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Quantum electrodynamics effects on singlet S-states of helium in the order $m\,\alpha^6$

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Abstract

Using the effective Hamiltonian approach a complete expression is derived, that is suited for the numerical evaluation of the $m\,\alpha^6$ correction to the energy of singlet n^1S_0-states of the helium atom.

I. INTRODUCTION

In last years energies of the ground 1^1S_0 and excited 2^1S_0 states in helium have been precisely measured in [1–4]. The verification of theoretical predictions is limited by the unknown $m\,\alpha^6$ correction [5]. It is the purpose of this paper to present a new approach to the bound state in quantum electrodynamics and derive a complete expression for energy levels in the order $m\,\alpha^6$ of the singlet S-states of the helium atom. This problem has not yet been attacked in the literature. The Bethe–Salpeter formalism [6], although well established, does not actually give prescription, for the calculation of the Lamb shift in singlet S-states. The idea behind the effective Hamiltonian approach is to replace the complicated Hamiltonian of quantum electrodynamics by a simplified Hamiltonian, while preserving the matrix element of the resolvent,

$$\left\langle \boldsymbol{p}_1', \boldsymbol{p}_2' | \frac{1}{E - H_{QED}} | \boldsymbol{p}_1, \boldsymbol{p}_2 \right\rangle^{(n)} = \left\langle \boldsymbol{p}_1', \boldsymbol{p}_2' | \frac{1}{E - H_{EF}(E)} | \boldsymbol{p}_1, \boldsymbol{p}_2 \right\rangle^{(n)} . \quad (1)$$

The superscript $^{(n)}$ denotes the fact, that this equation holds up to the specified order n in α. In this α expansion we assume that external momenta $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ and energy E are of order $m\,\alpha$ and $m\,\alpha^2$ respectively. There is a freedom in the choice of an effective Hamiltonian, as long as Eq. (1) holds. We introduce two regulators l and λ to allow the expansion of the effective Hamiltonian in all momenta. Without these regulators the expansion of for example $\sqrt{p^2+m^2}$ up to the order $p^6 \sim (m\,\alpha)^6$ would be not possible. This method has already been applied for the case of positronium [8,9], and we will use here several results which has been obtained in these works. Moreover, in the preceding paper [7] we have considered much simpler case of triplet S-states. For singlet S-states the wave function does not vanish at

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$\boldsymbol{r}_1 = \boldsymbol{r}_2$, which makes the effective electron–electron interaction more singular. To eliminate singularities in the effective Hamiltonian we regularize the electron–nucleus potential by

$$-\frac{Z\,\alpha}{r} \to -\left(\frac{Z\,\alpha}{r}\right)_l \equiv -\frac{Z\,\alpha}{r}\left(1 - e^{-L\,r}\right)\,. \tag{2}$$

where $L = l\,m\,\alpha$ and the propagator of the photon, which is exchanged between electrons, by

$$\frac{1}{k^2} \to \frac{1}{k^2}\,\frac{\Lambda^2}{\boldsymbol{k}^2 + \Lambda^2} \Rightarrow \frac{\alpha}{r} \to \left(\frac{\alpha}{r}\right)_\lambda \equiv \frac{\alpha}{r}\,\left(1 - e^{-\Lambda\,r}\right)\,, \tag{3}$$

where $\Lambda = \lambda\,m\,\alpha$. l and λ are artificially introduced parameters which are understood to be independent on α and asymptotically large. Parameter l simulates a finite nuclear size. Although we know that all nuclei have a finite charge distribution, it is not our goal to study this effect. The corresponding energy shift is already known with the more than sufficient precision, since it is proportional to the electron charge density at the origin $r_i = 0$. The parameter l cancels out between various matrix elements, in the same way as it in hydrogen [8], when instead of the Dirac equation one uses an effective Hamiltonian. Such a cancellation was explicitly demonstrated also for triplet S-states in helium [7], and in the case of singlet states it goes in analogous way. However the cancelation of λ dependence is much more complex, but this subject was analyzed in detail for the similar calculation in positronium. After getting this experience we are ready to derive the complete set of operators for the $m\,\alpha^6$ correction to the energy of singlet S-states in helium.

The effective Hamiltonian has the form

$$H_{EF} = H_0 + H^{(4)} + H^{(5)} + H^{(6)} + \alpha^2\,\delta^3(r)\,M_5 + \alpha^3\,\delta^3(r)\,M_6\,, \tag{4}$$

and is obtained from the expansion of the QED resolvent in momenta. While $H^{(i)}$ come from the low momentum region M_j are the extra terms, that incorporate the high momenta $p \sim m$ region, that has been forgotten by the regularizations in (2) and (3). The corrections to energy are given by:

$$E^{(4)} = \langle\phi|H^{(4)}|\phi\rangle\,, \tag{5}$$

$$E^{(5)} = \langle\phi|H^{(5)}|\phi\rangle + \langle\phi|\alpha^2\,\delta^3(r)\,M_5|\phi\rangle\,, \tag{6}$$

$$\begin{aligned} E^{(6)} = {} & \langle\phi|H^{(6)}|\phi\rangle + \langle\phi|H^{(4)}\,\frac{1}{(E_0 - H_0)'}\,H^{(4)}|\phi\rangle \\ & + \langle\phi|\alpha^2\,\delta^3(r)\,M_5^{(1)}|\phi\rangle + \langle\phi|\alpha^2\,\delta^3(r)\,M_6|\phi\rangle\,. \end{aligned} \tag{7}$$

