularization brings in essential simplifications, since almost any other regularization would bring in power-like divergences and hence require additional subtractions. This so-called hard scale contribution gives rise to four-fermion operators in the low-scale Lagrangian or, equivalently, to the $\delta(r)$ terms in the effective quantum mechanical Hamiltonian.

Technically, this calculation is similar to the derivation of the matching coefficient of the vector quark-antiquark current in QCD and its NRQCD counterpart, described e.g. in [34,35]. Here we outline the main steps of this calculation.

An arbitrary Feynman integral which contributes to the hard scale part of the calculation can be written as

$$I(a_1, ...a_9) = \int \frac{\mathrm{d}^D k_1}{(2\pi)^D} \frac{\mathrm{d}^D k_2}{(2\pi)^D} \frac{1}{S_1^{a_1} S_2^{a_2} S_3^{a_3} S_4^{a_4} S_5^{a_5} S_6^{a_6} S_7^{a_7} S_8^{a_8} S_9^{a_9}}, \tag{68}$$

where

$$\begin{aligned}
&S_1 = k_1^2, \qquad S_2 = k_2^2, \qquad S_3 = (k_1 - k_2)^2, \qquad S_4 = k_1^2 + 2pk_1, \\
&S_5 = k_2^2 + 2pk_2, \qquad S_6 = k_1^2 - 2pk_1, \qquad S_7 = k_2^2 - 2pk_2, \\
&S_8 = (k_1 - k_2)^2 + 2p(k_1 - k_2), \qquad S_9 = (k_1 - k_2)^2 - 2p(k_1 - k_2),
\end{aligned} \tag{69}$$

and $a_1, \ldots, a_9$ are integers. In practice we encounter diagrams with only at most 6 different propagators, so that at least 3 exponents a_i are zero. Applying the integration by parts technique [36] to an integral $I(\{a_i\})$, one obtains a set of relations among integrals with various values of indices $\{a_i\}$. Using these relations one can express any $I(\{a_i\})$ in terms of a few master integrals. This is most easily done using symbolic manipulation programs.

The result for the hard scale recoil corrections (Fig. 2) to the HFS reads [9]

$$\Delta_{\mathrm{hard}} E_{\mathrm{hfs}} = \frac{\pi\alpha^3}{3m^2}\psi^2(0)\left(-\frac{1}{\epsilon} + 4\ln m - \frac{51\zeta(3)}{\pi^2} + \frac{10}{\pi^2} - 6\ln 2\right). \tag{70}$$

C. HFS for excited S states

The result for the HFS of the ground state can be used to obtain the HFS for an arbitrary excited state. The non–trivial dependence on the principal quantum number n arises only from the soft scale contributions. Therefore, one has to repeat the quantum mechanical calculation of the non-relativistic part using any convenient regularization (we use a cut-off at $1/m \ll r_0 \ll 1/m\alpha$) and compare the result with the known formula for $n = 1$, Eq. (8). One finds

$$\Delta_{\mathrm{rec}} E_{\mathrm{hfs}}(n) = \frac{m\alpha^6}{n^3}\left[[div] - \frac{1}{6}\left(\ln\frac{\alpha}{n} + \Psi(n) + \gamma_E\right) + \frac{7}{12n} - \frac{1}{2n^2}\right], \tag{71}$$

The quantity $[div]$ in the above equation stands for the unknown and n-independent constant, easily determined by requiring that for n=1 Eq. (8) is reproduced. We then obtain the final result for the recoil corrections to the HFS splitting for an arbitrary nS state, Eq. (9).

IV. SPIN-AVERAGED ENERGY LEVELS

To obtain $\mathcal{O}(m\alpha^6)$ corrections to the triplet and singlet energy levels separately, we have to calculate $E_{\mathrm{aver}}(n)$ (cf. Eq. (2)). An appropriate formula for this calculation is

$$E_{\mathrm{aver}} = \frac{3\,E_{\mathrm{triplet}} + E_{\mathrm{singlet}}}{4} \to \frac{d\,E_{d-\mathrm{plet}} + E_{\mathrm{singlet}}}{d+1}.$$

It is known [37,38,30] that the recoil corrections $E_{\rm aver}$ do not contain $\ln(\alpha)$ at the order $m\alpha^6$. In dimensional regularization this means that the hard-scale and soft-scale contributions are separately finite.[5]

Conceptually, determination of $E_{\rm aver}$ is very similar to the calculation of the HFS discussed above in detail. The only difference is that several new operators appear, which contribute to $E_{\rm aver}$ but not to the HFS.

A. The ground state average energy shift

We begin with the correction to $E_{\rm aver}$ induced by the relativistic corrections to the dispersion law, $\omega_p = \sqrt{\boldsymbol{p}^2+m^2}$ (Fig. 1(g)). Expanding ω_p in $|\boldsymbol{p}|/m$, we obtain:

$$\omega_p = m + \frac{\boldsymbol{p}^2}{2m} - \frac{\boldsymbol{p}^4}{8m^3} + \frac{\boldsymbol{p}^6}{16m^5} + \dots. \tag{72}$$

The last term induces a correction of the appropriate order:

$$\Delta_{\rm disp} E_{\rm aver} = \frac{1}{8m^5}\left\langle \boldsymbol{p}^6 \delta^{(d)}(\boldsymbol{p}-\boldsymbol{p}')\right\rangle = -\frac{3}{64}\frac{\pi\alpha^3}{m^2}\psi^2(0). \tag{73}$$

The $\mathcal{O}(v^4)$ spin-independent part of the tree level Coulomb exchange amplitude (cf. Eq. (A1) and Fig. 1(a); we neglect terms odd in $\boldsymbol{p}$, whose average vanishes in an S-state),

$$\overline{V}_C(\boldsymbol{p}',\boldsymbol{p}) = -\frac{\pi\alpha}{16m^4}\left(7\left(\boldsymbol{p}^2+\boldsymbol{p}'^2\right) + \frac{5(\boldsymbol{p}^2-\boldsymbol{p}'^2)^2}{\boldsymbol{q}^2}\right), \tag{74}$$

gives rise to the following correction:

$$\Delta_{\rm C} E_{\rm aver} = \frac{5\pi\alpha^3}{32m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) + \frac{7}{5}\right). \tag{75}$$

