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# Effective Hamiltonian approach to the bound state: energy of helium $n^3S_1$-states in the order $m\,\alpha^6$

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## Abstract

An effective Hamiltonian approach is applied for the calculation of bound state energies of the helium atom. A complete set of nonrelativistic operators is derived for the $m\,\alpha^6$ correction to the energy of triplet $n^3S_1$-states.

## I. INTRODUCTION

The helium atom is one of the simplest systems, where quantum electrodynamics (QED) effects could be studied with the high precision [1]. The presence of the electron–electron interaction is an essential ingredient in the comparison of helium to hydrogenic systems and brings QED calculations to the next level of difficulty. A long standing problem is the treatment of the electron–electron interaction on the same footing as the electron–nucleus interaction. Commonly accepted Bethe-Salpeter formalism [2] is a well starting point for the derivation of various QED corrections in the helium atom. This treatment has been developed by Araki [3] and independly by Sucher [4] for the complete calculation of $m\,\alpha^5$ correction to energy levels. Although, this correction could be presented in a compact form, the calculation of the one term: the Bethe–logarithm, has not yet been performed with the satisfactory precision. The extension to the next order of $m\,\alpha^6$ has been achieved by Douglas and Kroll [5] but only for the fine splitting between triplet P-levels. Using the Bethe-Salpeter equation they have derived corresponding nonrelativistic operators, which can be treated in a standard perturbation calculus using Schrödinger wave functions. These operators are the extension of Breit Hamiltonian [6] to the order of $m\,\alpha^6$. Usually, such an nonrelativistic expansion gives a very singular operators which could not for example be evaluated in the second order of perturbation calculus. However, triplet P-state wave functions are much more regular at small distances, making matrix elements of these operators finite at order $m\,\alpha^6$ for the difference between P-levels.

In last years several transitions involving triplet S-states in helium have been precisely measured: $2^3S_1-2^3P_J$ by Shiner and coworkers in [7], $2^3S_1-3^3P_J$ by Inguscio and coworkers in [8], and $2^3S_1-3^3D_1$ by the Paris group in [9]. From the last measurement authors derived $2^3S_1$ Lamb shift which is two orders more precise than the current theoretical predictions.

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In this paper we derive a complete set of operators for the calculation of energies of helium triplet $n^3S_1$-states at order $m\,\alpha^6$ and demonstrate the cancelation of all divergences. The similar set of operators for singlet S-states will be presented in the next paper. However, the treatment for singlet states is much more complex. One has to regularize the electron–electron interaction to keep matrix elements finite. The divergence in some chosen parameter $\lambda$ is canceled by the terms derived from the high energy scattering amplitude. The third paper will be devoted to the fine structure in order $m\,\alpha^7$.

Here, in chapter II we outline the effective Hamiltonian approach. In chapter III, we derive all the corresponding operators. The cancelation of divergences for triplet states is shown in chapter IV. Short concluding remarks and a comparison to existing literature are left to the chapter V.

## II. EFFECTIVE HAMILTONIAN APPROACH

The key idea of this approach for the calculation of bound state energies is the replacement of the Hamiltonian of the full quantum electrodynamics, with the simplified Hamiltonian which acts only in the subspace of two-particle states with all momenta being of the order of the inverse of the size of the bound state [10]. This new simplified Hamiltonian depends on some artificial parameter $\lambda$, to keep its matrix element finite. For triplet states this divergence simply cancels between different matrix elements. In our case we regularize the Coulomb potential coming from the nucleus by the replacement

$$-\frac{Z\,\alpha}{r} \to -\frac{Z\,\alpha}{r}\left(1-e^{-\lambda\,m\,\alpha\,r}\right)\,. \tag{1}$$

The effective Hamiltonian is constructed using the following condition, which is to be valid up to the specified order $n$ in $\alpha$:

$$\left\langle \boldsymbol{p}_1',\boldsymbol{p}_2'\right|\frac{1}{E-H_{QED}}\left|\boldsymbol{p}_1,\boldsymbol{p}_2\right\rangle^{(n)} = \left\langle \boldsymbol{p}_1',\boldsymbol{p}_2'\right|\frac{1}{E-H_{EF}(E)}\left|\boldsymbol{p}_1,\boldsymbol{p}_2\right\rangle^{(n)}\,. \tag{2}$$

$|\boldsymbol{p}_1,\boldsymbol{p}_2\rangle$ on the left hand side denotes two particle states with momenta $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$, and a photon vacuum, while on right hand side it denotes a momentum state of two electrons only. In the $\alpha$ expansion in Eq. (2) we keep the energy $E$ and momenta $p,p'$ of the order $\alpha^2$ and $\alpha$ respectively. In the actual calculation $H_{EF}$ is obtained by an expansion of the resolvent in the Coulomb potential $V$ up to the third power and by an expansion in all momenta $p^i$. The effective Hamiltonian has the form

$$H_{EF} = H_0 + H^{(4)} + H^{(5)} + H^{(6)}\,, \tag{3}$$

where $H_0$ is a nonrelativistic Hamiltonian for helium with the regularized potential

$$H_0 = \frac{p_1^2}{2\,m} + \frac{p_2^2}{2\,m} - \frac{Z\,\alpha}{r_1}\left(1-e^{-\Lambda\,r_1}\right) - \frac{Z\,\alpha}{r_2}\left(1-e^{-\Lambda\,r_2}\right) + \frac{\alpha}{r}\,, \tag{4}$$

where $\Lambda = m\,\alpha\,\lambda$, $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, and $H^{(4)}$ is a leading relativistic Breit Hamiltonian and $H^{(5)}, H^{(6)}$ are higher order corrections in $m\,\alpha^5$ and $m\,\alpha^6$ orders respectively. The dependence

of the effective Hamiltonian on the energy $E$ could be neglected up to the order $m\,\alpha^6$, and we can put $E$ equal to $E_0$ the bound state energy. The correction to energy in the order $m\,\alpha^6$ could be written as

$$E^{(6)} = \left\langle \phi \left| H^{(4)} \frac{1}{(E_0 - H_0)'} H^{(4)} \right| \phi \right\rangle + \langle \phi | H^{(6)} | \phi \rangle \,. \tag{5}$$

