Effective Hamiltonian approach to the bound state: Positronium hyperfine structure

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(Received 17 March 1997)

An effective Hamiltonian approach is developed for the perturbative calculation of bound state energies in quantum electrodynamics. In this approach a recoil correction of order $\alpha^2 E_F$ to the hyperfine structure of hydrogenic systems with the arbitrary mass ratio is obtained. In the case of the positronium it amounts to $\Delta E = \frac{1}{3} m\alpha^6 [1.130(5) - \frac{1}{2}\ln\alpha]$. [S1050-2947(97)06807-8]

PACS number(s): 36.10.Dr, 06.20.Jr, 12.20.Ds, 31.30.Jv

I. INTRODUCTION

The treatment of bound states in quantum electrodynamics is a challenging task. Particularly interesting are systems consisting of two or three bodies where the calculation comparable with the precision of measurements could be performed. The Bethe-Salpeter formalism is a good starting point for the derivation and a subsequent calculation of various corrections to energy levels of simple atomic systems. This approach with its application to the positronium was presented in detail by Adkins in [1]. We present here an alternative approach based on an effective Hamiltonian. Our approach joins three original ideas of Lepage nonrelativistic quantum electrodynamics [2], calculations of Khriplovich and co-workers [3] using Breit Hamiltonians, and ours which was used in the evaluation of hydrogen Lamb shift [4] and hyperfine splitting [5]. We construct an effective Hamiltonian in the two-body subspace with the regularized Coulomb potential by introducing an extra parameter λ. This Hamiltonian is obtained by the Breit expansion of effective two-body interactions and by adding δ-like terms derived from corresponding S-matrix elements. The presence of a regulator ensures that the Breit Hamiltonian is finite. We apply this approach to the Dirac-Coulomb equation, to present the perturbative calculation of hydrogen energy levels in α^6 order. Next, we demonstrate our method on a less simple model described by the Hamiltonian $H=\sqrt{p^2+m^2}-\alpha/r$. This model resembles some features of real two-body systems. The calculation of its nS energy levels through the order of α^6 is presented in detail. After these simple examples we consider a hyperfine structure of a two-body system in the order of α^6 with the arbitrary mass ratio and check results against already known special cases of the muonium and positronium ground state hyperfine structure (hfs). In the summary we analyze the possible extension of this approach to the calculation of corresponding corrections to the helium energy levels.

II. DIRAC-COULOMB ENERGY LEVELS FROM PERTURBATIVE APPROACH

The Dirac-Coulomb Hamiltonian is given by the expression

$$H_{\rm DC} = \boldsymbol{\alpha}\cdot\mathbf{p} + \beta m - \frac{\alpha}{r}. \tag{1}$$

The corresponding eigenvalue problem $H_{\rm DC}|\psi\rangle = E|\psi\rangle$ has the following solution:

$$E(n,j) = m\left(1 + \frac{\alpha^2}{[n-j-\frac{1}{2}+\sqrt{(j+\frac{1}{2})^2-\alpha^2}]^2}\right)^{-1/2}, \tag{2}$$

where n is the principal number and j is the total angular momentum of the electron. The expansion of E in α reads

$$E(n,j) = m\left\{1 - \frac{\alpha^2}{2n^2} + \alpha^4\left[\frac{3}{8n^4} - \frac{1}{2(\frac{1}{2}+j)n^3}\right] + \alpha^6\left[-\frac{5}{16n^6} + \frac{3}{4(\frac{1}{2}+j)n^5} - \frac{3}{8(\frac{1}{2}+j)^2 n^4} - \frac{1}{8(\frac{1}{2}+j)^3 n^3}\right]\right\}. \tag{3}$$

We would like here to calculate the energy levels up to the order of α^6 using perturbative methods as an introduction to the more complex positronium case. The leading term $-m\alpha^2/(2n^2)$ is derived from the Schrödinger-Coulomb Hamiltonian H_S,

$$H_S = \frac{p^2}{2m} - \frac{\alpha}{r}. \tag{4}$$

The first relativistic correction could be calculated from the Foldy-Wouthuysen transformed Hamiltonian, namely,

$$\Delta H^{(4)} = -\frac{1}{8m^3}p^4 + \frac{\pi\alpha}{2m^2}\delta^3(r) + \frac{\alpha}{4m^2r^3}\boldsymbol{\sigma}\cdot\mathbf{L}. \tag{5}$$

where $\boldsymbol{\sigma}$ are Pauli matrices and $\mathbf{L}$ is an angular-momentum operator. The correction to energy

$$\Delta E^{(4)} = \langle\phi|\Delta H^{(4)}|\phi\rangle \tag{6}$$

coincides with the third term in Eq. (3). The problem appears in the evaluation of the next order correction, i.e., $\Delta E^{(6)}$. Matrix elements of, for example, $\langle\phi|p^6|\phi\rangle$ and

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$$\left\langle\phi\left|\delta^{(3)}(r)\frac{1}{(E-H_S)'}\delta^{(3)}(r)\right|\phi\right\rangle \tag{7}$$

are divergent for S states. This divergence, when properly regularized, would cancel out where all terms are summed up. So, we modify the Coulomb potential near the singularity by the following replacement in Eq. (1):