Virtual transitions to negative energy states induced by the Coulomb exchanges, Fig. 1(h), generate an effective spin-independent operator

$$V_{C-}(\boldsymbol{r}) = -\frac{1}{4m^3}[\boldsymbol{p}, C(r)]^2. \tag{76}$$

This operator describes the energy shift due to a creation of an additional e^+e^- pair by the Coulomb field of either electron or positron. The resulting energy shift is

$$\Delta_{C-} E_{\rm aver} = -\frac{\pi\alpha^3}{4m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha)\right). \tag{77}$$

The spin-independent part of the tree level magnetic exchange, Fig. 1(b), induces the following shift in the energy levels:

---

[5]Because of power-like singularities, this is not necessarily the case in other regularization schemes.

$$\Delta_{\rm M}E_{\rm aver} = \frac{2\pi\alpha}{m^4}\left\langle(\boldsymbol{p}'^2+\boldsymbol{p}^2)\left(\frac{\boldsymbol{p}\boldsymbol{p}'}{\boldsymbol{q}^2}-\frac{(\boldsymbol{p}\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p}')}{\boldsymbol{q}^4}\right)\right\rangle = \frac{\pi\alpha^3}{2m^2}\psi^2(0)\left(\frac{1}{\epsilon}-4\ln(m\alpha)+\frac{1}{2}\right). \quad (78)$$

To account for the retardation in the magnetic photon propagation, Fig. 1(c,d,e), we use the approach described in the HFS case. Our starting point is similar to Eq. (28), except that now the full expression for the currents must be used, rather than just their spin-dependent part. We obtain

$$\Delta_{\rm ret}E_{\rm aver} = \frac{\pi\alpha^3}{8m^2}\psi^2(0)\left(\frac{1}{\epsilon}-4\ln(m\alpha)-8\right). \quad (79)$$

The next contribution comes from the exchange of two magnetic photons with creation of an additional e^+e^- pair in the intermediate state, Fig. 1(i). We find

$$\Delta_{\rm MM-}E_{\rm aver} = -\frac{\pi\alpha^3}{2m^2}\psi^2(0)\left(\frac{1}{\epsilon}-4\ln(m\alpha)-3\right). \quad (80)$$

We proceed further with the correction to $E_{\rm aver}$, induced by the second iteration of the S-wave Breit Hamiltonian. The calculation closely follows the HFS case. We arrive at the following result:

$$\Delta^{(2)}_{\rm S}E_{\rm aver} = -\frac{\pi\alpha^3}{12m^2}|\psi(0)|^2\left(\frac{1}{\epsilon}-4\ln(m\alpha)+\frac{433}{24}\right). \quad (81)$$

The iteration of the D-wave part of the Breit Hamiltonian only influences the energy levels of the triplet state because of the total angular momentum $(\boldsymbol{L}+\boldsymbol{S})$ conservation. For this reason, to obtain the required correction to $E_{\rm aver}$ it is sufficient to multiply Eq. (67) by the factor $d/(d+1)$. We find

$$\Delta^{(2)}_{D}E_{\rm aver} = \frac{5\pi\alpha^3}{96m^2}\psi^2(0)\left(\frac{1}{\epsilon}-4\ln(m\alpha)-\frac{119}{30}\right). \quad (82)$$

It is easy to see that in 3 dimensions the spin-dependent operators do not contribute to $E_{\rm aver}$. However, since we work with divergent integrals and use dimensional regularization, this is no longer valid for $d\neq 3$. In this case an "anomalous" situation arises: spin-dependent operators provide contributions of the form $(d-3)/\epsilon$ to $E_{\rm aver}$, which are finite as $\epsilon\to 0$. Part of these contributions has already been accounted for in the corrections induced by the Breit Hamiltonian. The remaining contributions give

$$\Delta_{\rm anom}E_{\rm aver} = -\frac{15}{64}\frac{\pi\alpha^3}{m^2}\psi^2(0). \quad (83)$$

The hard scale contribution, Fig. 2, is calculated in the same way as for the HFS. One finds:

$$\Delta_{\rm hard}E_{\rm aver} = -\frac{\pi\alpha^3}{3m^2}\psi^2(0)\left(\frac{13}{8}+\frac{9\zeta(3)}{\pi^2}+\frac{33}{2\pi^2}\right). \quad (84)$$

The sum of all contributions presented above provides the $\mathcal{O}(m\alpha^6)$ pure recoil correction to the ground state energy:

$$\Delta_{\rm rec}E_{\rm aver} = -\frac{m\alpha^6}{8}\left(\frac{901}{576}+\frac{11}{2\pi^2}+\frac{3\zeta(3)}{\pi^2}\right) = -\frac{m\alpha^6}{8}(2.48688\ldots), \quad (85)$$

in very good agreement with the numerical result of Eq. (20) in [11], $-\frac{m\alpha^6}{8}(2.484(5))$.

B. Energy levels for arbitrary n

To generalize the result Eq. (85) for arbitrary n, we proceed according to the program outlined in Section III C. We repeat the calculation of the soft-scale contributions to $E_{\rm aver}$ for arbitrary n using a different regularization scheme. Namely, we set $d = 3$ and cut off the divergent integrals over r from below at some $r_0 \ll 1/(m\alpha)$. The transition to three dimensions simplifies the calculation. We find

$$\Delta_{\rm rec} E_{\rm aver}(n) = -\frac{m\alpha^6}{8n^3}\left([div] + \frac{69}{64n^3} - \frac{8}{3n^2} + \frac{2}{n}\right). \tag{86}$$

The n-independent term in the above equation is regularization dependent. It cannot be determined by considering the soft-scale contributions alone. Nevertheless, by matching Eq. (86) to the shift for the ground state Eq. (85), the "value" of the divergent constant $[div]$ is completely determined. We obtain

$$\Delta_{\rm rec} E_{\rm aver}(n) = -\frac{m\alpha^6}{8n^3}\left(\frac{83}{72} + \frac{11}{2\pi^2} + \frac{3\zeta(3)}{\pi^2} + \frac{69}{64n^3} - \frac{8}{3n^2} + \frac{2}{n}\right). \tag{87}$$

This is our main result for the recoil corrections to the energy levels of positronium. It agrees with the partially numerical result derived in [11].