The Breit Hamiltonian, neglecting terms proportional to $\delta^3(r)$ which vanish for triplet states, is

$$H^{(4)} = H_A + H_B + H_C + H_D \,, \tag{6}$$

$$H_A = -\frac{1}{8\,m^3}\,(p_1^4 + p_2^4) + \frac{Z\,\alpha\,\pi}{2\,m^2}\,(\delta^3(r_1) + \delta^3(r_2))_\lambda - \frac{\alpha}{2\,m^2}\,p_1^i \left( \frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3} \right) p_2^j \,, \tag{7}$$

$$H_B = \left[ \frac{Z\,\alpha}{4\,m^2} \left( \frac{\boldsymbol{r}_1}{r_1^3} \times \boldsymbol{p}_1 + \frac{\boldsymbol{r}_2}{r_2^3} \times \boldsymbol{p}_2 \right) - \frac{3\,\alpha}{4\,m^2}\,\frac{\boldsymbol{r}}{r^3} \times (\boldsymbol{p}_1 - \boldsymbol{p}_2) \right] \frac{\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2}{2} \,, \tag{8}$$

$$H_C = \left[ \frac{Z\,\alpha}{4\,m^2} \left( \frac{\boldsymbol{r}_1}{r_1^3} \times \boldsymbol{p}_1 - \frac{\boldsymbol{r}_2}{r_2^3} \times \boldsymbol{p}_2 \right) + \frac{\alpha}{4\,m^2}\,\frac{\boldsymbol{r}}{r^3} \times (\boldsymbol{p}_1 + \boldsymbol{p}_2) \right] \frac{\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2}{2} \,, \tag{9}$$

$$H_D = \frac{\alpha}{4\,m^2} \left( \frac{\boldsymbol{\sigma}_1\,\boldsymbol{\sigma}_2}{r^3} - 3\,\frac{\boldsymbol{\sigma}_1 \cdot \boldsymbol{r}\;\boldsymbol{\sigma}_2 \cdot \boldsymbol{r}}{r^5} \right) . \tag{10}$$

Each part leads to intermediate states with a different quantum number, therefore their contribution to energy separate out, and thus

$$E_A = \langle H_A\,\frac{1}{(E_0 - H_0)'}\,H_A \rangle \,, \tag{11}$$

$$E_{BCD} = \langle H_B\,\frac{1}{(E_0 - H_0)'}\,H_B \rangle + \langle H_C\,\frac{1}{(E_0 - H_0)'}\,H_C \rangle + \langle H_D\,\frac{1}{(E_0 - H_0)'}\,H_D \rangle \,. \tag{12}$$

The subscript $\lambda$ in the expression for $E_A$ denotes the regularized $\delta^3(r)$, namely

$$4\,\pi\,\delta^3(r)_\lambda \equiv \Delta\left( -\frac{1 - e^{-\Lambda\,r}}{r} \right) . \tag{13}$$

Without this regularization the matrix element in Eq. (11) would be divergent. Other parts $H_B, H_C, H_D$ do not require any regularization. The expression for $H^{(6)}$ is much more complex. It consists of electron–nucleus terms, electron–electron terms, few three–body terms and the radiative correction

$$H^{(6)} = H_{EN}(1) + H_{EN}(2) + H_{EE} + H_{TB} + H_{RC} \,. \tag{14}$$

The electron–nucleus part $H_{EN}$ could also be derived from the Dirac equation using the Fouldy–Wouthuysen transformation. The unregularized expression which is valid for $S$-states is [10]

$$\begin{aligned} H_{EN} = {} & \frac{p^6}{16\,m^5} - \frac{1}{8\,m^3} \left[ \boldsymbol{p}; \frac{Z\,\alpha}{r} \right]^2 - \frac{3}{64\,m^4} \left( p^2 \left[ \boldsymbol{p}; \left[ \boldsymbol{p}; \frac{Z\,\alpha}{r} \right] \right] + \left[ \boldsymbol{p}; \left[ \boldsymbol{p}; \frac{Z\,\alpha}{r} \right] \right] p^2 \right) \\ & - \frac{5}{128\,m^4} \left[ p^2; \left[ p^2; \frac{Z\,\alpha}{r} \right] \right] . \end{aligned} \tag{15}$$

$H_{EN}$ for the regularized potential is obtained by the replacement (1). The derivation of remaining parts $H_{EN}$, $H_{TB}$ and $H_{RC}$ is presented in the following section.

## III. TIME–ORDERED PERTURBATION TECHNIQUE

For the calculation of the effective Hamiltonian in the order $m\,\alpha^6$ we use the time–ordered perturbation technique and calculate diagrams in Fig.1. The first group i.e. (1-6) has already been derived for the positronium [10]. The only difference here lies in the lack of assumption that $\boldsymbol{p}_1 \neq -\boldsymbol{p}_2$. 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 $\delta$-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.