H_0 is a nonrelativistic Hamiltonian with the regularized Coulomb interactions

$$H_0 = \frac{p_1^2}{2\,m} + \frac{p_2^2}{2\,m} - \left(\frac{Z\,\alpha}{r_1}\right)_l - \left(\frac{Z\,\alpha}{r_2}\right)_l + \left(\frac{\alpha}{r}\right)_\lambda\,. \tag{8}$$

$H^{(4)}$ is a leading regularized relativistic Breit Hamiltonian

$$H^{(4)} = H_A + H_B + H_C + H_D\,, \tag{9}$$

$$\begin{aligned} H_A =& -\frac{1}{8\,m^3}\,(p_1^4+p_2^4) + \frac{Z\,\alpha\,\pi}{2\,m^2}\,\bigl(\delta^3(r_1)+\delta^3(r_2)\bigr)_l \\ & -\frac{\alpha}{2\,m^2}\,p_1^i\left(\frac{\delta^{ij}}{r}+\frac{r^i\,r^j}{r^3}\right)_\lambda p_2^j - \frac{\pi\,\alpha}{m^2}\,\delta^3(r)_\lambda - \frac{2\,\pi\,\alpha}{3\,m^2}\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,\delta^3(r)_\lambda\,, \end{aligned} \tag{10}$$

$$H_B = \left[\frac{Z\,\alpha}{4\,m^2}\left(\frac{\boldsymbol{r}_1}{r_1^3}\times\boldsymbol{p}_1+\frac{\boldsymbol{r}_2}{r_2^3}\times\boldsymbol{p}_2\right)-\frac{3\,\alpha}{4\,m^2}\,\frac{\boldsymbol{r}}{r^3}\times(\boldsymbol{p}_1-\boldsymbol{p}_2)\right]\frac{\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2}{2}\,, \tag{11}$$

$$H_C = \left[\frac{Z\,\alpha}{4\,m^2}\left(\frac{\boldsymbol{r}_1}{r_1^3}\times\boldsymbol{p}_1-\frac{\boldsymbol{r}_2}{r_2^3}\times\boldsymbol{p}_2\right)+\frac{\alpha}{4\,m^2}\,\frac{\boldsymbol{r}}{r^3}\times(\boldsymbol{p}_1+\boldsymbol{p}_2)\right]\frac{\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2}{2}\,, \tag{12}$$

$$H_D = \frac{\alpha}{4\,m^2}\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3}-3\,\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{r}\,\boldsymbol{\sigma}_2\cdot\boldsymbol{r}}{r^5}\right)_\lambda\,. \tag{13}$$

The subscript λ and l denotes a regularized form of the corresponding expression

$$4\,\pi\,\delta^3(r)_\lambda \equiv \Delta\left(-\frac{1-e^{-\Lambda\,r}}{r}\right), \tag{14}$$

$$\frac{1}{2}\left(\frac{\delta^{ij}}{r}+\frac{r^i\,r^j}{r^3}\right)_\lambda \equiv \int\frac{d^3k}{(2\,\pi)^3}\,\frac{\Lambda^2}{k^2+\Lambda^2}\,\frac{4\,\pi}{k^2}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)e^{-i\,k\,r}\,, \tag{15}$$

$$\left(\frac{\delta^{ij}}{r^3}-3\,\frac{r^i\,r^j}{r^5}\right)_\lambda \equiv \int\frac{d^3k}{(2\,\pi)^3}\,\frac{\Lambda^2}{k^2+\Lambda^2}\,\frac{4\,\pi}{k^2}\left(k^i\,k^j-\frac{\delta^{ij}}{3}k^2\right)e^{-i\,k\,r}\,. \tag{16}$$

We have corrected here in the Eq. (15), the corresponding equation in the former paper [8], where it was lack of factor 1/2. $H^{(5)}$ does not contribute in the order of interest. $H^{(6)}$ consists of electron–nucleus terms, electron–electron terms, three–body terms and the radiative correction

$$H^{(6)} = H_{EN}(1) + H_{EN}(2) + H_{EE} + H_{TB} + H_{RC}\,. \tag{17}$$

The derivation of $H^{(6)}$ is presented in the following section. H_{EE} and H_{TB} Hamiltonians are obtained from the time ordered diagrams in Fig. 1, by expanding in all momenta up to the order $m\,\alpha^6$. M_5 and M_6 are given by the forward scattering amplitude of two electrons, which exchange two and three photons respectively. These amplitudes require subtraction of terms already included in H_{EF} and then become finite. M_i depend on λ as the $H^{(i)}$ Hamiltonians. Nevertheless this dependence cancels out in the complete expression for the QED correction to energy levels in the limit of large λ.