V. RADIATIVE RECOIL CORRECTIONS

So far in this paper we have been considering pure recoil effects. Another class of the $\mathcal{O}(m\alpha^6)$ corrections to positronium energy levels and their HFS are the so-called radiative recoil corrections, where one of the three exchanged photons is created and absorbed by the same particle (see Fig. 3).

Our technique is very convenient for the calculation of these corrections. The key point is that at $\mathcal{O}(m\alpha^6)$ the radiative recoil corrections do not receive any contribution from the non-relativistic scales. Thus it is sufficient to calculate the diagrams shown in Fig. 3 (supplemented by the electric charge, electron wave function and mass renormalization) exactly at the threshold. For the same reason, the n-dependence of the radiative recoil corrections comes only from the $1/n^3$ behavior of the nS-wave function at the origin. Some details of this calculation are described in Section III B in the context of the HFS. We obtain

$$\Delta_{\rm rad\ rec} E_{\rm hfs} = \frac{m\alpha^6}{n^3}\left[\frac{\zeta(3)}{2\pi^2} - \frac{79}{48} + \frac{41}{36\pi^2} + \frac{4}{3}\ln 2\right], \tag{88}$$

$$\Delta_{\rm rad\ rec} E_{\rm aver} = \frac{m\alpha^6}{n^3}\left[\frac{9\zeta(3)}{8\pi^2} + \frac{97}{144} - \frac{1025}{432\pi^2}\right], \tag{89}$$

respectively for corrections to the HFS and to the average energy, in full agreement with the analytic results of Ref. [28]. For completeness, we give here separately the contributions of electron vacuum polarization effects to radiative recoil corrections [39,28,40] (they are included in (88,89)):

$$\Delta^{\rm vac\ pol}_{\rm rad\ rec} E_{\rm hfs} = \frac{m\alpha^6}{n^3}\frac{5}{9\pi^2}, \qquad \Delta^{\rm vac\ pol}_{\rm rad\ rec} E_{\rm aver} = \frac{m\alpha^6}{n^3}\left(\frac{1}{36} - \frac{5}{27\pi^2}\right). \tag{90}$$

VI. SUMMARY AND CONCLUSIONS

The main new results of the present paper are the analytic formulas (9) and (87) for the pure recoil $\mathcal{O}(m\alpha^6)$ corrections to the HFS and spin–averaged energy levels of positronium nS states. These recoil effects provide the last pieces needed to present complete analytical formulas for the total corrections to $E_{\rm aver}$ and $E_{\rm hfs}$. We use the parameterization introduced in Eq. (2),

$$E(J,n) = E_{\rm aver}(n) + \left(\frac{1}{4} - \delta_{J0}\right) E_{\rm hfs}(n), \tag{91}$$

and find

$$\begin{aligned} E_{\rm aver}(n) = & -\frac{m\alpha^2}{4n^2} + \frac{m\alpha^4}{16n^3}\left(\frac{11}{4n} - 1\right) \\ & + \frac{m\alpha^5}{8\pi n^3}\left[-6\ln\alpha - \frac{16}{3}\ln k_0(n,0) + \frac{14}{3}\left(\ln\frac{4}{n} + \Psi(n) + \gamma_E\right) - \frac{37}{45} - 3\ln 2 + \frac{7}{3n}\right] \\ & + \frac{m\alpha^6}{32n^3}\left[-\ln\frac{\alpha}{n} - \Psi(n) - \gamma_E + \frac{141}{4}\frac{\zeta(3)}{\pi^2} + \left(\frac{137}{6} - \frac{68}{\pi^2}\right)\ln 2 + \frac{1421}{27\pi^2}\right. \\ & \qquad \left. - \frac{2435}{432} - \frac{7}{n} + \frac{17}{12n^2} - \frac{69}{16n^3}\right], \end{aligned} \tag{92}$$

and

$$\begin{aligned} E_{\rm hfs}(n) = & \frac{7}{12}\frac{m\alpha^4}{n^3} - \frac{m\alpha^5}{\pi n^3}\left(\frac{8}{9} + \frac{1}{2}\ln 2\right) + \frac{m\alpha^6}{n^3}\left[-\frac{5}{24}\left(\ln\frac{\alpha}{n} + \Psi(n) + \gamma_E\right) + \frac{1367}{648\pi^2}\right. \\ & \left. - \frac{4297}{3456} + \left(\frac{221}{144} + \frac{1}{2\pi^2}\right)\ln 2 - \frac{53}{32\pi^2}\zeta(3) + \frac{5}{8n} - \frac{85}{96n^2}\right]. \end{aligned} \tag{93}$$

We have also recalculated the radiative recoil corrections, Eqs. (88,89), confirming recent result of Ref. [28]. Let us make a technical remark. In dimensional regularization, used in this paper, the calculation of the radiative recoil corrections is particularly simple. Since there are no low-scale contributions to the radiative recoil corrections, it suffices to calculate corresponding Feynman graphs exactly at the threshold. No matching or subtractions are required.

Formulas (92,93), together with P state energy levels given in Appendix C, can be used to compute quantities which can be directly confronted with experimental data. We use the following values for the Rydberg [41] and fine structure [42] constants:

$$R_\infty = \frac{m\alpha^2}{2} = 3\,289\,841\,960.394(27)\ \text{MHz}, \qquad \alpha = 1/137.035\,999\,59(51). \tag{94}$$

In addition to the full corrections $\mathcal{O}(m\alpha^6)$ we include the leading logarithmic terms $\mathcal{O}(m\alpha^7\ln^2\alpha)$ found in [43] for HFS, and in [44] for the spin-averaged energy levels:

$$\Delta_{LL}E(J,n) = -\left(\frac{193}{5} + 7\,(1 - 4\delta_{J0})\right)\frac{m\alpha^7\ln^2\alpha}{32\pi n^3}\delta_{l0}. \tag{95}$$

For the most precisely measured quantity, the Ps ground state HFS, we find

$$\Delta\nu = 203\,392.01(46) \text{ MHz}. \tag{96}$$

The $\mathcal{O}(m\alpha^6)$ recoil corrections to this observable have been subject of some debate. In the literature three different results have been reported [5,10,29].[6] Our result for this correction, Eq. (8), evaluates numerically to $m\alpha^6\left(-\frac{1}{6}\ln\alpha + 0.37632\right)$. This is in excellent agreement with Ref. [10], where for the non-logarithmic part of the correction a number 0.3767(17) was obtained. The framework of our calculation is similar to Ref. [10]. However, in that study a different regularization method was used. The agreement of the results gives us confidence in their correctness.