Let's start the calculation from the single Coulomb exchange, *i.e.* diagram 1 in Fig. 1. We denote by $\mathcal{V}$ the algebraic expression that corresponds to diagram, namely the effective interaction potential, and by $V$ its $m\,\alpha^6$ part. The correction to energy is obtained by taking the matrix element $\Delta E = \langle\phi|V|\phi\rangle$. The initial expression is

$$\mathcal{V}_1 = \frac{4\,\pi\,\alpha}{q^2}\,u^+(p_1')u(p_1)\;u^+(p_2')u(p_2)\,, \tag{16}$$

where

$$\boldsymbol{q}\!=\boldsymbol{p}_1' - \boldsymbol{p}_1 = \boldsymbol{p}_2 - \boldsymbol{p}_2'\,. \tag{17}$$

$\mathcal{V}_1$ is expanded in momenta up to $p^4$, and we will keep only the terms that give $\alpha^6$ correction. The free bispinor $u$ is

$$u(p) = \begin{pmatrix} \sqrt{\frac{E(p)+m}{2\,E(p)}} \\ \frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{\sqrt{2\,E(p)\,(E(p)+m)}} \end{pmatrix}\,, \tag{18}$$

where $E(p) = \sqrt{p^2+m^2}$. The scalar product after expansion in momenta takes a form

$$\begin{aligned} u^+(p')u(p) = 1 &- \frac{q^2}{8\,m^2} + \frac{i}{4\,m^2}\,\boldsymbol{p}'\times\boldsymbol{p}\cdot\boldsymbol{\sigma} \\ &+\frac{5}{128\,m^4}\,(p^2-p'^2)^2 + \frac{3}{64\,m^4}\,(q^2 - 2\,i\,\boldsymbol{p}'\times\boldsymbol{p}\cdot\boldsymbol{\sigma})\,(p'^2+p^2) + \ldots\,. \end{aligned} \tag{19}$$

In the further calculations, we make use of the fact that our state has angular momentum $l = 0$ and spin $s = 1$. It allows to omit $\delta^3(r)$ and $\delta^3(r)/r$ terms, since the spatial wave function is antisymmetric, and replace the product $\sigma_1^i \sigma_2^j$ by $\boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 \delta^{ij}/3$.

The single Coulomb exchange $V_1$ after $p$–expansion is

$$V_1 = \frac{4\pi\alpha}{q^2}\frac{1}{64\,m^4}\Big\{q^4 - \frac{4}{3}\,(\boldsymbol{p}_1' \times \boldsymbol{p}_1)\cdot(\boldsymbol{p}_2' \times \boldsymbol{p}_2)\,(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) + \frac{5}{2}\left[(p_2'^2 - p_2^2)^2 + (p_1'^2 - p_1^2)^2\right] + 3\,q^2\left(p_1^2 + p_1'^2 + p_2^2 + p_2'^2\right)\Big\}\,. \tag{20}$$

We have neglected terms proportional to $\boldsymbol{\sigma}\cdot\boldsymbol{L}$ that vanish on S-states. For triplet states also the last term in the above vanishes. The contribution to energy in the coordinate representation becomes

$$V_1 = \frac{1}{64\,m^4}\Big\{-\Delta(4\pi\alpha\,\delta^3(r)) + \frac{5}{2}\Big[p_2^2;\Big[p_2^2;\frac{\alpha}{r}\Big]\Big] + \frac{5}{2}\Big[p_1^2;\Big[p_1^2;\frac{\alpha}{r}\Big]\Big] + \frac{4}{3}\left(p_1^i\,p_2^j\frac{\alpha}{r}\,p_1^j\,p_2^i - p_1^i\,p_2^i\frac{\alpha}{r}\,p_1^j\,p_2^j\right)\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\Big\}\,. \tag{21}$$

The next contribution is the double Coulomb exchange, diagram 2 in Fig. 1.

$$\mathcal{V}_2 = \int\frac{d^3q_1}{(2\pi)^3}\int\frac{d^3q_2}{(2\pi)^3}\,\frac{4\pi\alpha}{q_1^2}\,\frac{4\pi\alpha}{q_2^2}\,(2\pi)^3\,\delta^3(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{q})\,u^+(p_1')\,\Lambda_-(p_1'')\,u(p_1)\,u^+(p_2')\,\Lambda_+(p_2'')\,u(p_2)\,\frac{-1}{2\,m + E_0 - E(p_1) - E(p_1'') - E(p_1') - E(p_2'')} + (1\leftrightarrow 2)\,, \tag{22}$$

where $p_1'' = p_1 + q_2$, $p_2'' = p_2 - q_1$, and

$$\Lambda_+(p) = \frac{E(p) + \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta\,m}{2\,E(p)}\,, \tag{23}$$

$$\Lambda_-(p) = \frac{E(p) - \boldsymbol{\alpha}\cdot\boldsymbol{p} - \beta\,m}{2\,E(p)} \tag{24}$$

are projection operators. In the leading order in the $p$–expansion their matrix element is

$$u^+(p_2')\,\Lambda_+(p_2'')\,u(p_2) = 1\,, \tag{25}$$

$$u^+(p_1')\,\Lambda_-(p_1'')\,u(p_1) = -\frac{1}{4\,m^2}(\boldsymbol{\sigma}_1\cdot\boldsymbol{q}_1)\,(\boldsymbol{\sigma}_1\cdot\boldsymbol{q}_2)\,. \tag{26}$$

Moreover, we can neglect $p$ dependence in the denominator and $V_2$ becomes

$$V_2 = \int\frac{d^3q_1}{(2\pi)^3}\int\frac{d^3q_2}{(2\pi)^3}\,(2\pi)^3\,\delta^3(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{q})\,\frac{1}{2\,m}\,\frac{4\pi\alpha}{q_1^2}\,\frac{4\pi\alpha}{q_2^2}\,\frac{(-1)}{4\,m^2}\,(\boldsymbol{\sigma}_1\cdot\boldsymbol{q}_1)\,(\boldsymbol{\sigma}_1\cdot\boldsymbol{q}_2) + (1\leftrightarrow 2)\,. \tag{27}$$

