Recoil Effects in Positronium Energy Levels to Order α^6

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Corrections to the positronium energy levels of order α^6 due to photon exchanges are calculated in the effective Hamiltonian approach. The quoted results are valid for all S-states and arbitrary mass ratios. We further present implications on the comparison of theory and experiment.

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I. INTRODUCTION

Positronium is a fundamental system for the study of quantum electrodynamics theory (QED). Consisting of an electron and a positron, it includes only negligible contributions from strongly interacting particles. For these reasons, one can calculate the positronium energy levels with a high accuracy, unlimited by the finite nuclear size effect. In contrast, theoretical predictions for the Lamb shift and hyperfine structure of hydrogen are limited by the uncertainty in the proton electric and magnetic formfactors. Therefore positronium opens a window for high precision QED tests. The ground state hyperfine structure (HFS) and the sharp 1^3S_1-2^3S_1 two-photon transition are particularly interesting.

The theoretical treatment of bound states is a distinguished problem in quantum electrodynamics (QED). The Bethe-Salpeter equation [1] provides a starting point for most of the calculations. In a previous paper [2], we introduced a different approach to bound state QED and calculated a recoil correction of order α^6 to the HFS of nS-states. In this letter we complete the calculation of recoil corrections to the positronium S-levels. Our effective Hamiltonian approach is based on Lepage's idea of nonrelativistic quantum electrodynamics [3], on Khriplovich and coworkers calculations using Breit expansions [4], and on our previous calculations of the hydrogen Lamb shift and the hyperfine structure [5]. We construct an effective Hamiltonian, where all momenta are of the order of $m\,\alpha$, by introducing a cutoff parameter λ. The high momentum region is accounted for by adding δ-like terms. Coefficients for these terms are determined by comparing resolvents constructed from the QED Hamiltonian and those constructed from the effective Hamiltonian. The equivalence of both resolvents ensures that the poles, i.e. the energy levels, are at the same position. The calculation of Khriplovich *et al.* of the positronium P-levels [4] was performed without any cutoff. Such a treshold was not required since the P-wave function vanishes at the origin, however, for S-states the corresponding corrections would diverge, and therefore a cutoff is necessary to keep all the terms finite and meaningful.

II. POSITRONIUM ENERGY LEVELS

The main structure of the positronium spectrum is obtained from the nonrelativistic Hamiltonian:

$$H_S = \frac{p^2}{2\,\mu} - \frac{\alpha}{r}\,, \tag{1}$$

where μ denotes the reduced mass of the system and is equal to half of the electron mass for positronium. The corresponding eigenenergies are:

$$E_n = -\frac{\mu\,\alpha^2}{2\,n^2} = -\frac{m\,\alpha^2}{4\,n^2}\,. \tag{2}$$

Leading relativistic effects, of order α^4, are correctly described by the Breit interaction (cf. Eq. (10)). These include relativistic corrections to the kinetic energy, as well as to the spin-orbit, spin-spin, and annihilation effects. In the following, we consider only triplet S-states, i.e. states with $L = 0$ and $S = 1$. These relativistic corrections sum to [6]:

$$E^{(4)} = \frac{m\,\alpha^4}{2\,n^3}\,\left(\frac{11}{32\,n} + \frac{1}{6}\right)\,. \tag{3}$$

There are many sources for corrections of the order of α^5. For triplet S-states they are: electron and positron self-energy, the vacuum polarization, two-photon exchange, and a one-loop correction to the one-photon annihilation [7]. The complete formula describing these terms is [8]:

$$E^{(5)} = \frac{m\,\alpha^5}{8\,\pi\,n^3}\left\{\frac{14}{3}\left[\ln\left(\frac{2}{n}\right) + \Psi(n) + C + \frac{1}{2\,n}\right]\right.$$
$$\left. -\frac{13}{5} + \frac{2}{3}\,\ln 2 - \frac{16}{3}\,\ln k_0(n) - 6\,\ln(\alpha)\right\}, \tag{4}$$

where Ψ is a logarithmic derivative of Euler Γ function and C denotes the Euler constant. The calculation of the α^6 correction has not yet been completed. The leading terms, enhanced by $\ln\alpha$, come from two sources. First,