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

The Schrödinger equation with this potential is no longer solvable, but it is not a problem. One calculates all corrections to the energy in the limit of large λ. The λ divergent terms are kept till they cancel out in the final expression. The Foldy-Wouthuysen transformation could be extended to obtain higher order terms in the regularized Hamiltonian $\Delta H^{(6)}$. An equivalent method for finding higher order terms, which is at the base of our approach, relies on the resolvent. One finds such an effective Hamiltonian that the corresponding resolvents are equal up to the specified order of α^n in the limit of infinitely large λ, namely,

$$\left\langle +,p,\beta\left|\frac{1}{E-H_{\rm DC}}\right|\beta',p',+\right\rangle^{(n)} = \lim_{\lambda\to\infty}\left\langle p,\beta\left|\frac{1}{E-H_{EF}(\lambda,E)}\right|p',\beta'\right\rangle^{(n)}, \tag{9}$$

where $\langle +,p,\beta|$ denotes a four-component bispinor corresponding to a positive energy solution of the free Dirac equation, and $\langle p,\beta|$ denotes a two-component spinor. In the α expansion in Eq. (9) we keep energy E and momenta p,p' of order α^2 and α, respectively. The first terms describing corrections to the energy take a form

$$\Delta E=\langle\phi|\Delta H(E_0)|\phi\rangle+\langle\phi|\Delta H(E_0)\frac{1}{(E_0-H_S)'}\Delta H(E_0)|\phi\rangle + \langle\phi|\Delta H(E_0)|\phi\rangle\left.\frac{d}{dE}\right|_{E=E_0}\langle\phi|\Delta H(E)|\phi\rangle. \tag{10}$$

Using Eq. (9) one obtains for $\Delta H^{(6)}$

$$\Delta H^{(6)}=\frac{p^6}{16m^5}-\frac{1}{8m^3}\left[\mathbf{p};\frac{\alpha}{r}\right]^2-\frac{3}{64m^4}\left(p^2\left[\mathbf{p};\left[\mathbf{p};\frac{\alpha}{r}\right]\right]+\left[\mathbf{p};\left[\mathbf{p};\frac{\alpha}{r}\right]\right]p^2\right)-\frac{5}{128m^4}\left[p^2;\left[p^2;\frac{\alpha}{r}\right]\right]+\frac{3}{32m^4}\boldsymbol{\sigma}\cdot\mathbf{L}\left(p^2\frac{\alpha}{r^3}+\frac{\alpha}{r^3}p^2\right). \tag{11}$$

$\Delta H^{(6)}$ for the regularized potential is obtained by the replacement (8). The terms proportional to $\boldsymbol{\sigma}\cdot\mathbf{L}$ do not need to be regularized because they act on states with $l\neq 0$. Having $\Delta H^{(4)}$ and $\Delta H^{(6)}$ the correction to energy in the order of α^6 could be expressed as

$$\Delta E^{(6)}=\langle\phi|\Delta H^{(6)}|\phi\rangle+\left\langle\phi\left|\Delta H^{(4)}\frac{1}{(E-H)'}\Delta H^{(4)}\right|\phi\right\rangle. \tag{12}$$

The state ϕ in the above fulfills the Schrödinger equation with the regularized potential and from now it has $l=0$. We subsequently use this equation and commutation rules to express Eq. (12) in terms of known matrix elements:

$$\langle H\rangle=E=-\frac{1}{2n^2}, \tag{13}$$

$$\left\langle\frac{1}{r}\right\rangle=\frac{1}{n^2}, \tag{14}$$

$$\left\langle\frac{1}{r^2}\right\rangle=\frac{2}{n^3}, \tag{15}$$

$$\left\langle\mathbf{p}\,\frac{1}{r^2}\mathbf{p}\right\rangle=\frac{8}{3n^3}-\frac{2}{3n^5}, \tag{16}$$

$$\left\langle\frac{1}{r}\,4\pi\delta^3(r)\right\rangle_\lambda=\left\langle\frac{1}{r^4}\right\rangle_\lambda+2\left\langle\frac{1}{r^3}\right\rangle_\lambda-\frac{8}{3n^3}-\frac{4}{3n^5}. \tag{17}$$

The subscript λ means the expression to be regularized, i.e.,

$$\left\langle\frac{1}{r^4}\right\rangle_\lambda\equiv\langle V'^{\,2}\rangle, \tag{18}$$

$$\left\langle\frac{1}{r^3}\right\rangle_\lambda\equiv-\langle V^3\rangle, \tag{19}$$

$$\left\langle\frac{1}{r}4\pi\delta^3(r)\right\rangle_\lambda\equiv-\langle V\Delta(V)\rangle. \tag{20}$$

The first term in Eq. (12) denoted by $\Delta E_1^{(6)}$ is transformed to the following form:

$$\Delta E_1^{(6)}=\frac{1}{32}\left\langle\frac{1}{r^4}\right\rangle_\lambda+\frac{1}{8}\left\langle\frac{1}{r^3}\right\rangle_\lambda+\frac{1}{2n^3}-\frac{7}{8n^5}-\frac{5}{16n^6}. \tag{21}$$

The calculation of the second term in Eq. (12) denoted by $\Delta E_2^{(6)}$ is more complicated. $\Delta H^{(4)}$ is to be regularized according to Eq. (8), namely,

$$4\pi\alpha\delta^3(r)\to 4\pi\alpha\delta^3(r)_\lambda\equiv\Delta(V). \tag{22}$$

$\Delta E_2^{(6)}$ could be rewritten as

$$\Delta E_2^{(6)}=\left\langle\phi\left|\frac{p^4}{8}\frac{1}{(E-H)'}\frac{p^4}{8}\right|\phi\right\rangle+\left\langle\phi\left|\frac{\pi}{2}\delta^3(r)_\lambda\frac{1}{(E-H)'}\frac{\pi}{2}\delta^3(r)_\lambda\right|\phi\right\rangle-2\left\langle\phi\left|\frac{p^4}{8}\frac{1}{(E-H)'}\frac{\pi}{2}\delta^3(r)_\lambda\right|\phi\right\rangle=E_A+E_B+E_C. \tag{23}$$

Each matrix element is divergent when λ goes to infinity. We extract this divergence in the form of the matrix element of $\langle 1/r^3\rangle$ and $\langle 1/r^4\rangle$, and the remainders become finite.