Its Fourier transform is:

$$V_2 = \frac{\alpha^2}{4\,m^3\,r^4}\,. \tag{28}$$

The next contribution is the exchange of a single transverse photon in the no retardation limit, diagram 3 in Fig. 1.

$$\mathcal{V}_3 = -\frac{4\,\pi\,\alpha}{q^2}\,[u^+(p_1')\,\boldsymbol{\alpha}^i\,u(p_1)]\,[u^+(p_2')\,\boldsymbol{\alpha}^j\,u(p_2)]\left(\delta^{ij} - \frac{q^i\,q^j}{q^2}\right). \tag{29}$$

As in the case of single Coulomb exchange one expands the current in momenta:

$$\begin{aligned} u^+(p')\,\boldsymbol{\alpha}^i\,u(p) = {} & \frac{1}{2\,m}\,(p^i + p'^i) + \frac{i}{2\,m}(\boldsymbol{\sigma}\times\boldsymbol{q})^i - \frac{1}{16\,m^3}\left[p^i\,(p'^2 + 3\,p^2) + p'^i\,(p^2 + 3\,p'^2)\right] \\ & + \frac{i}{16\,m^3}\left[(\boldsymbol{p}'\times\boldsymbol{\sigma})^i\,(p^2 + 3\,p'^2) - (\boldsymbol{p}\times\boldsymbol{\sigma})^i\,(p'^2 + 3\,p^2)\right]. \end{aligned} \tag{30}$$

When this current is replaced by the expanded form $V_3$ becomes:

$$\begin{aligned} V_3 = {} & \frac{1}{4\,m^4}\,\frac{4\,\pi\,\alpha}{q^2}\left(\delta^{ij} - \frac{q^i\,q^j}{q^2}\right)p_1^i\,p_2^j\,(p_1^2 + p_1'^2 + p_2^2 + p_2'^2) \\ & + \frac{1}{48\,m^4}\,\frac{4\,\pi\,\alpha}{q^2}\left[2\,q^2\,(p_1^2 + p_1'^2 + p_2^2 + p_2'^2) + (p_1'^2 - p_1^2)^2 + (p_2'^2 - p_2^2)^2\right]\boldsymbol{\sigma}_1\,\boldsymbol{\sigma}_2\,. \end{aligned} \tag{31}$$

For triplet state the first term is square brackets vanishes. In configuration space $V_3$ takes the form

$$\begin{aligned} V_3 = {} & \frac{\alpha}{8\,m^4}\left[p_1^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right)p_2^j\,(p_1^2 + p_2^2) + (p_1^2 + p_2^2)\,p_1^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right)p_2^j\right] \\ & + \frac{\boldsymbol{\sigma}_1\,\boldsymbol{\sigma}_2}{48\,m^4}\left\{\left[p_1^2;\left[p_1^2;\frac{\alpha}{r}\right]\right] + \left[p_2^2;\left[p_2^2;\frac{\alpha}{r}\right]\right]\right\}. \end{aligned} \tag{32}$$

The most tricky is the calculation of the retardation part in the single transverse photon exchange, diagram 4 in Fig 1. The initial expression is

$$\begin{aligned} \mathcal{V}_4 = {} & 4\,\pi\,\alpha\int\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij} - \frac{k^i\,k^j}{k^2}\right)\left(\frac{p_1^i}{m} + \frac{i\,(\boldsymbol{\sigma}_1\times\boldsymbol{k})^i}{2\,m}\right) \\ & \left\{e^{i\,k\,r_1}\left(\frac{1}{E_0 - k - H_0} + \frac{1}{k}\right)e^{-i\,k\,r_2}\right\}\left(\frac{p_2^j}{m} - \frac{i\,(\boldsymbol{\sigma}_2\times\boldsymbol{k})^j}{2\,m}\right) + (1\leftrightarrow 2)\,. \end{aligned} \tag{33}$$

$$= \mathcal{V}_4^A + \mathcal{V}_4^B \tag{34}$$

Lets consider first the spin independent part $\mathcal{V}_4^A$. The expression in braces requires subtraction of the term that contributes in the lower order, namely this term, which is obtained by the dipole approximation

$$\left\{e^{i\,k\,r_1}\left(\frac{1}{E_0 - k - H_0} + \frac{1}{k}\right)e^{-i\,k\,r_2} - \left(\frac{1}{E_0 - k - H_0} + \frac{1}{k}\right)\right\}. \tag{35}$$

Moreover, we need only the second term in the retardation expansion (notice two dotted lines in the corresponding diagram):

$$\frac{1}{E_0-k-H_0}+\frac{1}{k}=\frac{(H_0-E_0)}{k^2}-\frac{(H_0-E_0)^2}{k^3}+\dots\,, \tag{36}$$

and the spin independent part $V_4^A$ becomes

$$V_4^A=-4\,\pi\,\alpha\int\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)$$
$$\frac{p_1^i}{m}\left\{e^{i\,k\,r_1}\,\frac{(H_0-E_0)^2}{k^3}e^{-i\,k\,r_2}-\frac{(H_0-E_0)^2}{k^3}\right\}\frac{p_2^j}{m}+(1\leftrightarrow 2)\,. \tag{37}$$

The $k$–integral could be performed using the formula:

$$\int\frac{d^3k}{(2\,\pi)^3}\,\frac{1}{k^4}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)(e^{i\,k\,r}-1)=\frac{1}{32\,\pi\,r}\,(r^i\,r^j-3\,r^2\,\delta^{ij})\,. \tag{38}$$