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the one-photon annihilation contribution [9] can be written as

$$\Delta E^{(6)} = \frac{m\,\alpha^6}{n^3}\left(-\frac{1}{24}\ln(\alpha) + K(n)\right)\,, \tag{5}$$

where $K(n)$ denotes a constant term. The second term results from the spin dependent part of the three photon exchange [10]. A complete formula is obtained from [2] by putting $m_1 = m_2 = m$ and dividing by 4 to get the shift of the triplet state:

$$\Delta E^{(6)} = \frac{m\,\alpha^6}{12\,n^3}\left[1.130(5) + \frac{1}{2}\left(\ln(n) - \Psi(n) - C\right)\right.$$
$$\left. -\frac{3}{2\,n^2} + \frac{7}{4\,n} - \frac{1}{4} - \frac{1}{2}\ln(\alpha)\right]. \tag{6}$$

The calculation of the spin independent part of $\Delta E^{(6)}$ is presented in the following section. As it was found in [11], this contribution does not lead to $\ln(\alpha)$ terms.

III. DETAILS OF THE CALCULATION

Some details of the method used in our work have been described in [2]. There are two energy regions in the integrals which generate the α^6 term. The low energy scale is given by the inverse of Bohr radius, and the high energy scale is governed by the electron mass. In our method an artificial parameter λ is introduced to separate these two regions and allow the use of expansions specific to each energy region. There is a freedom, how the parameter λ is introduced. Our choice is the following:

$$\frac{1}{k^2} \to \frac{1}{k^2}\,\frac{\Lambda^2}{\boldsymbol{k}^2 + \Lambda^2}\,, \tag{7}$$

where $\Lambda = \lambda\,\mu\,\alpha$. This replacemend defines the low energy part. In the case of the Coulomb interaction it takes the form:

$$V = -\frac{\alpha}{r} \to -\frac{\alpha}{r}\left(1 - e^{-\lambda\,\mu\,\alpha\,r}\right)\,. \tag{8}$$

Since the value of λ is arbitrary, after the expansion in α, we can also expand in $1/\lambda$. This allows the calculation of all necessary matrix elements, without knowledge of the exact wave function in the modified Coulomb potential.

In the first step one finds an effective Hamiltonian

$$H_{EF} = \frac{p^2}{2\,\mu} - \frac{\alpha}{r}\left(1 - e^{-\lambda\,\mu\,\alpha\,r}\right) + \Delta H^{(4)} + \Delta H^{(5)}$$
$$+\Delta H^{(6)} + \alpha^2 M_5\,\delta^3(r) + \alpha^3\,M_6\,\delta^3(r)\,. \tag{9}$$

The $\Delta H^{(i)}$ account for the low momentum region, while the M_j coefficients account for the contributions from for high momentum regime. All terms depend on λ. $\Delta H^{(4)}$ is a Breit Hamiltonian

$$\Delta H^{(4)} = -\frac{p^4}{8\,m_1^3} - \frac{p^4}{8\,m_2^3} + \frac{\pi\,\alpha}{2}\left(\frac{1}{m_1^2} + \frac{1}{m_2^2}\right)\delta^3(r)$$
$$-\frac{\alpha}{2\,m_1\,m_2\,r}\left(p^2 + \frac{r^i\,r^j}{r^2}\,p^i\,p^j\right) - \frac{\alpha}{4\,m_1\,m_2}$$
$$\cdot\left(\frac{\boldsymbol{\sigma}_1\,\boldsymbol{\sigma}_2}{r^3} - \frac{3\,\boldsymbol{\sigma}_1\boldsymbol{r}\;\boldsymbol{\sigma}_2\boldsymbol{r}}{r^5} - \frac{8}{3}\,\pi\,\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\,\delta^3(r)\right)\,, \tag{10}$$