II. CONTRIBUTIONS TO EFFECTIVE HAMILTONIAN AT THE ORDER $M\,\alpha^6$

For the derivation of the effective Hamiltonian we use time ordered perturbation technique, which was used in QED before Feynman has introduced covariant perturbation approach based on his propagators. Time ordered perturbation technique has been rediscovered by Khriplovich [10] in his calculation of P-levels in positronium. It is much easier in the application, than the Bethe-Salpeter equation and leads quickly to the results. The Bethe-Salpeter equation has been used by Douglas and Kroll for the derivation of $m\,\alpha^6$ effective operators to fine structure of P-levels [11]. We have rederived their result and obtained full agreement.

As in the case of triplet S-states we use diagrams to represent various corrections. They are shown in Fig. 1. There are rules to derive an expression from the corresponding time ordered diagram. We use the Coulomb gauge, so have a Coulomb photon (the dashed line) and the transverse one (the wavy line), the dotted line denotes something else, to be explained later. The vertex for the Coulomb exchange is e ($-e$ for the positron) which is multiplied by $(2\,\pi)^3\,\delta^3(\Sigma_i \boldsymbol{p}_i)$ to conserve three-dimensional momentum. The dashed line is $1/q^2$, the Fourier transform of the Coulomb potential. The vertex for the transverse photon is $e\,\alpha^i$ ($-e\,\alpha^i$ for the positron) times the corresponding δ-function to preserve momentum. The wavy line is $1/(2\,q)\,(\delta^{ij}-q^i\,q^j/q^2)$. There are projection operators between the vertices on electron lines onto positive or negative energy states, depending on the time arrow. The additional terms are energy denominators. Each denominator is equal to $E-\Sigma_i E_i$, where the sum goes over all intermediate state. Such a factor is between two Coulomb exchanges, between emission and absorption of the transverse photon, and between the transverse vertex and the Coulomb exchange. There is also a factor -1 for any electron positron pair creation. When the transverse photon is involved, the leading term in the denominator is the photon energy, and for the most cases one can neglect other terms in the denominator, and we denote it by a vertical wavy line. Since there are two possibilities, any of the electrons could first emit a photon and the second absorbs, the overall factor is $-2/q$. We have introduced a dotted line which denotes both the Coulomb exchange *and* the expansion of the energy denominator with respect to the kinetic energy. The whole expression is enclosed by $u^+(p')$ and $u(p)$, the free fermion bispinors, which correspond to outer lines.

The electron–nucleus part H_{EN} could be derived from the Dirac equation using the Fouldy–Wouthuysen transformation, but it could also be obtained from the first two diagrams on Fig. 1. We may assume for a while that a lower line denotes a static nucleus, while the upper one denotes one of the electrons. The first term V_K comes from the expansion of kinetic energy operator $E(p)=\sqrt{p^2+m^2}$ in p^2

$$V_K = \frac{p^6}{16\,m^5}\,. \tag{18}$$

The single Coulomb exchange V_C is

$$V_C = -\frac{Z\,e^2}{q^2}\,\bar{u}(p')\gamma^0 u(p)\,, \tag{19}$$

where $\boldsymbol{q}$ is a momentum exchange from $\boldsymbol{p}$ to $\boldsymbol{p}'$, $\boldsymbol{q}=\boldsymbol{p}'-\boldsymbol{p}$ and $u(p)$ is a positive energy solution of the free Dirac equation. We need only the $m\,\alpha^6$ part, so after the expansion in momentum and neglect of spin dependent terms V_C becomes

$$V_C = -\frac{Z\,e^2}{q^2+L^2}\left[\frac{5}{128\,m^4}(p'^2-p^2)^2+\frac{3}{64\,m^4}(p^2+p'^2)\,q^2\right]\,. \tag{20}$$

Double Coulomb contribution is

$$V_{CC} = -\int \frac{d^3 q_1}{(2\,\pi)^3} \int \frac{d^3 q_2}{(2\,\pi)^3}\, \frac{4\,\pi\,\alpha}{q_1^2+L^2}\, \frac{4\,\pi\,\alpha}{q_2^2+L^2}\, (2\,\pi)^3\, \delta^3(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{q})$$
$$\frac{u^+(p')\,\Lambda_-(p+q_1)\,u(p)}{m+E-E(p)-E(p+q_1)-E(p')}\,, \tag{21}$$

where

$$\Lambda_-(p) = \frac{E(p)-\boldsymbol{\alpha}\cdot\boldsymbol{p}-\beta\,m}{2\,E(p)} \tag{22}$$

is a projection operator. In the leading order in the p–expansion, its matrix element is

$$u^+(p_1')\,\Lambda_-(p+q_1)\,u(p_1) = -\frac{1}{4\,m^2}(\boldsymbol{\sigma}_1\cdot\boldsymbol{q}_1)\,(\boldsymbol{\sigma}_1\cdot\boldsymbol{q}_2)\,. \tag{23}$$