$$E_A=-\frac{1}{4}\left\langle\left(\frac{1}{r^2}+\frac{2E}{r}\right)\frac{1}{(H-E)'}\left(\frac{1}{r^2}+\frac{2E}{r}\right)\right\rangle-\frac{1}{8}\left\langle\frac{1}{r^4}\right\rangle_\lambda -\frac{1}{2}\left\langle\frac{1}{r^3}\right\rangle_\lambda+\frac{2}{n^5}-\frac{1}{2\,n^6}, \tag{24}$$

$$E_B=\frac{1}{16}\left\langle \mathbf{p}\cdot\mathbf{p}\left(\frac{1}{r}\right)\frac{1}{(H-E)'}\mathbf{p}\left(\frac{1}{r}\right)\cdot\mathbf{p}\right\rangle-\frac{1}{32}\left\langle\frac{1}{r^4}\right\rangle_\lambda-\frac{1}{8}\left\langle\frac{1}{r^3}\right\rangle_\lambda +\frac{1}{6n^3}+\frac{1}{3n^5}, \tag{25}$$

$$E_C=-\frac{1}{8}\left\langle\left(\frac{1}{r^2}+\frac{2E}{r}\right)\frac{1}{(H-E)'}\mathbf{p}\left(\frac{1}{r}\right)\cdot\mathbf{p}\right\rangle +\frac{1}{8}\left\langle \mathbf{p}\cdot\mathbf{p}\left(\frac{1}{r}\right)\frac{1}{(H-E)'}\left(\frac{1}{r^2}+\frac{2E}{r}\right)\right\rangle+\frac{1}{8}\left\langle\frac{1}{r^4}\right\rangle_\lambda +\frac{1}{2}\left\langle\frac{1}{r^3}\right\rangle_\lambda-\frac{1}{3n^3}-\frac{5}{3n^5}+\frac{1}{4n^6}, \tag{26}$$

where $\mathbf{p}(1/r)$ denotes $[\mathbf{p};1/r]$. All the divergent terms cancel out in $\Delta E^{(6)}$,

$$\Delta E^{(6)}=\Sigma+\frac{1}{3n^3}-\frac{5}{24n^5}+\frac{1}{16n^6}, \tag{27}$$

$$\Sigma=-\frac{1}{4}\left\langle\left[\frac{1}{r^2}+\frac{2E}{r}-\frac{1}{2}\mathbf{p}\cdot\mathbf{p}\left(\frac{1}{r}\right)\right]\frac{1}{(H-E)'} \times\left[\frac{1}{2}\mathbf{p}\left(\frac{1}{r}\right)\cdot\mathbf{p}+\frac{1}{r^2}+\frac{2E}{r}\right]\right\rangle. \tag{28}$$

Σ is already finite, it is calculated with the help of a relation which holds for $l=0$,

$$\mathbf{p}\left(\frac{1}{r}\right)\cdot\mathbf{p}=-i\left[H-E;\frac{\mathbf{r}}{r}\cdot\mathbf{p}\right]-\frac{1}{r^2}, \tag{29}$$

and using the fact that the radial Schrödinger equation could be solved for any real, positive α and l,

$$\Sigma=-\frac{11}{24n^3}-\frac{3}{8n^4}+\frac{23}{24n^5}-\frac{3}{8n^6}. \tag{30}$$

The complete correction to energy in the order of α^6,

$$\Delta E^{(6)}=-\frac{1}{8n^3}-\frac{3}{8n^4}+\frac{3}{4n^5}-\frac{5}{16n^6}, \tag{31}$$

coincides with the corresponding term in the expansion of the Dirac-Coulomb energy in powers of α, Eq. (3). This calculation shows that the Dirac-Coulomb energy levels could be calculated perturbatively with the use of an effective Hamiltonian. The cancellation effect, i.e., the cancellation of all divergent terms is a specific feature of the Dirac equation. In the case of the positronium, for example, the λ divergence does not cancel out. This means that there are some extra terms, which are forgotten in the nonrelativistic expansion. Before passing to the positronium we consider first a model which resembles some features of the positronium system and demonstrate that the effective Hamiltonian approach works for the calculation of its energy levels.

III. ENERGY LEVELS OF A MODEL HAMILTONIAN

The model, which demonstrates an effective Hamiltonian approach, is given by

$$H=\sqrt{p^2+m^2}-m-\frac{\alpha}{r}. \tag{32}$$

The corresponding eigenvalue problem is not solvable. To calculate energy levels in the order of α^6 one introduces an effective Hamiltonian H_{EF} which is determined by the condition (9),

$$H_{EF}=\frac{p^2}{2m}-\frac{\alpha}{r}(1-e^{-\lambda m\alpha r})-\frac{p^4}{8m^3}+\frac{p^6}{16m^5}+\alpha^2M_5\delta^3(r) +\alpha^3M_6\delta^3(r). \tag{33}$$

p^4 and p^6 terms are obtained by the expansion of the square root in Eq. (32). These extra M_i terms are necessary to fulfill the condition (9). It is our ansatz that they are proportional to the $\delta^3(r)$. The coefficients are calculated by comparing the difference in the forward scattering amplitude at zero momentum between H and H_{EF} and they depend on our regulator λ. This Hamiltonian is used to determine energy levels:

$$E^{(2)}=-\frac{m\alpha^2}{2n^2}, \tag{34}$$

$$\Delta E^{(4)}=\left\langle\phi\left|-\frac{p^4}{8m^3}\right|\phi\right\rangle, \tag{35}$$

$$\Delta E^{(5)}=\langle\phi|\alpha^2M_5\delta^3(r)|\phi\rangle, \tag{36}$$

$$\Delta E^{(6)}=\left\langle\phi\left|\frac{p^6}{16m^5}\right|\phi\right\rangle+\left\langle\phi\left|\frac{p^4}{8m^3}\frac{1}{(E-H)'}\frac{p^4}{8m^3}\right|\phi\right\rangle +\langle\phi|\alpha^2M_5\delta^3(r)|\phi\rangle^{(6)}+\langle\phi|\alpha^3M_6\delta^3(r)|\phi\rangle. \tag{37}$$