Comparing Eq. (96) with the experimental results, Eqs. (4,5), we observe a significant deviation of the order of $3-4$ experimental errors. It is not very likely that the uncalculated higher order effects alone can account for this discrepancy. The size of the $\mathcal{O}(m\alpha^6)$ corrections gives no indication of bad behavior of the perturbative expansion. On the other hand, the leading logarithmic term $\mathcal{O}(m\alpha^7\ln^2\alpha)$ is sizable. A calculation of the subleading terms at this order remains an important theoretical challenge.

For another experimentally interesting quantity, the energy interval of the $1S-2S$ transition, we get

$$E(2^3S_1) - E(1^3S_1) = 1233\,607\,222.33(65) \text{ MHz}. \tag{97}$$

in fair agreement with the experimental result, Eq. (6).

Other quantities, for which high precision measurements have been made or are being planned, have recently been reviewed in [28]. In Table I we update the theory predictions for those observables. Our predictions are in good agreement with [28]. We have been able to decrease the error bars by including the analytical results (92,93) and the value of the leading quadratic logarithms (95).

Finally we would like to comment on our error estimates. The errors due to uncertainties in the fine structure constant and the electron mass are well below 0.1 MHz level. The dominant theoretical error source is the uncalculated remainder of the perturbation expansion. Although 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 [43]. It remains very important to calculate the remaining, non-leading terms in $\mathcal{O}(m\alpha^7)$. For the present analysis we assume that the leading logs $\mathcal{O}(m\alpha^7\ln^2\alpha)$ dominate the higher order contributions and take half their size as the theoretical error estimate.

The spectrum of the nS and nP positronium energy levels is now known analytically, including effects $\mathcal{O}(m\alpha^6)$. Our calculation for the nS levels was made possible by new theoretical tools which have their roots in the recent perturbative calculations in high-energy physics. We hope that these methods will find further applications.

The agreement between theoretical predictions and experimental results in Ps spectroscopy is impressive with a few exceptions. One can only hope to find something new and unexpected by trying to put these exceptions in line with the overall picture. We look

[6] After our HFS calculation was completed, we were informed about an independent numerical calculation of the recoil corrections [45]. Although that study is still in progress, its preliminary results seem to agree with Ref. [10] and the present paper.

forward to future improved measurements of positronium energy levels and their confrontation with QED.

Acknowledgments

We are grateful to A. Burichenko for informing us about his results prior to publication. We thank S. Karshenboim, K. Pachucki and E. Remiddi for reading the manuscript and helpful comments. K.M. would like to thank the High Energy Theory Group at Brookhaven National Laboratory for hospitality during the final stage of this project. This research was supported in part by the U.S. Department of Energy under grant number DE-AC02-98CH10886, by BMBF under grant number BMBF-057KA92P, by Graduiertenkolleg "Teilchenphysik" at the University of Karlsruhe and by the Russian Foundation for Basic Research under grant number 98-02-17913.

APPENDIX A: TREE–LEVEL ELECTRON–POSITRON POTENTIAL

We present here formulas for the potential arising from a single Coulomb or magnetic photon exchange between an electron and a positron, valid to $\mathcal{O}(v^4)$. The virtual annihilation is not taken into account here. We also drop those terms which annihilate the S–state wave function. These formulas, valid in d-dimensions, are useful in the derivations of HFS and spin–averaged energy levels.

For a single Coulomb exchange between two particles of opposite charges, Fig. 1(a), the minus on–shell scattering amplitude is

$$-A_C(\boldsymbol{p}',\boldsymbol{p}) = -\frac{4\pi\alpha}{\boldsymbol{q}^2}\rho(\boldsymbol{p}',\boldsymbol{p})\rho(-\boldsymbol{p}',-\boldsymbol{p}), \tag{A1}$$

where $\boldsymbol{p}$ and $\boldsymbol{p}'$ are spatial momenta of the incoming and outgoing electron; $\boldsymbol{q}=\boldsymbol{p}'-\boldsymbol{p}$; and the charge density is $\rho(\boldsymbol{p}',\boldsymbol{p}) = u^+(\boldsymbol{p}')u(\boldsymbol{p})$. In momentum representation a single Coulomb photon exchange gives rise to the potential

$$U_C(\boldsymbol{p},\boldsymbol{p}') = -\frac{4\pi\alpha}{\boldsymbol{q}^2}\left\{1-\frac{\boldsymbol{q}^2}{4m^2}+\frac{5\left(\boldsymbol{p}^2-\boldsymbol{p}'^2\right)^2+6\boldsymbol{q}^2\left(\boldsymbol{p}^2+\boldsymbol{p}'^2\right)+\boldsymbol{q}^4+[\boldsymbol{\sigma}\boldsymbol{p}',\boldsymbol{\sigma}\boldsymbol{p}][\boldsymbol{\sigma}'\boldsymbol{p}',\boldsymbol{\sigma}'\boldsymbol{p}]}{64m^4}\right\}. \tag{A2}$$

In the leading nonrelativistic approximation Eq. (A2) gives the Coulomb potential.

Next we consider a magnetic photon exchange, Fig. 1(b). We neglect retardation effects. The scattering amplitude is

$$-A_M(\boldsymbol{p}',\boldsymbol{p}) = \frac{4\pi\alpha}{\boldsymbol{q}^2}j_i(\boldsymbol{p}',\boldsymbol{p})j_j(-\boldsymbol{p}',-\boldsymbol{p})\left(\delta_{ij}-\frac{q_iq_j}{\boldsymbol{q}^2}\right), \tag{A3}$$

where $\boldsymbol{j}(\boldsymbol{p}',\boldsymbol{p}) = u^+(\boldsymbol{p}')\boldsymbol{\alpha}u(\boldsymbol{p})$ is the matrix element of the current. The resulting potential is