Moreover, we can neglect p and E dependence in the denominator, so V_{CC} becomes

$$V_{CC} = -\frac{1}{8\,m^3}\int \frac{d^3 q_1}{(2\,\pi)^3}\int \frac{d^3 q_2}{(2\,\pi)^3}\,(2\,\pi)^3\,\delta^3(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{q})\frac{4\,\pi\,\alpha}{q_1^2}\,\frac{4\,\pi\,\alpha}{q_2^2}\,(\boldsymbol{\sigma}_1\cdot\boldsymbol{q}_1)\,(\boldsymbol{\sigma}_1\cdot\boldsymbol{q}_2)\,. \tag{24}$$

The complete expression for H_{EN} is the sum of V_K, V_C and V_{CC}. In position representation it has a form

$$H_{EN} = \frac{p^6}{16\,m^5} - \frac{1}{8\,m^3}\left[\boldsymbol{p};\left(\frac{Z\,\alpha}{r}\right)_l\right]^2 - \frac{5}{128\,m^4}\left[p^2;\left[p^2;\left(\frac{Z\,\alpha}{r}\right)_l\right]\right]$$
$$-\frac{3}{64\,m^4}\left(p^2\left[\boldsymbol{p};\left[\boldsymbol{p};\left(\frac{Z\,\alpha}{r}\right)_l\right]\right] + \left[\boldsymbol{p};\left[\boldsymbol{p};\left(\frac{Z\,\alpha}{r}\right)_l\right]\right]p^2\right), \tag{25}$$

where by square brackets $[A;B]$ one denotes a commutator $A\,B-B\,A$. Together with the lower order part $H = -\frac{p^4}{8\,m^3}+\frac{Z\,\alpha\,\pi}{2\,m^2}\,\delta^3_l(r)$, H_{EN} gives a correction to energy in the perfect agreement with that obtained from the Dirac equation [8].

The next contribution we consider is the retardation part in the single transverse photon exchange E_T. This part requires a separate treatment as in the positronium case [9]. The reason for this, is the fact, that single transverse term contributes at very low photon energies $k \approx m\,\alpha^2$. The initial expression which could be derived from the nonrelativistic quantum electrodynamics is

$$E_T = 4\,\pi\,\alpha\int\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)$$
$$\times\left\langle\phi\left|\frac{p_1^i}{m}\left\{e^{i\,k\,r_1}\left(\frac{1}{E_0-k-H_0}+\frac{1}{k}\right)e^{-i\,k\,r_2}\right\}\frac{p_2^j}{m}\right|\phi\right\rangle + (1\leftrightarrow 2)\,, \tag{26}$$

where H_0 and ϕ here are (exceptionally) without any regulator. We divide it into three parts:

$$E_{TL} = 4\,\pi\,\alpha\int\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\frac{\Lambda^2}{k^2+\Lambda^2}$$

$$\times \left\langle \phi \left| \frac{p_1^i}{m} \left(\frac{1}{E_0 - k - H_0} + \frac{1}{k} \right) \frac{p_2^j}{m} \right| \phi \right\rangle + (1 \leftrightarrow 2)\,, \tag{27}$$

$$E_{TM} = 4\,\pi\,\alpha \int \frac{d^3k}{(2\,\pi)^3\,2\,k} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2} \right) \frac{\Lambda^2}{k^2 + \Lambda^2}$$
$$\left\langle \phi \left| \frac{p_1^i}{m} \left\{ e^{i\,k\,r_1} \left(\frac{1}{E_0 - k - H_0} + \frac{1}{k} \right) e^{-i\,k\,r_2} - \left(\frac{1}{E_0 - k - H_0} + \frac{1}{k} \right) \right\} \frac{p_2^j}{m} \right| \phi \right\rangle + (1 \leftrightarrow 2), \tag{28}$$

$$E_{TH} = 4\,\pi\,\alpha \int \frac{d^3k}{(2\,\pi)^3\,2\,k} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2} \right) \frac{k^2}{k^2 + \Lambda^2}$$
$$\times \left\langle \phi \left| \frac{p_1^i}{m} \left\{ e^{i\,k\,r_1} \left(\frac{1}{E_0 - k - H_0} + \frac{1}{k} \right) e^{-i\,k\,r_2} \right\} \frac{p_2^j}{m} \right| \phi \right\rangle . \tag{29}$$