These matrix elements are calculated in a way similar to that in the previous case:

$$\Delta E^{(4)}=-\frac{m\alpha^4}{n^3}\left(1-\frac{3}{8n}\right), \tag{38}$$

$$\left\langle\phi\left|\frac{p^6}{16m^5}\right|\phi\right\rangle=\frac{1}{4}\left\langle\frac{1}{r^4}\right\rangle_\lambda+\frac{1}{2}\left\langle\frac{1}{r^3}\right\rangle_\lambda-\frac{3}{2n^5}+\frac{5}{16n^6}, \tag{39}$$

$$\left\langle \phi \left| \frac{p^4}{8m^3} \frac{1}{(E-H)'} \frac{p^4}{8m^3} \right| \phi \right\rangle = -\frac{1}{8}\left\langle \frac{1}{r^4} \right\rangle_\lambda - \frac{1}{2}\left\langle \frac{1}{r^3} \right\rangle_\lambda - \frac{1}{n^3} - \frac{3}{2n^4} + \frac{3}{n^5} - \frac{5}{8n^6}. \quad (40)$$

The matrix element $\langle 1/r^4 \rangle_\lambda$ does not cancel out in the sum, so we give its value

$$\left\langle \frac{1}{r^4} \right\rangle_\lambda = \frac{8}{n^3}\left[\frac{\lambda}{4} + \ln\left(\frac{3}{\lambda}\right) - \frac{11}{12} + \frac{1}{6n^2} + \frac{1}{2n} + \Psi(n) + C - \ln(n) \right]. \quad (41)$$

To complete the evaluation of energy levels one needs to determine M_5 and M_6. M_5 is given by the two-photon subtracted forward scattering amplitude at zero momentum,

$$M_5 = \int \frac{d^3p}{(2\pi)^3} \left\{ \frac{(4\pi)^2}{p^4} \left[\frac{1}{m-\sqrt{p^2+m^2}} + \frac{1}{2m} + \frac{2m}{p^2} \right] - \frac{(4\pi)^2}{p^4} \frac{\Lambda^4}{(p^2+\Lambda^2)^2} \frac{p^2}{8m^3} \right\} = \frac{1}{m^2}\left(\frac{8}{3} - \frac{\pi\Lambda}{4m} \right), \quad (42)$$

where $\Lambda = \lambda m \alpha$. The corresponding correction to the energy in the order of α^5 is

$$\Delta E^{(5)} = \frac{m\alpha^5}{n^3} \frac{8}{3\pi}. \quad (43)$$

M_6 is given by three-photon subtracted forward scattering amplitude,

$$\begin{aligned} M_6 = -\frac{1}{\pi^3} \int \frac{d^3p_1 d^3p_2}{p_1^4 p_2^4} \Bigg\{ & \frac{1}{q^2}[(m+\sqrt{m^2+p_1^2})(m+\sqrt{m^2+p_2^2}) - 4m^2 - p_1^2 - p_2^2] \\ & - \frac{\Lambda^2}{p_1^2+\Lambda^2} \frac{1}{q^2} \frac{\Lambda^2}{q^2+\Lambda^2} \frac{\Lambda^2}{p_2^2+\Lambda^2} \frac{(p_1^2p_2^2 - p_1^4 - p_2^4)}{4m^2} \\ & - \frac{1}{p_2^2}[2m(m+\sqrt{m^2+p_2^2}) - 4m^2 - p_2^2] \\ & + \frac{\Lambda^2}{p_1^2+\Lambda^2} \frac{1}{p_2^2} \frac{\Lambda^4}{(p_2^2+\Lambda^2)^2} \frac{(-p_2^4)}{4m^2} \\ & - \frac{1}{p_1^2}[2m(m+\sqrt{m^2+p_1^2}) - 4m^2 - p_1^2] \\ & + \frac{\Lambda^2}{p_2^2+\Lambda^2} \frac{1}{p_1^2} \frac{\Lambda^4}{(p_1^2+\Lambda^2)^2} \frac{(-p_1^4)}{4m^2} \Bigg\} \\ = \frac{\pi}{m^2}\left[\ln\left(\frac{\Lambda}{m}\right) - \frac{3}{2} + \frac{7}{\pi^2}\zeta(3) - \frac{2}{\pi^2} - \ln(3) \right]. \end{aligned} \quad (44)$$

The matrix element of the M_5 term in the order of α^6 requires additional treatment,

$$\langle \phi | \alpha^2 \delta^3(r) M_5 | \phi \rangle^{(6)} = \phi_\lambda^2(0)\alpha^2\left(-\frac{\pi\lambda\alpha}{4m^2} \right) = \frac{m\alpha^6}{n^3}\left(1 - \frac{\lambda}{4} \right). \quad (45)$$

We can now sum up all the terms in α^6 order. The result is

$$\Delta E^{(6)} = \frac{m\alpha^6}{n^3}\left[\ln(\alpha) + \frac{7}{\pi^2}\zeta(3) - \frac{2}{\pi^2} - \frac{33}{16} + \left(\Psi(n) + C - \ln(n) - \frac{1}{n} + \frac{5}{3n^2} - \frac{5}{16n^3} - \frac{17}{48} \right) \right]. \quad (46)$$

The correction to energy $\Delta E^{(6)}$ contains $\ln(\alpha)$, so the expansion in α is nonanalytic. It is the general feature of the bound state problems in QED. There are two energy scales in the problem: the binding energy and the electron mass. This effective Hamiltonian approach splits these two scales and allows us to treat them separately.