After simple transformations $V_4^A$ is

$$V_4^A=-\frac{\alpha}{8}\,\frac{p_1^i}{m}\left\{(H_0-E_0)\left(\frac{r^i\,r^j}{r}-3\,\delta^{ij}\,r\right)(H_0-E_0)+(H_0-E_0)\left[\frac{p_2^2}{2\,m}\,;\,\frac{r^i\,r^j}{r}-3\,\delta^{ij}\,r\right]\right.$$
$$\left.+\left[\frac{r^i\,r^j}{r}-3\,\delta^{ij}\,r\,;\,\frac{p_1^2}{2\,m}\right](H_0-E_0)+\left[\frac{p_2^2}{2\,m}\,;\,\left[\frac{r^i\,r^j}{r}-3\,\delta^{ij}\,r\,;\,\frac{p_1^2}{2\,m}\right]\right]\right\}\frac{p_2^j}{m}\,. \tag{39}$$

The spin dependent part $V_4^B$ is obtained from (33) using (36)

$$V_4^B=-8\,\pi\,\alpha\int\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\frac{(\boldsymbol{\sigma}_1\times\boldsymbol{k})^i}{2\,m}\,e^{i\,k\,r_1}\,\frac{(H_0-E_0)^2}{k^3}e^{-i\,k\,r_2}\frac{(\boldsymbol{\sigma}_2\times\boldsymbol{k})^j}{2\,m}\,. \tag{40}$$

Since only the term proportional to $\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2$ does not vanish on S-states, could be further transform to

$$V_4^B=\frac{1}{24\,m^4}\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\left[p_1^2\,;\,\left[p_2^2\,;\,\frac{\alpha}{r}\right]\right]\,. \tag{41}$$

The next contribution is a group of diagrams No. 5 in Fig. 1. It consists of four diagrams with different time ordering on both electron lines and next four with "Z" on lower line. Lets first consider the upper electron line. By $q_1$ and $q_2$ we denote momenta transfered by transverse and Coulomb photon respectively.

$$u^+(p_1')\,\alpha^j\,\Lambda_-(p_1+q_2)\,u(p_1)+u^+(p_1')\,\Lambda_-(p_1'-q_2)\,\alpha^j\,u(p_1)=-\frac{i}{m}\,(\boldsymbol{q}_2\times\boldsymbol{\sigma}_1)^j\,. \tag{42}$$

The lower electron line is

$$u^+(p_2')\,\alpha^i\,\Lambda_+(p_2'+q_1)\,u(p_2)+u^+(p_2')\,\Lambda_+(p_2-q_1)\,\alpha^i\,u(p_2)=\frac{1}{m}(p_2^i+p_2'^i)+\frac{i}{m}\,(\boldsymbol{q}_1\times\boldsymbol{\sigma}_2)^i\,. \tag{43}$$

Only the last term in (43) contributes for S-states. The effective interaction $V_5$ is:

$$V_5 = 2 \int \frac{d^3q_1}{(2\,\pi)^3} \int \frac{d^3q_2}{(2\,\pi)^3}\,(2\,\pi)^3\,\delta^3(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{q})\,\frac{4\,\pi\,\alpha}{q_2^2}\,\frac{(-4\,\pi\,\alpha)}{2\,q_1^2}\left(\delta^{ij}-\frac{q_1^i\,q_1^j}{q_1^2}\right)$$
$$\frac{1}{2\,m}\,\frac{-i}{m}\,(\boldsymbol{q}_2\times\boldsymbol{\sigma}_1)^j\,\frac{i}{m}\,(\boldsymbol{q}_1\times\boldsymbol{\sigma}_2)^i \tag{44}$$
$$= -\frac{1}{3\,m^3}\int \frac{d^3q_1}{(2\,\pi)^3} \int \frac{d^3q_2}{(2\,\pi)^3}\,(2\,\pi)^3\,\delta^3(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{q})\,\frac{4\,\pi\,\alpha}{q_1^2}\,\frac{4\,\pi\,\alpha}{q_2^2}\,(\boldsymbol{q}_1\cdot\boldsymbol{q}_2)\,(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\,. \tag{45}$$

The factor 2 in front of the first integral comes from the fact that $Z$ is on upper or on the lower electron line. For triplet S-states in configuration space $V_5$ is

$$V_5 = \frac{\alpha^2}{3\,m^3\,r^4}\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,. \tag{46}$$

The next contribution is double transverse photon exchange with single $Z$, diagram 6 in Fig. 1. This contribution consists of twelve diagrams. They reduce to two diagrams upon nonretardation limit.

$$V_6 = \int \frac{d^3q_1}{(2\,\pi)^3} \int \frac{d^3q_2}{(2\,\pi)^3}\,(2\,\pi)^3\,\delta^3(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{q})\,\frac{4\,\pi\,\alpha}{q_1^2}\left(\delta^{ik}-\frac{q_1^i\,q_1^k}{q_1^2}\right)\frac{4\,\pi\,\alpha}{q_2^2}\left(\delta^{jk}-\frac{q_2^j\,q_2^k}{q_2^2}\right)\frac{1}{2\,m}$$
$$\left[\frac{(2\,\boldsymbol{p}_2+i\,\boldsymbol{q}_1\times\boldsymbol{\sigma}_2)^i}{2\,m}\,\frac{(2\,\boldsymbol{p}_2'+i\,\boldsymbol{q}_2\times\boldsymbol{\sigma}_2)^j}{2\,m}+\frac{(2\,\boldsymbol{p}_1-i\,\boldsymbol{q}_1\times\boldsymbol{\sigma}_1)^i}{2\,m}\,\frac{(2\,\boldsymbol{p}_1'-i\,\boldsymbol{q}_2\times\boldsymbol{\sigma}_1)^j}{2\,m}\right]. \tag{47}$$