E_{TL} contributes in the limit of large λ only at the order $m\,\alpha^5$, so we can skip it. In the expression for E_{TM} one expands the denominator

$$\frac{1}{E_0 - k - H_0} + \frac{1}{k} = \frac{(H_0 - E_0)}{k^2} - \frac{(H_0 - E_0)^2}{k^3} + \ldots\,, \tag{30}$$

and takes only the second term, (others do not contribute),

$$E_{TM} = -4\,\pi\,\alpha \int \frac{d^3k}{(2\,\pi)^3\,2\,k} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2} \right) \frac{\Lambda^2}{k^2 + \Lambda^2}$$
$$\left\langle \phi \left| \frac{p_1^i}{m} \left\{ e^{i\,k\,r_1} \frac{(H_0 - E_0)^2}{k^3} e^{-i\,k\,r_2} - \frac{(H_0 - E_0)^2}{k^3} \right\} \frac{p_2^i}{m} \right| \phi \right\rangle + (1 \leftrightarrow 2)\,. \tag{31}$$

The k integral is replaced by the expression

$$\int \frac{d^3k}{(2\,\pi)^3}\,\frac{1}{k^4} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2} \right) (e^{i\,k\,r} - 1)\,\frac{\Lambda^2}{k^2 + \Lambda^2} \equiv \frac{1}{32\,\pi} \left(\frac{r^i\,r^j}{r} - 3\,\delta^{ij}\,r \right)_\lambda . \tag{32}$$

After using commutation relations E_{TM} becomes

$$E_{TM} = -\frac{\alpha}{8} \left\langle \phi \left| \frac{p_1^i}{m} \left\{ (H_0 - E_0) \left(\frac{r^i\,r^j}{r} - 3\,\delta^{ij}\,r \right)_\lambda (H_0 - E_0) \right. \right. \right.$$
$$+ (H_0 - E_0) \left[\frac{p_2^2}{2\,m}\,;\, \left(\frac{r^i\,r^j}{r} - 3\,\delta^{ij}\,r \right)_\lambda \right] + \left[\left(\frac{r^i\,r^j}{r} - 3\,\delta^{ij}\,r \right)_\lambda ;\, \frac{p_1^2}{2\,m} \right] (H_0 - E_0)$$
$$\left. \left. \left. + \left[\frac{p_2^2}{2\,m}\,;\, \left[\left(\frac{r^i\,r^j}{r} - 3\,\delta^{ij}\,r \right)_\lambda ;\, \frac{p_1^2}{2\,m} \right] \right] \right\} \frac{p_2^j}{m} \right| \phi \right\rangle . \tag{33}$$

The high energy part E_{TH} in the momentum space is

$$E_{TH} = 4\,\pi\,\alpha\,\langle \phi | \delta^3(r) | \phi \rangle \int \frac{d^3k}{(2\,\pi)^3\,2\,k} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2} \right) \frac{k^2}{k^2 + \Lambda^2} \int \frac{d^3q}{(2\,\pi)^3} \int \frac{d^3q'}{(2\,\pi)^3}\,q'^i\,q^j$$
$$(2\,\pi)^3\,\delta^3(q + q' + k)\,\frac{4\,\pi\,\alpha}{q'^4}\,\frac{4\,\pi\,\alpha}{q^4} \left(\frac{1}{k} - \frac{1}{k + q^2/(2\,m) + q'^2/(2\,m)} \right) + (1 \leftrightarrow 2)\,. \tag{34}$$

One performs integrals in q and q' and obtains

$$E_{TH} = -4\,\alpha^3\,\langle\phi|\delta^3(r)|\phi\rangle \int \frac{dk}{k^3}\,\frac{k^2}{k^2+\Lambda^2}\,\left[\frac{\pi}{2} - \frac{1}{z} + \left(\frac{1}{z^2}-1\right)\,\arctan(z)\right]\,, \tag{35}$$

where

$$z = \frac{m}{k}\Big/\sqrt{\frac{1}{4}+\frac{m}{k}}\,. \tag{36}$$

One goes to the limit of large λ after performing k integral, therefore $1/\Lambda$ and $1/\sqrt{\Lambda}$ drop out and E_{TH} becomes

$$E_{TH} = \frac{\pi\,\alpha^3}{m^2}\,\langle\phi|\delta^3(r)|\phi\rangle\,\left(\frac{\ln(\lambda\,\alpha)}{2} - 1.96830\right)\,. \tag{37}$$

The retardation and spin independent part of single transverse photon exchange E_T is the sum of Eq. (33) and Eq. (37)

$$E_T = E_{TM} + E_{TH}\,. \tag{38}$$

For the calculation of all remaining terms we assume that H_0 depends on regulators λ, l as in (8), so are ϕ and E_0 as well. The algebraic expressions have been already derived in the former paper [7]. Here, we have to take into account the regularization of the photon propagator according to Eq. (3), and keep also the terms proportional to $\delta^3(r)$, which have been neglected before. We denote by V the expression that corresponds to a diagram, namely the effective interaction potential. The correction to energy is obtained by taking the matrix element $\Delta E = \langle\phi|V|\phi\rangle$. The first contribution is a single Coulomb exchange, the diagram 1 in Fig. 1.