IV. POSITRONIUM HYPERFINE STRUCTURE

We will present here an effective Hamiltonian approach to the calculation of recoil effects of order α^2 to the positronium hyperfine structure. By recoil effects we mean all Feynman diagrams with photon exchanges, without photons created and absorbed by the same particle. We neglect also diagrams with closed fermion loops, they have already been calculated. The derivation of the effective Hamiltonian, from which one finds the energy spectrum, consists of two steps. The starting point is the Hamiltonian of full QED. The first step is the construction of an intermediate Hamiltonian in the two-body subspace and the reference frame with total momentum equal to zero,

$$\left\langle \mathbf{p}', -\mathbf{p}' \left| \frac{1}{E - H_{\rm QED}} \right| \mathbf{p}, -\mathbf{p} \right\rangle = \left\langle \mathbf{p}' \left| \frac{1}{E - H'_{EF}(E)} \right| \mathbf{p} \right\rangle, \quad (47)$$

where this equation holds for any momentum and up to three-photon exchange, i.e., up to the order α^3. In the second step we limit momenta and energy to be of the order α and α^2, respectively, by introducing parameter λ as it was in Eq. (9),

$$\left\langle \mathbf{p}' \left| \frac{1}{E - H'_{EF}(E)} \right| \mathbf{p} \right\rangle^{(n)} = \lim_{\lambda\to\infty} \left\langle \mathbf{p}' \left| \frac{1}{E - H_{EF}(\lambda, E)} \right| \mathbf{p} \right\rangle^{(n)}. \quad (48)$$

This effective Hamiltonian H_{EF} is obtained in parts by the application of Breit expansion to the higher order, and by adding the forward scattering amplitude terms. Since higher order terms would be divergent, we regularize the photon propagator by introducing a factor:

$$\frac{1}{k^2} \to \frac{1}{k^2} \frac{\Lambda^2}{\mathbf{k}^2 + \Lambda^2}, \quad (49)$$

where $\Lambda = \lambda\mu\alpha$ and μ is a reduced mass. This construction allows for an extension of the calculation of Khriplovich and co-workers [3] to the states with a zero angular momentum. In the case of, for example, P states the wave function vanishes at origin and all the Breit-type terms are finite and the contribution from M_i vanishes. In the case of S states we have to include also δ-like terms that correspond to the forward scattering amplitude to obtain a complete H_{EF},

$$H_{EF}=\frac{p^2}{2\mu}-\frac{\alpha}{r}(1-e^{-\lambda\mu\alpha r})+\Delta H^{(4)}+\Delta H^{(6)}+\alpha^2 M_5\delta^3(r)+\alpha^3 M_6\delta^3(r). \tag{50}$$

We start the calculation with the second order contribution from the Breit Hamiltonian for two charged particles with masses m_1 and m_2. We will keep both masses different for comparing with other results. The regularized Breit Hamiltonian reads

$$\Delta H^{(4)}\equiv H_B=-\frac{p^4}{8m_1^3}-\frac{p^4}{8m_2^3}+\frac{\pi\alpha}{2}\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)\delta^3(r)_\lambda-\frac{\alpha}{2m_1m_2r}\left(p^2+\frac{r^ir^j}{r^2}p^ip^j\right)_\lambda-\frac{\alpha}{4m_1m_2}\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3}-\frac{3\boldsymbol{\sigma}_1\cdot\mathbf{r}\ \boldsymbol{\sigma}_2\cdot\mathbf{r}}{r^5}-\frac{8}{3}\pi\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta^3(r)\right)_\lambda, \tag{51}$$

where $\delta^3(r)_\lambda$ was defined in Eq. (20), and

$$\frac{1}{r}\left(p^2+\frac{r^ir^j}{r^2}p^ip^j\right)_\lambda=\int\frac{d^3k}{(2\pi)^3}\frac{\Lambda^2}{k^2+\Lambda^2}\frac{4\pi}{k^2}\left(\delta^{ij}-\frac{k^ik^j}{k^2}\right)\times e^{-ikr}p^ip^j, \tag{52}$$

$$\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3}-\frac{3\boldsymbol{\sigma}_1\cdot\mathbf{r}\ \boldsymbol{\sigma}_2\cdot\mathbf{r}}{r^5}\right)_\lambda=\int\frac{d^3k}{(2\pi)^3}\frac{\Lambda^2}{k^2+\Lambda^2}\frac{4\pi}{k^2}\times\left(k^ik^j-\frac{\delta^{ij}}{3}k^2\right)e^{-ikr}\sigma_1^i\sigma_2^j. \tag{53}$$

The second order correction to hyperfine structure is a sum of five terms calculated as follows.

$$E_A=2\left\langle\left(-\frac{p^4}{8m_1^3}-\frac{p^4}{8m_2^3}\right)\frac{1}{(E-H)'}\times\frac{8}{3}\pi\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta^3(r)_\lambda\right\rangle\frac{\alpha}{4m_1m_2}=\frac{\mu^6\alpha^6}{6m_1m_2}\left(\frac{1}{m_1^3}+\frac{1}{m_2^3}\right)\times\left\{4\left\langle\frac{1}{r^4}\right\rangle_\lambda+16\left\langle\frac{1}{r^3}\right\rangle_\lambda+\frac{16}{3n^3}+\frac{48}{n^4}-\frac{136}{3n^5}\right\}, \tag{54}$$

$$E_B=2\left\langle\frac{\pi\alpha}{2}\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)\delta^3(r)_\lambda\frac{1}{(E-H)'}\times\frac{8}{3}\pi\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta^3(r)_\lambda\right\rangle\frac{\alpha}{4m_1m_2}=-\frac{\mu^5\alpha^6}{6m_1m_2}\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)\times\left\{2\left\langle\frac{1}{r^4}\right\rangle_\lambda+8\left\langle\frac{1}{r^3}\right\rangle_\lambda-\frac{40}{3n^3}+\frac{24}{n^4}-\frac{8}{3n^5}\right\}, \tag{55}$$

$$E_C=2\left\langle-\frac{\alpha}{2m_1m_2r}\left(p^2+\frac{r^ir^j}{r^2}p^ip^j\right)_\lambda\frac{1}{(E-H)'}\times\frac{8}{3}\pi\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta^3(r)_\lambda\right\rangle\frac{\alpha}{4m_1m_2}=\frac{4\mu^5\alpha^6}{3m_1^2m_2^2}\left\{2\left\langle\frac{1}{r^3}\right\rangle_\lambda+\frac{4}{n^3}\ln\left(\frac{4}{3}\right)+\frac{12}{n^3}+\frac{12}{n^4}-\frac{10}{n^5}\right\}, \tag{56}$$