In the configuration space it becomes:

$$V_6 = \frac{1}{2\,m^3}\,p_1^i\,\frac{\alpha^2}{4\,r^2}\Big(\delta^{ij}+3\frac{r^i\,r^j}{r^2}\Big)p_1^j+\frac{1}{2\,m^3}\,p_2^i\,\frac{\alpha^2}{4\,r^2}\Big(\delta^{ij}+3\frac{r^i\,r^j}{r^2}\Big)p_2^j+\frac{\alpha^2}{2\,m^3\,r^4}\,. \tag{48}$$

Other two body diagrams do not contribute in order $m\,\alpha^6$. Therefore, further diagrams are connected to three body interactions. Diagram 7 in Fig. 1 is a two–Coulomb exchange. It is similar to the diagram No. 2 so we skip a simple rederivation. The expression for $V_7$ is

$$V_7 = \frac{1}{4\,m^3}\left[\boldsymbol{\sigma}_1\cdot\boldsymbol{p}_1\,;\,\frac{Z\,\alpha}{r}\right]\left[\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\,;\,\frac{\alpha}{r}\right]+(1\to 2) = -\frac{Z\,\alpha^2}{4\,m^3}\,\frac{\boldsymbol{r}}{r^3}\left(\frac{\boldsymbol{r}_1}{r_1^3}-\frac{\boldsymbol{r}_2}{r_2^3}\right). \tag{49}$$

The last diagram, No. 8, is a single Coulomb–single transverse exchange. It is similar to the diagram No. 5.

$$V_8 = \frac{1}{6\,m^3}\left[\boldsymbol{p}_1\,;\,\frac{Z\,\alpha}{r}\right]\cdot\left[\boldsymbol{q}\,;\,\frac{\alpha}{r}\right]\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2+(1\to 2) = -\frac{Z\,\alpha^2}{6\,m^3}\,\frac{\boldsymbol{r}}{r^3}\left(\frac{\boldsymbol{r}_1}{r_1^3}-\frac{\boldsymbol{r}_2}{r_2^3}\right). \tag{50}$$

The effective Hamiltonians $H_{EE}$ and $H_{TB}$ are expressed in terms of $V_i$

$$H_{EE} = \Sigma_{i=1}^6 V_i\,, \tag{51}$$
$$H_{TB} = V_7+V_8\,. \tag{52}$$

The radiative correction $H_{RC}$ consists of the one–loop and two–loop terms, that could be obtained from the hydrogen Lamb shift

$$H_{RC} = H_{RC1} + H_{RC2}\,, \tag{53}$$

$$H_{RC1} = \frac{\pi\,\alpha\,(Z\,\alpha)^2}{m^2}\left(\frac{139}{32} - 2\,\ln(2) + \frac{5}{48}\right)\left[\delta^3(r_1) + \delta^3(r_2)\right]\,, \tag{54}$$

$$H_{RC2} = \frac{\alpha^2\,(Z\,\alpha)}{\pi\,m^2}\left(-\frac{4358}{1296} - \frac{10}{27}\,\pi^2 + \frac{3}{2}\,\pi^2\,\ln(2) - \frac{9}{4}\,\zeta(3)\right)\left[\delta^3(r_1) + \delta^3(r_2)\right]\,. \tag{55}$$

The radiative correction to electron–electron interaction does not contribute for triplet S-states in the order $m\,\alpha^6$.

## IV. CANCELATION OF ELECTRON–NUCLEUS DIVERGENCES

The mechanism for the cancelation of electron–nucleus divergences in helium is the same as in hydrogen. The cancelation in hydrogen was demonstrated in [10] and we follow here that method. The dangerous terms are $E_A$ in (11) and

$$E_{EN} = \langle H_{EN}(1) + H_{EN}(2)\rangle\,, \tag{56}$$

We extract the potentially divergent terms in the form of

$$\left(\frac{(Z\,\alpha)^2}{r_i^4}\right)_\lambda \equiv \left\{\nabla_i\left[\frac{Z\,\alpha}{r_i}\left(1 - e^{-\Lambda\,r_i}\right)\right]\right\}^2\,, \tag{57}$$

$$\left(\frac{(Z\,\alpha)^3}{r_i^3}\right)_\lambda \equiv \left[\frac{Z\,\alpha}{r_i}\left(1 - e^{-\Lambda\,r_i}\right)\right]^3\,. \tag{58}$$

In further calculations we simply skip the subscript $\lambda$ what should nor lead to any confusion. Whenever expression is divergent it should be regularized according to (1), (13), (57), and (58). Lets first consider the term

$$\mathcal{E}_1 = \frac{1}{16\,m^5}\,\langle p_1^6 + p_2^6\rangle\,. \tag{59}$$

It is transformed using $p_1^2 + p_2^2 = 2m[E_0 - V + (H_0 - E_0)]$ and a Schrödinger equation,

$$\begin{aligned}
\mathcal{E}_1 &= \frac{1}{16\,m^5}\,\left\langle (p_1^2 + p_2^2)^3 - 3\,p_1^2\,p_2^2\,(p_1^2 + p_2^2)\right\rangle \\
&= \frac{1}{16\,m^5}\,\left\langle 2\,m\,(E_0 - V)\,(p_1^2 + p_2^2)\,2\,m\,(E_0 - V) - 3\,m\,(E_0 - V)\,p_1^2\,p_2^2 - 3\,m\,p_1^2\,p_2^2\,(E_0 - V)\right\rangle \\
&= \frac{1}{16\,m^5}\,\Big\langle 2\,m^2\,[E_0 - V\,;\,[p_1^2 + p_2^2\,;\,E_0 - V]] + 2\,m^2\,(E_0 - V)^2\,(p_1^2 + p_2^2) \\
&\quad + 2\,m^2\,(p_1^2 + p_2^2)\,(E_0 - V)^2 - 3\,m\,p_1^2\,p_2^2\,(E_0 - V) - 3\,m\,(E_0 - V)\,p_1^2\,p_2^2\Big\rangle \\
&= \frac{1}{16\,m^5}\Big\{4\,m^2\,(\nabla_1 V)^2 + 4\,m^2\,(\nabla_2 V)^2 + [2\,m\,(E_0 - V)]^3 \\
&\quad - 3\,m\,p_1^2\,p_2^2\,(E_0 - V) - 3\,m\,(E_0 - V)\,p_1^2\,p_2^2\Big\}\,.
\end{aligned} \tag{60}$$