$$\begin{aligned} V_1 = \frac{1}{64\,m^4}\Bigl\{ & -\Delta[4\,\pi\,\alpha\,\delta^3(r)_\lambda] + \frac{5}{2}\Bigl[p_2^2;\Bigl[p_2^2;\Bigl(\frac{\alpha}{r}\Bigr)_\lambda\Bigr]\Bigr] + \frac{5}{2}\Bigl[p_1^2;\Bigl[p_1^2;\Bigl(\frac{\alpha}{r}\Bigr)_\lambda\Bigr]\Bigr] \\ & +3\,(p_1^2+p_2^2)\,4\,\pi\,\alpha\,\delta^3(r)_\lambda + 3\cdot 4\,\pi\,\alpha\,\delta^3(r)_\lambda\,(p_1^2+p_2^2) \\ & +\frac{4}{3}\,\Bigl[p_1^i\,p_2^j\,\Bigl(\frac{\alpha}{r}\Bigr)_\lambda\,p_1^j\,p_2^i - p_1^i\,p_2^i\,\Bigl(\frac{\alpha}{r}\Bigr)_\lambda\,p_1^j\,p_2^j\Bigr]\;\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\Bigr\}\,, \end{aligned} \tag{39}$$

where for singlet S-state $\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 = -3$. The second contribution is a double Coulomb exchange,

$$V_2 = \frac{1}{4\,m^3}\,\left[\frac{\partial}{\partial r}\,\left(\frac{\alpha}{r}\right)_\lambda\right]^2\,. \tag{40}$$

The third contribution is an exchange of a single transverse photon in the no retardation limit,

$$\begin{aligned} V_3 = {} & \frac{\alpha}{8\,m^4}\Bigl[p_1^i\,\Bigl(\frac{\delta^{ij}}{r}+\frac{r^i\,r^j}{r^3}\Bigr)_\lambda\,p_2^j\,(p_1^2+p_2^2) + (p_1^2+p_2^2)\,p_1^i\,\Bigl(\frac{\delta^{ij}}{r}+\frac{r^i\,r^j}{r^3}\Bigr)_\lambda\,p_2^j\Bigr] + \\ & \frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{48\,m^4}\Bigl\{2\,(p_1^2+p_2^2)\,4\,\pi\,\alpha\,\delta^3(r)_\lambda + 2\cdot 4\,\pi\,\alpha\,\delta^3(r)_\lambda\,(p_1^2+p_2^2) + \\ & \Bigl[p_1^2;\Bigl[p_1^2;\Bigl(\frac{\alpha}{r}\Bigr)_\lambda\Bigr]\Bigr] + \Bigl[p_2^2;\Bigl[p_2^2;\Bigl(\frac{\alpha}{r}\Bigr)_\lambda\Bigr]\Bigr]\Bigr\}\,. \end{aligned} \tag{41}$$

The fourth contribution is a spin dependent, retardation part of the single transverse photon exchange,

$$V_4 = \frac{1}{24\,m^4}\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\left[p_1^2\,;\,\left[p_2^2\,;\,\left(\frac{\alpha}{r}\right)_\lambda\right]\right]. \tag{42}$$

The fifth contribution is a single transverse and single Coulomb exchange,

$$V_5 = \frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{3\,m^3}\left[\frac{\partial}{\partial r}\left(\frac{\alpha}{r}\right)_\lambda\right]^2. \tag{43}$$

The sixth contribution is a double transverse photon exchange with the single Z,

$$V_6 = \frac{1}{2\,m^3}\left\{p_1^i\left[\frac{\alpha^2}{4\,r^2}\left(\delta^{ij}+3\frac{r^i\,r^j}{r^2}\right)\right]_\lambda p_1^j + p_2^i\left[\frac{\alpha^2}{4\,r^2}\left(\delta^{ij}+3\frac{r^i\,r^j}{r^2}\right)\right]_\lambda p_2^j + \left[\frac{\partial}{\partial r}\left(\frac{\alpha}{r}\right)_\lambda\right]^2\right\}, \tag{44}$$

where

$$\left[\frac{1}{r^2}\left(\delta^{ij}+3\frac{r^i\,r^j}{r^2}\right)\right]_\lambda = \left[\frac{\delta^{ik}}{r}+\frac{r^i\,r^k}{r^3}\right]_\lambda\left[\frac{\delta^{kj}}{r}+\frac{r^k\,r^j}{r^3}\right]_\lambda. \tag{45}$$

The seventh contribution is a three–body, double–Coulomb exchange,

$$V_7 = -\frac{Z\,\alpha^2}{4\,m^3}\,\frac{\boldsymbol{r}}{r^3}\left(\frac{\boldsymbol{r}_1}{r_1^3}-\frac{\boldsymbol{r}_2}{r_2^3}\right). \tag{46}$$

The eighth contribution is a three–body, single–Coulomb, single transverse photon exchange,

$$V_8 = -\frac{Z\,\alpha^2}{6\,m^3}\,\frac{\boldsymbol{r}}{r^3}\left(\frac{\boldsymbol{r}_1}{r_1^3}-\frac{\boldsymbol{r}_2}{r_2^3}\right). \tag{47}$$

Effective Hamiltonians H_{EE} and H_{TB} are expressed in terms of V_i

$$H_{EE} = \Sigma_{i=1}^6 V_i\,, \tag{48}$$

$$H_{TB} = V_7 + V_8\,, \tag{49}$$

and the E_T as given by Eq. (38) is treated separately.