$$E_D=\left\langle\frac{8}{3}\pi\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta^3(r)_\lambda\frac{1}{(E-H)'}\frac{8}{3}\pi\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta^3(r)_\lambda\right\rangle\times\left(\frac{\alpha}{4m_1m_2}\right)^2=\frac{2\mu^5\alpha^6}{9m_1^2m_2^2}\left\{2\left\langle\frac{1}{r^4}\right\rangle_\lambda+8\left\langle\frac{1}{r^3}\right\rangle_\lambda-\frac{40}{3n^3}+\frac{24}{n^4}-\frac{8}{3n^5}\right\}, \tag{57}$$

$$E_E=\left\langle\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3}-\frac{3\boldsymbol{\sigma}_1\cdot\mathbf{r}\ \boldsymbol{\sigma}_2\cdot\mathbf{r}}{r^5}\right)_\lambda\frac{1}{(E-H)'}\times\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3}-\frac{3\boldsymbol{\sigma}_1\cdot\mathbf{r}\ \boldsymbol{\sigma}_2\cdot\mathbf{r}}{r^5}\right)_\lambda\right\rangle\left(\frac{\alpha}{4m_1m_2}\right)^2 \tag{58}$$

$$=-\frac{\mu^5\alpha^6}{18n^3m_1^2m_2^2}\left\{4\lambda-20\ln\left(\frac{\lambda}{4}\right)-20\ln(n)+20\,[\Psi(n)+C]+6\ln\left(\frac{4}{3}\right)+\frac{3}{n^2}+\frac{10}{n}-\frac{61}{3}\right\}. \tag{59}$$

Matrix element $\langle 1/r^4\rangle_\lambda$ was given in Eq. (41), and

$$\left\langle\frac{1}{r^3}\right\rangle_\lambda=\frac{4}{n^3}\left[\ln\left(\frac{\lambda}{4}\right)+\ln\left(\frac{3}{4}\right)+\ln(n)-\Psi(n)-C+\frac{1}{2}-\frac{1}{2\,n}\right]. \tag{60}$$

The extension of the Breit Hamiltonian to the next order requires the calculation of diagrams presented in Fig. 1. Only some of them contribute to the hfs. The double-transverse–double-pair diagrams nominally contribute in the order of α^6 order but the retarded part and the single Coulomb exchange cancel out. Another cancellation effect allows us to treat the Z subdiagram as a point interaction. The calculation is done in the Coulomb gauge, as the most appropriate for

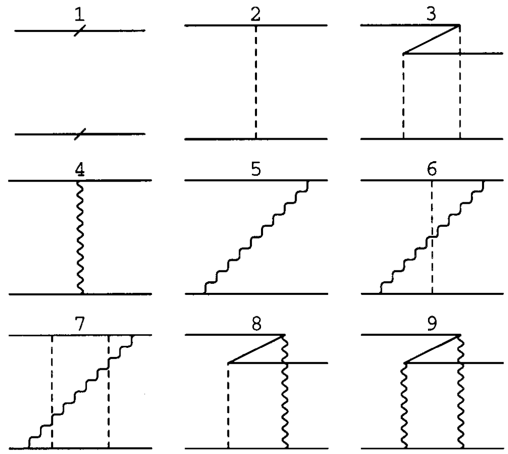

FIG. 1. Diagrams contributing to energy levels in α^6 order.

this problem. The dashed line denotes Coulomb interaction, and the wave line denotes transverse photon. The single Coulomb term is

$$E_2=\int\frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3}\phi(p)\phi(p')\frac{4\pi\alpha}{q^2}\frac{\Lambda^2}{\Lambda^2+q^2}\frac{1}{16m_1^2m_2^2}\times(\mathbf{p}'\times\mathbf{p}\cdot\boldsymbol{\sigma}_1)(\mathbf{p}'\times\mathbf{p}\cdot\boldsymbol{\sigma}_2)=\frac{\mu^5\alpha^6}{6m_1^2m_2^2}\left[\left\langle\frac{1}{r^3}\right\rangle_\lambda+\frac{2}{n^3}\ln\left(\frac{3}{4}\right)-\frac{1}{3n^3}-\frac{5}{3n^5}\right]. \tag{61}$$

The single transverse term without retardation is

$$E_4=\int\frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3}\phi(p)\phi(p')\frac{4\pi\alpha}{q^2}\frac{\Lambda^2}{\Lambda^2+q^2}\times\left(\delta^{ij}-\frac{q^iq^j}{q^2}\right)\frac{1}{4m_1m_2}\left\{\left[\frac{1}{4m_1^2}(p^2+p'^2)(\mathbf{q}\times\boldsymbol{\sigma}_1)^i-\frac{1}{8m_1^2}(p^2-p'^2)((\mathbf{p}+\mathbf{p}')\times\boldsymbol{\sigma}_1)^i\right](\boldsymbol{\sigma}_2\times\mathbf{q})^j+\left[\frac{1}{4m_2^2}(p^2+p'^2)(\mathbf{q}\times\boldsymbol{\sigma}_2)^i-\frac{1}{8m_2^2}(p^2-p'^2)((\mathbf{p}+\mathbf{p}')\times\boldsymbol{\sigma}_2)^i\right](\boldsymbol{\sigma}_1\times\mathbf{q})^j\right\}=\left\{-\frac{\mu^5\alpha^6}{3m_1m_2}\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)\left[3\left\langle\frac{1}{r^4}\right\rangle_\lambda+4\left\langle\frac{1}{r^3}\right\rangle_\lambda-\frac{16}{3n^3}-\frac{20}{3n^5}\right]\right\}. \tag{62}$$