which must be regularized according to the prescription in Eq. (7), otherwise matrix elements in Eq. (11) would be divergent. We will keep the two masses different throughout the calculation to permit a comparison with known corrections in the hydrogen atom. $\Delta H^{(5)}$ and $\Delta H^{(6)}$ are Breit-like Hamiltonians obtained by the higher order expansion in momenta. $\Delta H^{(6)}$ comes from time ordered diagrams presented in Fig. 1. This calculation is done in the Coulomb gauge, which is the most appropriate one for this problem. A dashed line denotes a Coulomb interaction, while a wavey line denotes a transverse photon. The nominal contribution from double transverse-double pair diagrams is of the order of α^5. The retarded part and the single Coulomb exchange cancel each other at order α^6. Another cancellation effect allows the "Z" subdiagram to be treated as a point interaction.

The contribution of the $\Delta H^{(i)}$ to the energy in the order of α^6 is calculated according to standard perturbation theory

$$\Delta E_L = \left\langle\phi|\Delta H^{(6)}|\phi\right\rangle + \left\langle\phi|\Delta H^{(4)}\,\frac{1}{(E-H)'}\,\Delta H^{(4)}|\phi\right\rangle\,. \tag{11}$$

All matrix elements are calculated analytically in the limit of large λ. As an example, consider the term

$$\left\langle\frac{p^4}{8}\,\frac{1}{(E-H)'}\,\frac{p^4}{8}\right\rangle =$$
$$-\frac{1}{8}\,\langle V'^2\rangle + \frac{1}{2}\,\langle V^3\rangle - \frac{1}{n^3} - \frac{3}{2\,n^4} + \frac{3}{n^5} - \frac{5}{8\,n^6}\,, \tag{12}$$

where V is defined in Eq. (8) and

$$\langle V'^2\rangle = \frac{8}{n^3}\left[\frac{\lambda}{4} + \ln\left(\frac{3}{\lambda}\right) - \frac{11}{12} + \frac{1}{6\,n^2} + \frac{1}{2\,n}\right.$$
$$\left. +\Psi(n) + C - \ln(n)\right],$$
$$\langle V^3\rangle = -\frac{4}{n^3}\left[\ln\left(\frac{\lambda}{4}\right) + \ln\left(\frac{3}{4}\right) + \frac{1}{2} - \frac{1}{2\,n}\right.$$
$$\left. + \ln(n) - \Psi(n) - C\right]. \tag{13}$$

The divergent terms those which are linear or logarithmic in λ, are canceled by the coefficients M_i:

$$\Delta E_H = \left\langle\phi|\alpha^2\,M_5\,\delta^3(r)|\phi\right\rangle^{(6)} + \left\langle\phi|\alpha^3\,M_6\,\delta^3(r)|\phi\right\rangle\,. \tag{14}$$

M_5 is obtained by comparing the two-photon scattering amplitudes derived from QED and from the effective Hamiltonian. In analogy, M_6 is obtained by comparing three photon scattering amplitudes. The contribution from M_5 to the energy in the order of α^6 is due to its linear divergence in λ

$$\langle\alpha^2\, M_5\, \delta^3(r)\rangle^{(6)} = \frac{\lambda\,\alpha^3}{2\,m_1\,m_2}\left(\frac{\mu^2}{m_1\,m_2} - 1\right)\,\phi^2_\lambda(0)\,, \quad (15)$$

where $\phi^2_\lambda(0) = \phi^2(0)\,(1-4/\lambda)$. It was convenient in this calculation to combine the λ dependence of the wave function at the origin with M_6. Therefore, M_5 only cancels out the linear divergence in λ in Eq. (11), and the expression for the high energy part is:

$$\Delta E_H = \frac{\alpha^6\,\mu^3}{n^3\,m_1\,m_2}\,T \quad (16)$$

$$\begin{aligned} T = \frac{1}{16\,\pi^4}\int d^3p_1\,d^3p_2\,\frac{1}{p_1^4\,q^2\,p_2^4}\Big\{&g(p_1,q,p_2) \\ -\frac{\Lambda^2}{p_1^2+\Lambda^2}\,\frac{\Lambda^2}{q^2+\Lambda^2}\,\frac{\Lambda^2}{p_2^2+\Lambda^2}\,&g^{(4)}(p_1,q,p_2) \\ -g(0,p_2,p_2) + \left(\frac{\Lambda^2}{p_2^2+\Lambda^2}\right)^2 &g^{(4)}(0,p_2,p_2) \\ -g(p_1,p_1,0) + \left(\frac{\Lambda^2}{p_1^2+\Lambda^2}\right)^2 &g^{(4)}(p_1,p_1,0)\Big\}. \quad (17)\end{aligned}$$

The function g is obtained from the forward scattering three-photon exchange amplitude at zero momentum by integration with respect to two photon energies and the subtraction of lower order terms which correspond to $H_S, \Delta H^{(4)}$ and $\Delta H^{(5)}$. The $g^{(4)}$ is a leading term in the power expansion of g in momenta, and is of the order p^4. The algebraic expression for g is very long, so special care has to be taken to generate a numerically stable expression without any spurious singularities. This was achieved by writing diagrams in mixed time-momentum representation, and by integrating with respect to the time coordinate of each vertex. This calculation directly corresponds to the standard Rayleigh-Schrödinger perturbation theory. For small momenta we take the leading term in the power expansion. There are additional terms which we subtract from g because they contribute at photon energies of order α^2. They are the nonrelativistic single transverse retardation diagrams No. 5, 6, 7 on Fig. 1. These term are ultraviolet finite and are calculated directly. The additional subtraction leads to logarithmic dependence on λ in (17). The three-dimensional numerical integration of T is done to quadrupole precision using Gaussian method with 15 and 30 points [12]. Errors are estimated by comparing both values. The sum of all terms leads to the expression which is the main result of this work:

$$\begin{aligned}\Delta E^{(6)} = \frac{\mu\,\alpha^6}{n^3}\,\Bigg[&\left(-\frac{1}{8} - \frac{5}{16\,n^3} + \frac{3}{4\,n^2} - \frac{3}{8\,n}\right) \\ &+ \frac{\mu^2}{m_1\,m_2}\left(F + \frac{3}{16\,n^3} - \frac{1}{4\,n^2}\right) \\ &- \frac{\mu^4}{m_1^2\,m_2^2}\,\left(\frac{1}{16\,n^3} + \frac{1}{3\,n^2} + \frac{2}{n}\right)\Bigg]. \quad (18)\end{aligned}$$

The first term corresponds to the Dirac formula for hydrogenic energy levels with the electron mass replaced by the reduced mass. The second term agrees with the recoil correction calculated in [13] and independly confirmed in [14]. F is a sum of n-independent terms but it depends on the mass ratio. For $m_1/m_2 \to 0$ F is $F = -0.727(1)$, which is very close to the number: $4\,\ln 2 - 7/2 = -0.727411$. We regard this agreement as a significant test of these calculations. For positronium $m_1 = m_2$, and thus

$$F = -1.573(5)\,. \quad (19)$$

Fig. 2 is a plot of F for intermediate values of m_1/m_2 The third term in Eq. (18) is completely new, and none of our tests could check its correctness. Eq. (18) completes the calculation of the pure photon exchange correction of the order of α^6. For positronium it becomes

$$\Delta E^{(6)} = \frac{m\,\alpha^6}{8\,n^3}\,\left(-2.073(5) - \frac{69}{64\,n^3} + \frac{8}{3\,n^2} - \frac{2}{n}\right)\,. \quad (20)$$