$$U_M(\boldsymbol{p},\boldsymbol{p}') = \frac{\pi\alpha}{m^2\boldsymbol{q}^2}\left(\frac{4}{\boldsymbol{q}^2}\left[(\boldsymbol{p}\boldsymbol{p}')^2 - \boldsymbol{p}^2\boldsymbol{p}'^2\right] - \frac{1}{4}[\boldsymbol{\sigma}\boldsymbol{q},\sigma^i][\boldsymbol{\sigma}'\boldsymbol{q},\sigma'^i]\right)$$
$$-\frac{\pi\alpha}{2m^4\boldsymbol{q}^2}\left\{(\boldsymbol{p}^2+\boldsymbol{p}'^2)\left(\frac{4}{\boldsymbol{q}^2}\left[(\boldsymbol{p}\boldsymbol{p}')^2 - \boldsymbol{p}^2\boldsymbol{p}'^2\right] - \frac{1}{4}[\boldsymbol{\sigma}\boldsymbol{q},\sigma^i][\boldsymbol{\sigma}'\boldsymbol{q},\sigma'^i]\right)\right.$$
$$\left. +\frac{\boldsymbol{p}^2-\boldsymbol{p}'^2}{16}\left([\boldsymbol{\sigma}\boldsymbol{q},\sigma^i][\boldsymbol{\sigma}'\boldsymbol{P},\sigma'^i] + [\boldsymbol{\sigma}\boldsymbol{P},\sigma^i][\boldsymbol{\sigma}'\boldsymbol{q},\sigma'^i]\right)\right\}. \tag{A4}$$

These formulas are valid in the center of mass frame. We use $\boldsymbol{p}$ and $\boldsymbol{p}'$ to denote incoming and outgoing electron momenta, and $\boldsymbol{q} \equiv \boldsymbol{p}' - \boldsymbol{p}$, $\boldsymbol{P} \equiv \boldsymbol{p}' + \boldsymbol{p}$. The primed σ-matrices act on the positron spinor.

APPENDIX B: USEFUL INTEGRALS

In this Appendix we present various integrals which were useful in the calculations presented in this paper. The following formulas have been used throughout the paper, especially for the tree level diagrams:

$$\begin{aligned}
\left\langle \boldsymbol{p}^2 \right\rangle &= -\frac{m^2\alpha^2}{4}\psi^2(0), \\
\left\langle \frac{\boldsymbol{p}^4}{\boldsymbol{q}^2} \right\rangle &= \frac{m^2\alpha^2}{16}\psi^2(0), \\
\left\langle \frac{\boldsymbol{p}^2\boldsymbol{p}'^2}{\boldsymbol{q}^2} \right\rangle &= \frac{m^2\alpha^2}{4}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) + \frac{1}{4}\right), \\
\left\langle \frac{(\boldsymbol{q}\boldsymbol{p})(\boldsymbol{q}\boldsymbol{p}')}{\boldsymbol{q}^2} \right\rangle &= -\frac{m^2\alpha^2}{8}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) - 1\right).
\end{aligned} \tag{B1}$$

In the remainder of this Appendix we describe some details of the D-wave contribution to the second iteration of the Breit Hamiltonian. First, we rewrite Eq. (64) in the following way:

$$\langle B_{ij}(\boldsymbol{p}'-\boldsymbol{k})g(k)B_{ij}(\boldsymbol{k}-\boldsymbol{p})\rangle = \left\langle B_{ij}(\boldsymbol{p}'-\boldsymbol{k})g(k)4\pi\frac{k_ik_j - 2k_ip_j + p_ip_j}{(\boldsymbol{k}-\boldsymbol{p})^2}\right\rangle$$
$$= \left\langle B_{ij}(\boldsymbol{q})p_ip_j - 2B_{ij}(\boldsymbol{p}'-\boldsymbol{k})g(k)\frac{4\pi(k_i-p_i)}{(\boldsymbol{k}-\boldsymbol{p})^2}p_j - B_{ij}(\boldsymbol{p}'-\boldsymbol{k})g(k)\frac{4\pi}{(\boldsymbol{k}-\boldsymbol{p})^2}p_ip_j\right\rangle. \tag{B2}$$

Here and below we use the Schrödinger equation in the form

$$\phi(p) = g(p)\frac{4\pi}{(\boldsymbol{p}-\boldsymbol{k})^2}\phi(k). \tag{B3}$$

Similarly, by rearranging terms in (65) we get

$$\left\langle B_{ij}(\boldsymbol{p}'-\boldsymbol{k}')g(k')\frac{4\pi}{(\boldsymbol{k}'-\boldsymbol{k})^2}g(k)B_{ij}(\boldsymbol{k}-\boldsymbol{p})\right\rangle$$

$$= \left\langle B_{ij}(\boldsymbol{p}'-\boldsymbol{k})g(k)\frac{4\pi}{(\boldsymbol{k}-\boldsymbol{p})^2}p_ip_j - 2B_{ij}(\boldsymbol{p}'-\boldsymbol{k}')g(k')\frac{4\pi}{(\boldsymbol{k}'-\boldsymbol{k})^2}k_ig(k)\frac{4\pi}{(\boldsymbol{k}-\boldsymbol{p})^2}p_j \right.$$
$$\left. +B_{ij}(\boldsymbol{p}'-\boldsymbol{k}')g(k')\frac{4\pi}{(\boldsymbol{k}'-\boldsymbol{k})^2}g(k)\frac{4\pi}{(\boldsymbol{k}-\boldsymbol{p})^2}p_ip_j \right\rangle , \tag{B4}$$

Using the symmetry with respect to $\boldsymbol{p} \leftrightarrow \boldsymbol{p}'$, we rewrite the first term in Eq. (B2),

$$\langle B_{ij}(\boldsymbol{q})p_ip_j\rangle = 4\pi \left\langle \frac{\boldsymbol{q}^2}{2} + \frac{(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{\boldsymbol{q}^2} - \frac{\boldsymbol{p}^2}{3} \right\rangle = 4\pi \left\langle -\frac{2}{3}\gamma^2 + \frac{(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{\boldsymbol{q}^2} \right\rangle . \tag{B5}$$