The radiative correction H_{RC} consists of one–loop and two–loop terms for the electron–nucleus and the electron–electron interaction. They could be obtained from the hydrogen [12] and the positronium [13] Lamb shift respectively

$$H_{RC} = H_{RC1}^N + H_{RC2}^N + H_{RC1}^E + H_{RC2}^E\,, \tag{50}$$

$$H_{RC1}^N = \frac{\alpha\,(Z\,\alpha)^2}{m^2}\,9.61837\left[\delta^3(r_1)+\delta^3(r_2)\right], \tag{51}$$

$$H_{RC2}^N = \frac{\alpha^2\,(Z\,\alpha)}{m^2}\,0.17155\left[\delta^3(r_1)+\delta^3(r_2)\right], \tag{52}$$

$$H_{RC1}^E = \frac{\alpha^3}{m^2}\,(14.33134 - 3.42651\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\,\delta^3(r)\,, \tag{53}$$

$$H_{RC2}^E = \frac{\alpha^3}{m^2}\,(-0.66526 + 0.08633\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\,\delta^3(r)\,. \tag{54}$$

The M_i counter terms are the high part, that is omitted by the regularizations in Eqs. (2,3). They have been calculated for positronium [8,9] and are the same in our case of helium, since the electron–nucleus interaction does not have the high energy part. It is essential piece of our method that M_i could be obtained in the limit of large λ from the scattering amplitude only. M_5 is given by the forward amplitude involving exchange of two photons between two electrons. More precisely, it is a subtracted amplitude by terms already incorporated in the effective Hamiltonian. Its α part is

$$M_5^{(1)} = \frac{\pi\,\lambda\,\alpha}{4\,m^2}\,\left(-3+\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{3}\right)\,. \tag{55}$$

We correct here the corresponding equation in [9], where it lacked of factor π. The contribution of $M_5^{(1)}$ to energy is calculated with regularized wave functions. M_6 in analogy is a forward amplitude involving exchange of three photon, and is calculated numerically. Together with $M_5^{(1)}$ it is

$$\langle\phi|\alpha^2\,\delta^3(r)\,M_5^{(1)}|\phi\rangle + \langle\phi|\alpha^3\,\delta^3(r)\,M_6|\phi\rangle = \frac{\pi\,\alpha^3}{m^2}\,\langle\delta^3(r)\rangle$$
$$\left\{\frac{\lambda}{4}\,\left(-3+\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{3}\right) + [\ln(\lambda\,\alpha)+1.04(1)]\,\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{3} + \left[-\frac{\ln(\lambda\,\alpha)}{2}+1.823(5)\right]\right\}\,, \tag{56}$$

where $\langle\delta^3(r)\rangle$ is calculated on the unregularized wave function. The complete correction to energy in the order $m\,\alpha^6$ as given by Eq. (7) and Eq. (38) does not depend on λ and l in the limit of large values. The linear divergence is canceled by $M_5^{(1)}$ and the logarithmic by M_6. The terms logarithmic in α are in Eqs. (37) and (56). They sum to

$$\Delta E^{(6)} = \frac{\pi\,\alpha^3}{m^2}\,\langle\phi|\delta^3(r)|\phi\rangle\,\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{3}\,\ln(\alpha)\,. \tag{57}$$

III. SUMMARY

The purpose of this work was to show the possibility of the calculation of higher order QED effects for singlet S-levels of the helium atom. There was no method so far, which allowed for such calculations at order $m\,\alpha^6$. We have presented the derivation of a complete set of operators that contributes to helium energy levels of singlet n^1S_0 states in that order. In this work we have based on the former calculations of energy levels in the positronium [8,9], and of triplet S-levels in the helium [7].

The further step is the numerical calculations of matrix elements with this complete set of operators. Since one needs to calculate numerically the limit of large λ and l, this calculation is significantly more difficult than for the fine splitting of P-levels, which has recently been performed in [15]. However, if one performs the calculations at some finite value of λ and l the error will be of order $1/\lambda + 1/l$. So, if we are interested in for example 10% accuracy, such a calculation seems to be achievable using known methods. These parameters λ and l regularize all integrals, eliminate singularities, so there is no need at this accuracy for high precision helium wave functions. The rather technical problem is the large number of these operators which contain many derivatives. It was suggested by Jonathan Sapirstein that B-spline method may be quite suitable for this purposes.