This expression contains few terms that are potentially divergent and are taken out:

$$\mathcal{E}_1 \approx \frac{1}{4\,m^3}\,\frac{(Z\,\alpha)^2}{r_1^4} + \frac{1}{4\,m^3}\,\frac{(Z\,\alpha)^2}{r_2^4} + \frac{1}{2\,m^2}\,\left(\frac{Z\,\alpha}{r_1}\right)^3 + \frac{1}{2\,m^2}\,\left(\frac{Z\,\alpha}{r_2}\right)^3 . \tag{61}$$

The second term is simple

$$\mathcal{E}_2 = \frac{1}{8\,m^3}\,\left[\frac{(Z\,\alpha)^2}{r_1^4} + \frac{(Z\,\alpha)^2}{r_2^4}\right] . \tag{62}$$

Further terms after these transformations are to long to write its explicit form, so we show only the divergent part. In the calculation of the third term

$$\mathcal{E}_3 = \frac{3}{64\,m^4}\left[p_1^2\,\Delta_1\left(\frac{Z\,\alpha}{r_1}\right) + \Delta_1\left(\frac{Z\,\alpha}{r_1}\right)p_1^2 + p_2^2\,\Delta_2\left(\frac{Z\,\alpha}{r_2}\right) + \Delta_2\left(\frac{Z\,\alpha}{r_2}\right)p_2^2\right] , \tag{63}$$

we use the identity

$$\begin{aligned}\left\langle \frac{Z\,\alpha}{r_1}\,4\,\pi\,Z\,\alpha\,\delta^3(r_1)\right\rangle \;=\; &\left\langle \frac{(Z\,\alpha)^2}{r_1^4} + 2\,m\,(E_0 - V)\,\frac{(Z\,\alpha)^2}{r_1^2}\right. \\ &\left. -p_2^2\,\frac{(Z\,\alpha)^2}{2\,r_1^2} - \frac{(Z\,\alpha)^2}{2\,r_1^2}\,p_2^2 - \boldsymbol{p}_1\,\frac{(Z\,\alpha)^2}{r_1^2}\,\boldsymbol{p}_1\right\rangle\end{aligned} \tag{64}$$

to find the divergent part

$$\mathcal{E}_3 \approx -\frac{3}{16\,m^3}\left[\frac{(Z\,\alpha)^2}{r_1^4} + \frac{(Z\,\alpha)^2}{r_2^4} + 2\,\left(\frac{Z\,\alpha}{r_1}\right)^3 + 2\,\left(\frac{Z\,\alpha}{r_1}\right)^3\right] . \tag{65}$$

The fourth term is

$$\mathcal{E}_4 = -\frac{5}{128\,m^4}\,\left(\left[p_1^2;\left[p_1^2;\frac{Z\,\alpha}{r_1}\right]\right] + \left[p_2^2;\left[p_2^2;\frac{Z\,\alpha}{r_2}\right]\right]\right) \approx -\frac{5}{32\,m^3}\left[\frac{(Z\,\alpha)^2}{r_1^4} + \frac{(Z\,\alpha)^2}{r_2^4}\right] . \tag{66}$$

Further potentially divergent terms are that in $E_A$, Eq. (11) i.e. in the second order contribution from $H_A$.

$$\mathcal{E}_5 = \left\langle \frac{1}{8\,m^3}\,(p_1^4 + p_2^4)\,\frac{1}{(E_0 - H_0)'}\,\frac{1}{8\,m^3}\,(p_1^4 + p_2^4)\right\rangle , \tag{67}$$

$$\mathcal{E}_6 = \left\langle \frac{Z\,\alpha\,\pi}{2\,m^2}[\delta^3(r_1) + \delta^3(r_2)]\,\frac{1}{(E_0 - H_0)'}\,\frac{Z\,\alpha\,\pi}{2\,m^2}[\delta^3(r_1) + \delta^3(r_2)]\right\rangle , \tag{68}$$

$$\mathcal{E}_7 = -2\,\left\langle \frac{1}{8\,m^3}\,(p_1^4 + p_2^4)\,\frac{1}{(E_0 - H_0)'}\,\frac{Z\,\alpha\,\pi}{2\,m^2}[\delta^3(r_1) + \delta^3(r_2)]\right\rangle . \tag{69}$$