IV. CONCLUSIONS

We have developed a novel approach to quantum electrodynamics of the bound states and calculated the photon exchange contribution to positronium energy levels in the order of α^6. Using Eq. (6) and Eq. (20), one can find a correction to the 1^3S_1-2^3S_1 transition in the order of α^6 beyond previously known $\ln\alpha$ terms which is

$$\Delta E = 3.5\ \text{MHz}\,. \quad (21)$$

The corrected theoretical prediction for the 1^3S_1-2^3S_1 transition becomes

$$E_{th} = 1\,233\,607\,224.9(8.2)\ \ \text{MHz}\,. \quad (22)$$

where the error is estimated assuming a coefficient 1/2 for the unknown terms of order $m\,\alpha^6$. The measurement of Fee *et al.* [15] gives

$$E_{exp} = 1\,223\,607\,216.4\,(3.2)\ \ \text{MHz}\,. \quad (23)$$

Although the agreement within an error is maintained, the new correction increases the deviation from the measured value. The theoretical predictions are still limited by unknown other terms in the order of α^6, such as radiative recoil or a single photon anihilation. Calculation of the latter one, has recently been completed by Adkins *et al* [16], and independly by Hoang *et al.* [17]. We point out that for positronium, the logarithmic corrections of order

$\alpha^7 \ln^2(\alpha^{-2})$ might be important at the current precision level.

An additional motivation for our work is the problem of the calculation of the helium energy levels in the order of α^6. There have been several high precision measurements of the Lamb shift of the singlet 1S ground state [18], and the metastable triplet 2S state [19]. It is a challenge for theorists to formulate a formalism for the calculation of this correction. We believe that the method developed here could be used in a more complex system like the helium atom.

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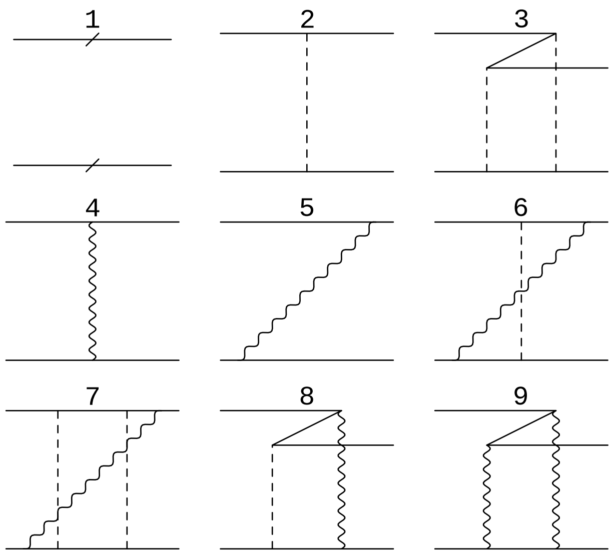

FIG. 1. Time ordered diagrams contributing to energy levels in α^6 order

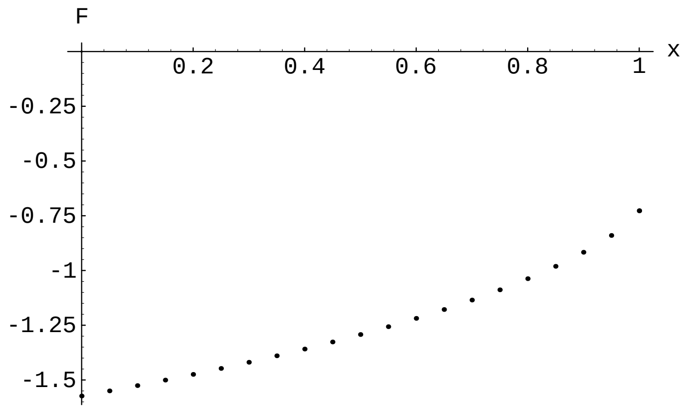

FIG. 2. Numerical values of F as a function of $x = (m_1 - m_2)^2/(m_1 + m_2)^2$