In the same way, the second term in Eq. (B2) is transformed to

$$\left\langle -2B_{ij}(\boldsymbol{p}'-\boldsymbol{k})g(k)\frac{4\pi(k_i-p_i)}{(\boldsymbol{k}-\boldsymbol{p})^2}p_j \right\rangle$$
$$= \left\langle \frac{8\pi}{d}g(k)\frac{4\pi(\boldsymbol{k}-\boldsymbol{p})\boldsymbol{p}}{(\boldsymbol{k}-\boldsymbol{p})^2} + 2p'_i\frac{4\pi}{(\boldsymbol{p}'-\boldsymbol{k})^2}\left(2k_j - p'_j\right)g(k)\frac{4\pi(k_i-p_i)}{(\boldsymbol{k}-\boldsymbol{p})^2}p_j \right\rangle . \tag{B6}$$

Considering the divergent part of this expression we find

$$\left\langle \frac{8\pi}{d}g(k)\frac{4\pi(\boldsymbol{k}-\boldsymbol{p})\boldsymbol{p}}{(\boldsymbol{k}-\boldsymbol{p})^2} \right\rangle = \frac{16\pi^2\alpha}{d}\psi^2(0)\left[G_0(0,0)+G_1(0,0)\right] . \tag{B7}$$

The sum of (64) and (65) reads

$$\Delta_{D0}E_{\rm hfs} + \Delta_{D1}E_{\rm hfs} = -\frac{\alpha(d-2)^2}{4m^4d}\left\langle \frac{16\pi^2\alpha}{d}\left[G_0(0,0)+G_1(0,0)\right] - \frac{8\pi\gamma^2}{3} + \frac{4\pi(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{\boldsymbol{q}^2} \right.$$
$$+2p'_i\frac{4\pi}{(\boldsymbol{p}'-\boldsymbol{k})^2}\left(2k_j-p'_j\right)g(k)\frac{4\pi(k_i-p_i)}{(\boldsymbol{k}-\boldsymbol{p})^2}p_j$$
$$-2B_{ij}(\boldsymbol{p}'-\boldsymbol{k}')g(k')\frac{4\pi}{(\boldsymbol{k}'-\boldsymbol{k})^2}k_ig(k)\frac{4\pi}{(\boldsymbol{k}-\boldsymbol{p})^2}p_j$$
$$\left. +B_{ij}(\boldsymbol{p}'-\boldsymbol{k}')g(k')\frac{4\pi}{(\boldsymbol{k}'-\boldsymbol{k})^2}g(k)\frac{4\pi}{(\boldsymbol{k}-\boldsymbol{p})^2}p_ip_j \right\rangle . \tag{B8}$$

Only two terms here contain the logarithmic divergence:

$$-\frac{4\pi^2\alpha^2(d-2)^2}{m^4d^2}\langle G_1(0,0)\rangle = \frac{\pi\alpha^3}{36m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) - \frac{2}{3}\right) , \tag{B9}$$
$$-\frac{\alpha(d-2)^2}{4m^4d}\left\langle \frac{4\pi(\boldsymbol{p}'\boldsymbol{q})(\boldsymbol{q}\boldsymbol{p})}{\boldsymbol{q}^2} \right\rangle = \frac{\pi\alpha^3}{24m^2}\psi^2(0)\left(\frac{1}{\epsilon} - 4\ln(m\alpha) - \frac{13}{3}\right) . \tag{B10}$$

All other terms are finite and we compute them in three dimensions. Here we list some useful integrals ($x \equiv k/\gamma$ and $a(x) \equiv \arctan(x)$):

$$\int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{p_i}{(\boldsymbol{k}-\boldsymbol{p})^2}\phi(p) = \frac{\gamma\psi(0)k_i}{k^3}\left(a(x) - \frac{x}{x^2+1}\right) ,$$

$$
\begin{aligned}
&\int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{p_ip_j}{(\boldsymbol{k}-\boldsymbol{p})^2}\phi(p) \\
&\qquad = \frac{\gamma\psi(0)}{k}\left[\frac{1}{2}\left(\frac{k_ik_j}{\boldsymbol{k}^2}-\frac{\delta_{ij}}{3}\right)\left(\frac{x^2+3}{x(x^2+1)}+\frac{x^2-3}{x^2}a(x)\right)+\frac{\delta_{ij}}{3}\left(a(x)-\frac{x}{x^2+1}\right)\right], \\
&\int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{\mathrm{d}^3k'}{(2\pi)^3}\frac{g(k')B_{ij}(\boldsymbol{k}'-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{k}')^2}\phi(p) = \frac{\gamma\psi(0)}{k}\left(\frac{k_ik_j}{\boldsymbol{k}^2}-\frac{\delta_{ij}}{3}\right)\left[\frac{a(x)}{2}\left(1+\frac{3}{x^2}\right)-\frac{3}{2x}\right].
\end{aligned}
\tag{B11}
$$

Using these above formulas in Eq. (B8) we find the final result for $\Delta_{D0}E_{\mathrm{hfs}}+\Delta_{D1}E_{\mathrm{hfs}}$.

APPENDIX C: P STATE ENERGY LEVELS

In this Appendix we present formulas for the energy levels of P states, to order $\mathcal{O}(m\alpha^6)$. Correcting some minor misprints in Ref. [31,32] one finds

$$
\begin{aligned}
E(n^3P_2) = &-\frac{m\alpha^2}{4n^2}-\frac{m\alpha^4}{4n^3}\left(\frac{13}{30}-\frac{11}{16n}\right)-\frac{m\alpha^5}{8\pi n^3}\left(\frac{4}{45}+\frac{16}{3}\ln k_0(n,1)\right) \\
&+\frac{m\alpha^6}{n^3}\left(-\frac{69}{512n^3}+\frac{559}{4800n^2}-\frac{169}{4800n}+\frac{20677}{432000}-\frac{3}{80}\ln 2+\frac{9\zeta(3)}{160\pi^2}+\frac{13}{128\pi^2}\right), \\
E(n^3P_1) = &-\frac{m\alpha^2}{4n^2}-\frac{m\alpha^4}{4n^3}\left(\frac{5}{6}-\frac{11}{16n}\right)-\frac{m\alpha^5}{8\pi n^3}\left(\frac{5}{9}+\frac{16}{3}\ln k_0(n,1)\right) \\
&+\frac{m\alpha^6}{n^3}\left(-\frac{69}{512n^3}+\frac{77}{320n^2}-\frac{25}{192n}+\frac{1}{48}\ln 2-\frac{\zeta(3)}{32\pi^2}-\frac{179}{3456\pi^2}+\frac{493}{17280}\right), \\
E(n^3P_0) = &-\frac{m\alpha^2}{4n^2}-\frac{m\alpha^4}{4n^3}\left(\frac{4}{3}-\frac{11}{16n}\right)-\frac{m\alpha^5}{8\pi n^3}\left(\frac{25}{18}+\frac{16}{3}\ln k_0(n,1)\right) \\
&+\frac{m\alpha^6}{n^3}\left(-\frac{69}{512n^3}+\frac{119}{240n^2}-\frac{1}{3n}-\frac{923}{4320}+\frac{1}{8}\ln 2-\frac{3}{16\pi^2}\zeta(3)-\frac{203}{576\pi^2}\right), \\
E(n^0P_1) = &-\frac{m\alpha^2}{4n^2}-\frac{m\alpha^4}{4n^3}\left(\frac{2}{3}-\frac{11}{16n}\right)-\frac{m\alpha^5}{8\pi n^3}\left(\frac{7}{18}+\frac{16}{3}\ln k_0(n,1)\right) \\
&+\frac{m\alpha^6}{n^3}\left(\frac{163}{4320}+\frac{23}{120n^2}-\frac{69}{512n^3}-\frac{1}{12n}\right).
\end{aligned}
\tag{C1}
$$