The retardation terms with 0,1,2 Coulomb exchanges is

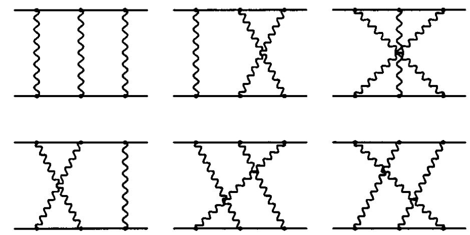

FIG. 2. Three-photon exchange forward scattering amplitude.

$$E_{567}=-e^2\int\frac{d^3k}{(2\pi)^3}\frac{1}{2k}\left(\delta^{ij}-\frac{k^ik^j}{k^2}\right)\frac{\Lambda^2}{\Lambda^2+k^2}\times\left\langle\frac{i}{2m_1}(\boldsymbol{\sigma}_1\times\mathbf{k})^i e^{i\mathbf{k}\cdot\mathbf{r}_1}\frac{1}{E-k-H}\frac{(-i)}{2m_2}(\boldsymbol{\sigma}_2\times\mathbf{k})^j e^{-i\mathbf{k}\cdot\mathbf{r}_2}\right\rangle^{(3)}+(1\leftrightarrow2)=-\frac{2\mu^5\alpha^6}{3m_1^2m_2^2}\left\langle\frac{1}{r^4}\right\rangle_\lambda. \tag{63}$$

The single Coulomb, single transverse, and single Z term is

$$E_8=-\int\frac{d^3p}{(2\pi)^3}\frac{d^3q_1}{(2\pi)^3}\frac{d^3q_2}{(2\pi)^3}\phi(p-q_1)\phi(p+q_2)\times\frac{\Lambda^2}{\Lambda^2+q_1^2}\frac{\Lambda^2}{\Lambda^2+q_2^2}\frac{e^2}{q_1^2}\frac{e^2}{q_2^2}\frac{1}{4m_1^2m_2}\left(\delta^{ij}-\frac{q_1^iq_1^j}{q_1^2}\right)\times(\boldsymbol{\sigma}_1\times\mathbf{q}_2)^i(\boldsymbol{\sigma}_2\times\mathbf{q}_1)^i+(1\leftrightarrow2)=\frac{2\mu^3\alpha^6}{3m_1m_2}\left\langle\frac{1}{r^4}\right\rangle_\lambda. \tag{64}$$

All other E_i terms do not contribute to hfs.

The high energy contribution denoted in analogy with the previous example by M_5 and M_6 is given by the subtracted two- and three-photon scattering amplitude, respectively, see Fig. 2. The expression for M_5 is simple,

$$M_5=-\frac{8}{m_2^2-m_1^2}\ln\left(\frac{m_2}{m_1}\right)+\frac{2\pi\lambda\alpha\mu^2}{3m_1^2m_2^2}. \tag{65}$$

The contribution from M_5 to energy in the order of α^6 reads

$$\langle\alpha^2M_5\delta^3(r)\rangle^{(6)}=\frac{2\lambda\alpha^6\mu^5}{3m_1^2m_2^2}\left(1-\frac{4}{\lambda}\right). \tag{66}$$

It was convenient in this calculation to combine the second term in parentheses in the above with M_6. Therefore M_5 will only cancel out the linear divergence in λ and the construction of the high energy part follows:

$$E_H=\frac{8}{3}\alpha^6\frac{\mu^5}{m_1^2m_2^2}T, \tag{67}$$

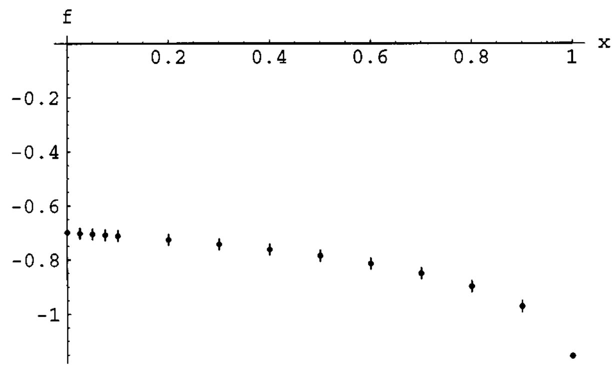

FIG. 3. Results of numerical integration of f in M_6, $x=(m_1-m_2)^2/(m_1+m_2)^2$; the value for $x=1$ is a known analytic result of Bodwin *et al.* [7].

$$T=\frac{1}{16\pi^4}\int d^3p_1 d^3p_2\frac{1}{p_1^4q^2p_2^4}\Bigg\{g(p_1,q,p_2)-\frac{\Lambda^2}{p_1^2+\Lambda^2}\frac{\Lambda^2}{q^2+\Lambda^2}\frac{\Lambda^2}{p_2^2+\Lambda^2}g^{(4)}(p_1,q,p_2)-g(0,p_2,p_2)+\left(\frac{\Lambda^2}{p_2^2+\Lambda^2}\right)^2g^{(4)}(0,p_2,p_2)-g(p_1,p_1,0)+\left(\frac{\Lambda^2}{p_1^2+\Lambda^2}\right)^2g^{(4)}(p_1,p_1,0)\Bigg\} \tag{68}$$

$$=-2\ln\left(\frac{\Lambda}{\mu}\right)+f(x), \tag{69}$$

where $x=(m_1-m_2)^2/(m_1+m_2)^2$. The function f is calculated numerically, and the results are presented in Fig. 3. The integration with respect to two-photon frequencies is done analytically, giving a long ($\approx$ 100 kB) algebraic expression, denoted by a function g in Eq. (68) that depends on p_1,p_2,q, three scalar momenta. Since the Λ dependence is exactly logarithmic we set $\Lambda=\mu$ in the numerical evaluation. Although this expression in Eq. (68) is finite, it is not numerically stable. Some singularities are avoided by the proper parametrization of the integral,