We use the equations

$$p_1^4 + p_2^4 = 4m^2[E_0 - V + (H_0 - E_0)]^2 - 2\,p_1^2\,p_2^2\,, \tag{70}$$

$$4\,\pi\,Z\,\alpha\,\delta^3(r_1) = -2\,\left[\boldsymbol{p}_1\,;\,\frac{Z\,\alpha}{r_1}\right]\boldsymbol{p}_1 + 2\,m\,\left[H_0 - E_0\,;\,\frac{Z\,\alpha}{r_1}\right] , \tag{71}$$

to separate out the divergent terms:

$$\mathcal{E}_5 \approx -\frac{1}{8\,m^3}\,\frac{(Z\,\alpha)^2}{r_1^4} - \frac{1}{8\,m^3}\,\frac{(Z\,\alpha)^2}{r_2^4} - \frac{1}{2\,m^2}\,\left(\frac{Z\,\alpha}{r_1}\right)^3 - \frac{1}{2\,m^2}\,\left(\frac{Z\,\alpha}{r_2}\right)^3\,, \tag{72}$$

$$\mathcal{E}_6 \approx -\frac{1}{32\,m^3}\,\frac{(Z\,\alpha)^2}{r_1^4} - \frac{1}{32\,m^3}\,\frac{(Z\,\alpha)^2}{r_2^4} - \frac{1}{8\,m^2}\,\left(\frac{Z\,\alpha}{r_1}\right)^3 - \frac{1}{8\,m^2}\,\left(\frac{Z\,\alpha}{r_2}\right)^3\,, \tag{73}$$

$$\mathcal{E}_7 \approx \frac{1}{8\,m^3}\,\frac{(Z\,\alpha)^2}{r_1^4} + \frac{1}{8\,m^3}\,\frac{(Z\,\alpha)^2}{r_2^4} + \frac{1}{2\,m^2}\,\left(\frac{Z\,\alpha}{r_1}\right)^3 + \frac{1}{2\,m^2}\,\left(\frac{Z\,\alpha}{r_2}\right)^3\,. \tag{74}$$

$$\tag{75}$$

All the divergent terms from $\mathcal{E}_i$ cancel out,

$$\Sigma_{i=1}^{7}\mathcal{E}_i \approx 0\,, \tag{76}$$

leaving a finite expression to be evaluated numerically.

## V. SUMMARY

The contribution to energy in the order $m\,\alpha^6$ is a sum of terms (11), (12), and (14). The electron nucleus terms in (11) and (14) require transformation to cancel out internal divergences, which was demonstrated in the previous chapter. This cancelations proves the lack of $\ln(\alpha)$ term for triplet states, what was first shown by Drake *et al.* in [11]. The correctness of the derived operators is verified by the comparison to the known positronium case [10], which is obtained by putting $Z \to 0$ and $\boldsymbol{p}_1 = -\boldsymbol{p}_2 = \boldsymbol{p}$. Some of the operators for helium S-levels have been first derived by Zhang in [12]. However, his set of operators is not complete, so we can not make a direct comparison. The further step is the numerical calculation of the corresponding matrix elements. Such a calculation has been performed recently with high precision for the fine structure of P-levels by Yan and Drake in [13], and their method could be applied to triplet S-states as well.

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## FIGURES

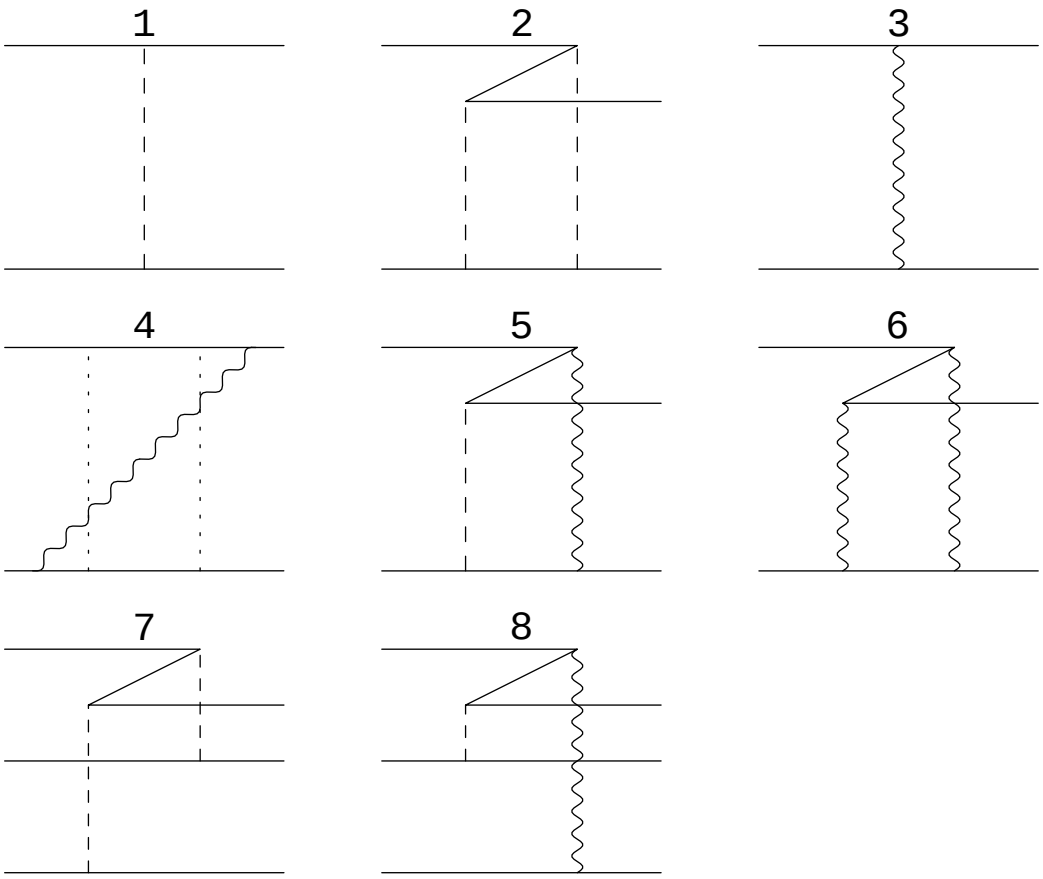


FIG. 1. Time ordered diagrams contributing to energy levels in order $m\,\alpha^6$. The middle horizontal line corresponds to helium, two outer horizontal lines correspond to two electrons. The wavy line is a transverse photon, the dashed line is a Coulomb photon, and the dotted line denotes retardation.