For the numerical evaluations we use the following values of Bethe logarithms $\ln\left[k_0(n,l)/R_\infty\right]$ [46]

$$
\begin{aligned}
\ln\left[k_0(1,0)/R_\infty\right] &= 2.984\,128\,555\,765\,498, \\
\ln\left[k_0(2,0)/R_\infty\right] &= 2.811\,769\,893\,120\,563, \\
\ln\left[k_0(2,1)/R_\infty\right] &= -0.030\,016\,708\,630\,213.
\end{aligned}
\tag{C2}
$$

REFERENCES

[1] A. P. Mills, Jr., in *The spectrum of atomic hydrogen: advances*, edited by G. W. Series (World Scientific, Singapore, 1988), Chap. 8.

[2] R. Barbieri and E. Remiddi, Nucl. Phys. **B141**, 413 (1978).

[3] F. Gross, Phys. Rev. **186**, 1448 (1969).

[4] G. P. Lepage, Phys. Rev. **A16**, 863 (1977).

[5] W. E. Caswell and G. P. Lepage, Phys. Lett. **167B**, 437 (1986).

[6] J. R. Sapirstein and D. R. Yennie, in *Quantum Electrodynamics*, edited by T. Kinoshita (World Scientific, Singapore, 1990), p. 560.

[7] A. Pineda and J. Soto, Nucl. Phys. Proc. Suppl. **64**, 428 (1998).

[8] A. Pineda and J. Soto, Phys. Rev. **D59** 016005, (1999).

[9] A. Czarnecki, K. Melnikov, and A. Yelkhovsky, Phys. Rev. Lett. **82** 311, (1999).

[10] K. Pachucki, Phys. Rev. **A56**, 297 (1997).

[11] K. Pachucki, Phys. Rev. Lett. **79**, 4120 (1997).

[12] R. Karplus and A. Klein, Phys. Rev. **87**, 848 (1952).

[13] T. Fulton and P. C. Martin, Phys. Rev. **95**, 811 (1954).

[14] S. N. Gupta, W. W. Repko, and C. J. Suchyta III, Phys. Rev. **D40**, 4100 (1989).

[15] A. P. Mills, Jr., Phys. Rev. **A27**, 262 (1983).

[16] A. P. Mills, Jr. and G. H. Bearman, Phys. Rev. Lett. **34**, 246 (1975).

[17] M. W. Ritter, P. O. Egan, V. W. Hughes, and K. A. Woodle, Phys. Rev. **A30**, 1331 (1984).

[18] M. S. Fee, A. P. Mills, Jr., S. Chu, E. D. Shaw, K. Danzmann, R. J. Chicherster, and D. M. Zuckerman, Phys. Rev. Lett. **70**, 1397 (1993).

[19] G. T. Bodwin and D. R. Yennie, Phys. Rep. **43**, 267 (1978).

[20] W. E. Caswell and G. P. Lepage, Phys. Rev. **A20**, 36 (1979).

[21] S. J. Brodsky and G. W. Erickson, Phys. Rev. **148**, 26 (1966).

[22] R. Barbieri, J. A. Mignaco, and E. Remiddi, Nuov. Cim. **11A**, 824 (1972).

[23] G. S. Adkins, M. H. T. Bui, and D. Zhu, Phys. Rev. **A37**, 4071 (1988).

[24] G. S. Adkins, Y. M. Aksu, and M. H. T. Bui, Phys. Rev. **A47**, 2640 (1993).

[25] G. S. Adkins, R. N. Fell, and P. M. Mitrikov, Phys. Rev. Lett. **79**, 3383 (1997).

[26] A. H. Hoang, P. Labelle, and S. M. Zebarjad, Phys. Rev. Lett. **79**, 3387 (1997).

[27] J. R. Sapirstein, E. A. Terray, and D. R. Yennie, Phys. Rev. **D29**, 2290 (1984).

[28] K. Pachucki and S. G. Karshenboim, Phys. Rev. Lett. **80**, 2101 (1998).

[29] G. S. Adkins and J. Sapirstein, Phys. Rev. **A58**, 3552 (1998).

[30] I. B. Khriplovich, A. I. Milstein, and A. S. Yelkhovsky, Phys. Scr. **T46**, 252 (1993).

[31] I. B. Khriplovich, A. I. Milstein, and A. S. Yelkhovsky, Phys. Rev. Lett. **71**, 4323 (1993).

[32] I. B. Khriplovich, A. I. Milstein, and A. S. Yelkhovsky, JETP **78**, 159 (1994).

[33] S. N. Gupta, *Quantum Electrodynamics* (Gordon and Breach, New York, 1977).

[34] A. Czarnecki and K. Melnikov, Phys. Rev. Lett. **80**, 2531 (1998).

[35] M. Beneke, A. Signer, and V. A. Smirnov, Phys. Rev. Lett. **80**, 2535 (1998).

[36] K. G. Chetyrkin and F. Tkachov, Nucl. Phys. **B192**, 159 (1981).

[37] R. N. Fell, Phys. Rev. Lett. **68**, 25 (1992).