The contribution to the energy seems to be dominated by the radiative one–loop correction H^{RC}, Eqs. (51-54). Hopefully, it could be easily calculated numerically, since it depends only on the wave function at $r_1 = 0$ and $r = 0$. These values were presented by Drake in [5], and for example

$$\langle\phi|\delta^3(r)|\phi\rangle = (m\,\alpha)^3 \begin{cases} 0.106\,345\,372\,2(2) \text{ for } 1^1S_0 \text{ state} \\ 0.008\,648\,437\,6(2) \text{ for } 2^1S_0 \text{ state}. \end{cases} \tag{58}$$

The previously unknown radiative correction $H^E_{RC} = H^E_{RC1} + H^E_{RC2}$ gives

$$\Delta E = \langle\phi|H^E_{RC}|\phi\rangle = \begin{cases} 47.0\,\text{MHz for } 1^1S_0 \text{ state} \\ 3.8\,\text{MHz for } 2^1S_0 \text{ state}, \end{cases} \tag{59}$$

which is larger than the logarithmic term in Eq. (57). This logarithmic term agrees with the result obtained formerly in [5] and, for example, it contributes 30.7 MHz for 1^1S_0 state. However, there is a discrepancy in the case of the hyperfine structure of the ground state in positronium that is relevant for singlet states of helium. Calculations of Caswell and Lepage in Ref. [14] and our in [8] disagree, and till now this problem has not been resolved.

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FIGURES

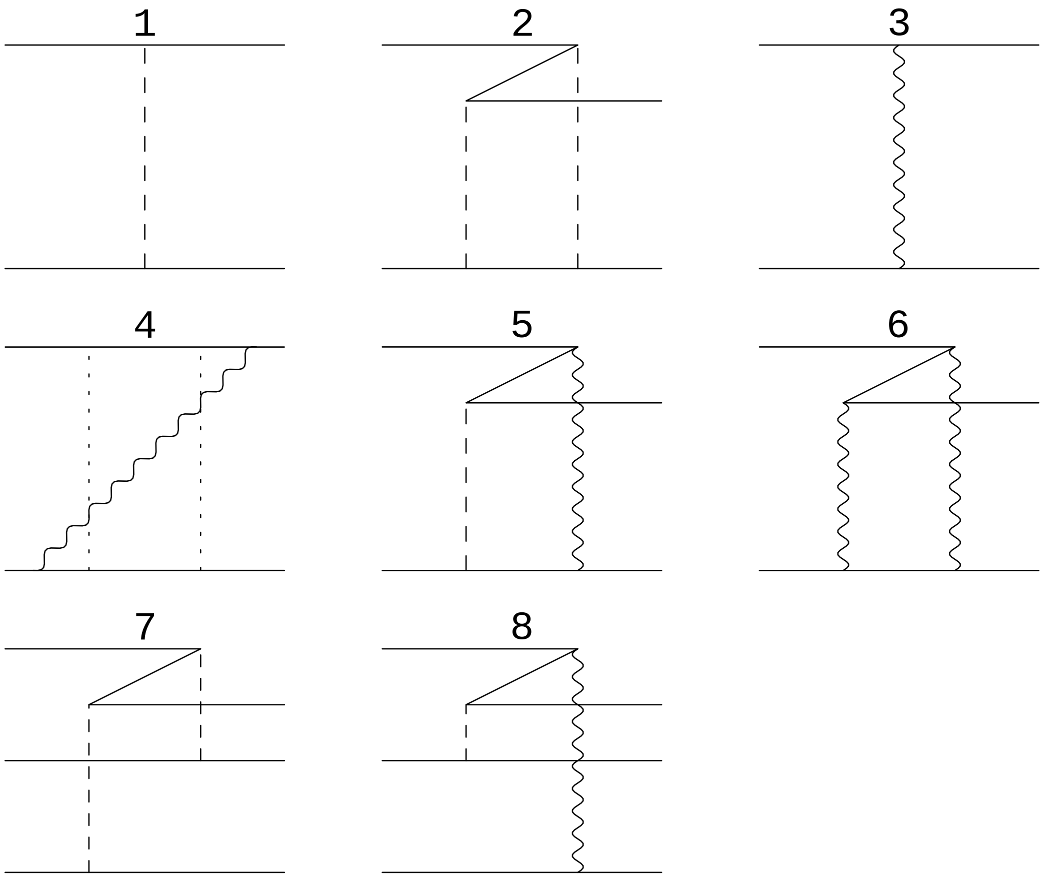

FIG. 1. Time ordered diagrams contributing to energy levels in order $m\,\alpha^6$. The middle horizontal line corresponds to helium, two outer horizontal lines correspond to two electrons. The wavy line is a transverse photon, the dashed line is a Coulomb photon, and the dotted line denotes retardation.