$$\frac{1}{16\pi^4}\int d^3p_1d^3p_2\frac{1}{p_1^2q^2p_2^2}f(p_1,p_2,q)=\frac{1}{2\pi^2}\int_0^\infty\frac{dD}{D}\int_0^\pi d\alpha\int_0^\pi d\beta\,\theta(\pi-\alpha-\beta)\times f(D\sin(\alpha),D\sin(\beta),D\sin(\alpha+\beta)), \tag{70}$$

and the other by a symmetrization of f in (p_1,p_2,q). The numerical work is performed in quadruple precision using three dimensional Gauss integration with 15 and 30 points [6]. Errors are estimated by comparing both values. Since there are spurious singularities at $m_1=m_2$ in the integrand, we calculate four points at small x and perform linear extrapolation. The result for $x=0$ is $f(0)=-0.70(2)$. We expect from independent analysis a log-type singularity around $x=1$, which agrees with the numerical results. The value for $x=1$ is a known result of Bodwin *et al.* [7] for the recoil correction to muonium hfs, and this forms a crucial test of our calculation.

The sum of all terms reads

$$\Delta E^{(6)}=\frac{8}{3n^3}\alpha^6\frac{\mu^3}{m_1m_2}\left[\frac{11}{6}-\frac{11}{6n^2}+\frac{3}{2n}\right]+\frac{8}{3n^3}\alpha^6\frac{\mu^5}{m_1^2m_2^2}\times\left[-2\ln(\alpha)+F(x)+\left(\frac{4}{3n^2}+\frac{1}{n}+2\ln(n)-2[\Psi(n)+C]-\frac{7}{3}\right)\right], \tag{71}$$

where

$$F(x)=\tfrac{139}{36}+\tfrac{13}{2}\ln(3)-\tfrac{17}{2}\ln(4)+f(x). \tag{72}$$

We recovered the Breit term and got an agreement with the result of Bodwin *et al.* [7]; see Fig. 3. For the ground state positronium hfs we obtained

$$\Delta E^{(6)}=\tfrac{1}{3}m\alpha^6(1.130(5)-\tfrac{1}{2}\ln(\alpha)). \tag{73}$$

It does not agree with the Lepage result 0.5(1) [2]. We were unable to identify the reason for this discrepancy. Our result is dominated by the Breit correction 1.5; the remaining terms are smaller due to the extra $\mu^2/(m_1m_2)$ factor.

V. CONCLUSIONS

We have developed an effective Hamiltonian approach to bound state problems in quantum electrodynamics and calculated recoil corrections to the hyperfine structure of hydrogenic systems in the order of α^6. This correction in the case of positronium contributes 6.22 MHz, which is a significant contribution in comparison to the precision of the most recent experimental result by Ritter *et al.* [8],

$$E=203\,389.10(74)\ \text{MHz}. \tag{74}$$

Remaining corrections of this order due to the single-photon anihilation channel are investigated by Sapirstein and Adkins [9].

The main motivation for our work is the calculation of 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 [10], and metastable triplet $2S$ state [11]. The last measurement by Dorrer *et al.* of the $2\,^3S_1$ Lamb shift [12],

$$E_L(2\,^3S_1)=4057.276(60)\ \text{MHz}, \tag{75}$$

is two orders of magnitude more precise than the current theoretical predictions, mostly limited by the unknown α^6 correction. It is a challenge for theorists to formulate a formalism for the calculation of this correction. There are already several partial results obtained by Zhang [13]. We think that our approach is very well suited for this problem. Positronium is a simpler system to start with. In fact its

Hamiltonian is a part of the helium effective Hamiltonian and, for example, the M_i terms remain exactly the same. Therefore this approach could be tested and verified here. In summary, the calculation of the α^6 correction to helium energy levels would be a significant step in testing QED.

ACKNOWLEDGMENTS

The author gratefully acknowledges useful discussions with J. Sapirstein and E. Remiddi. This work was supported by the Polish Committee for Scientific Research under Contract No. 2 P03B 024 11.

[1] G. S. Adkins, in *Relativistic, Quantum Electrodynamic, and Weak Interaction Effects in Atoms*, edited by W. Johnson, P. Mohr, and J. Sucher, AIP Conf. Proc. No. 189 (AIP, New York, 1989), p. 65.

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

[3] I. B. Khriplovich, A. I. Milstein, A. S. Yelkhovsky, Phys. Rev. Lett. **77**, 4323 (1993); A. S. Yelkhovsky, I. B. Khriplovich, and A. I. Milstein, Zh. Éksp. Teor. Fiz. **105**, 229 (1994) [JETP **78**, 159 (1994)].

[4] K. Pachucki, Ann. Phys. (N.Y.) **226**, 1 (1993).

[5] K. Pachucki, Phys. Rev. A **54**, 1994 (1996).

[6] The numerical integration was done on a Cray YMP in the Interdisciplinary Center of Mathematical and Computer Modeling (ICM) Warsaw University.

[7] G. T. Bodwin, D. R. Yennie, and M. Gregorio, Phys. Rev. Lett. **48**, 1799 (1982).

[8] M. Ritter, P. O. Egan, V. W. Hughes, and K. A. Woodle, Phys. Rev. A **30**, 1331 (1984).

[9] J. Sapirstein and G. Adkins (private communication).

[10] K. S. E. Eikema, W. Ubachs, W. Vassen, and W. Hogervorst, Phys. Rev. Lett. **76**, 1216 (1996).

[11] D. Shiner, R. Dixson, and P. Zhao, Phys. Rev. Lett. **72**, 1802 (1994); F. S. Pavone, F. Marin, P. De Natale, M. Inguscio, and F. Biraben, *ibid.* **73**, 42 (1994).

[12] C. Dorrer, F. Nez, B. de Beauvoir, L. Julien, and F. Biraben (unpublished).

[13] T. Zhang, Phys. Rev. A **54**, 1252 (1996).