[38] R. N. Fell, I. B. Khriplovich, A. I. Milstein, and A. S. Yelkhovsky, Phys. Lett. **A181**, 172 (1993).

[39] M. I. Eides and H. Grotch, Phys. Rev. **A52**, 1757 (1995).
[40] J. R. Sapirstein, E. A. Terray, and D. R. Yennie, Phys. Rev. **D29**, 2290 (1984).
[41] T. Udem, A. Huber, B. Gross, J. Reichert, M. Prevedelli, M. Weitz, and T. W. Hänsch, Phys. Rev. Lett. **79**, 2646 (1997).
[42] A. Czarnecki and W. J. Marciano, to appear in the Proceedings of the 5th Intl. Workshop on Tau Lepton Physics (TAU 98), Santander, Spain, 1998 [hep-ph/9810512].
[43] S. G. Karshenboim, JETP **76**, 41 (1993).
[44] K. Melnikov and A. Yelkhovsky, to be published.
[45] A. Burichenko, private communication.
[46] G. W. F. Drake and R. A. Swainson, Phys. Rev. **A41**, 1243 (1990).

TABLES

TABLE I. Theoretical predictions for experimentally relevant positronium transitions.

Transition	Theory [MHz]
$2^3S_1 - 1^3S_1$	1233 607 222.33(65)
$1^3S_1 - 1^1S_0$	203 392.01(46)
$2^3S_1 - 2^3P_0$	18498.22(9)
$2^3S_1 - 2^3P_1$	13012.38(9)
$2^3S_1 - 2^3P_2$	8626.69(9)
$2^3S_1 - 2^1P_1$	11185.35(9)
$2^3S_1 - 2^1S_0$	25424.67(6)

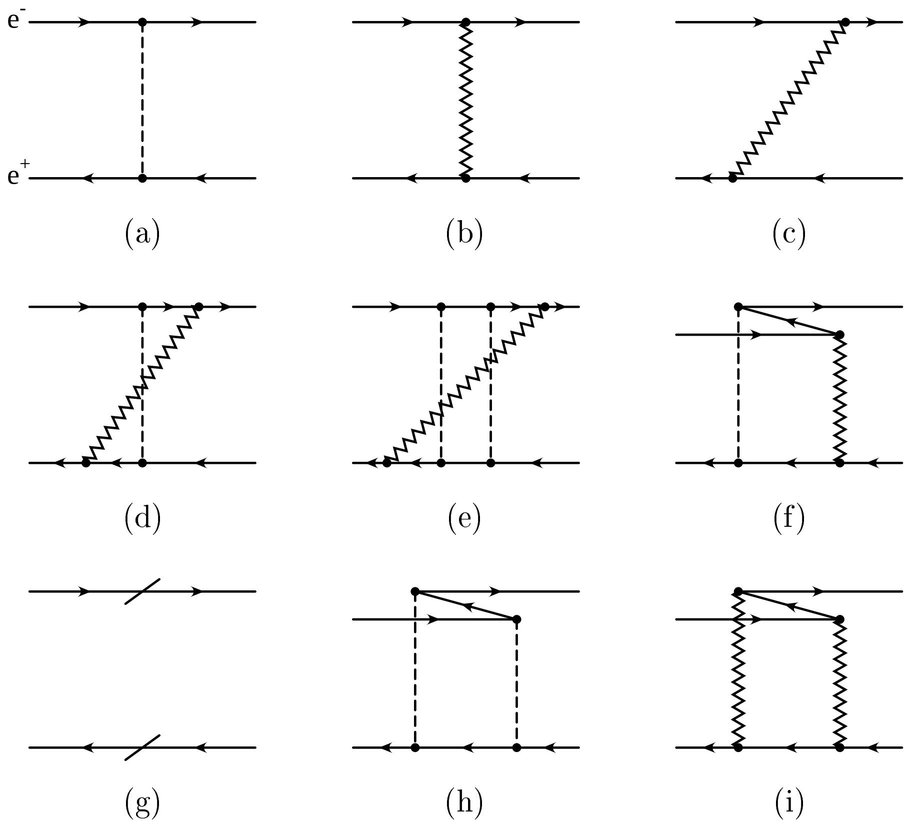

FIG. 1. Non-relativistic corrections to HFS and spin-averaged energy levels: (a,b) Coulomb and magnetic photon exchange; (c,d,e) retardation effects; (f) mixed Coulomb-magnetic exchange; (g) relativistic correction to the dispersion law; (h,i) double Coulomb and magnetic exchange.

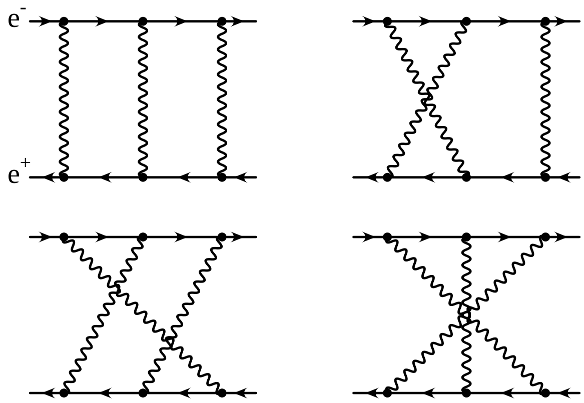

FIG. 2. Feynman diagrams representing pure recoil corrections to positronium HFS and spin-averaged energy levels. Wiggly lines denote photons in Feynman gauge.

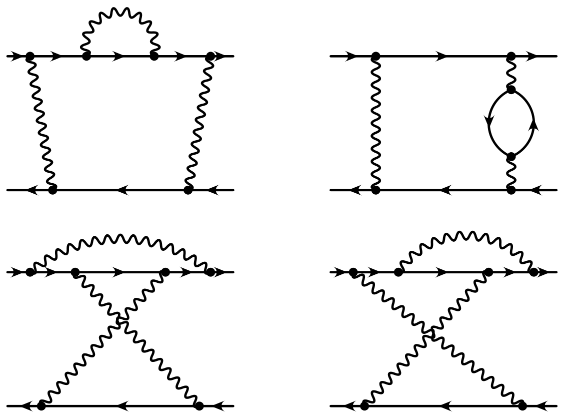

FIG. 3. Examples of radiative recoil corrections to positronium HFS and spin-averaged energy levels.