Ground State Energy of the Helium Atom

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Abstract. With an eye on the high accuracy ($\sim 10\,$MHz) evaluation of the ionization energy from the helium atom ground state, a complete set of order $m\alpha^6$ operators is built. This set is gauge and regularization scheme independent and can be used for an immediate calculation with a wave function of the helium ground state.

1 Introduction

Singlet states of the helium atom, especially its ground state, is probably the best place for precision studies of the electron-electron interaction at low energies. Recent measurements of $1^1S - 2^1P$ [1] and $1^1S - 2^1S$ [2] intervals have reached an unprecedented accuracy of about 10 *ppb*. The ground state ionization energy extracted from these measurements constitutes

$$\nu_{\rm exp}(1^1S) = 5\;945\;204\;238(45)\;\text{MHz} \tag{1}$$

and

$$\nu_{\rm exp}(1^1S) = 5\;945\;204\;356(48)\;\text{MHz}, \tag{2}$$

respectively. The most recent theoretical result,

$$\nu_{\rm th}(1^1S) = 5\;945\;204\;226(91)\;\text{MHz}, \tag{3}$$

obtained in [3] has twice larger uncertainty. The main source of this uncertainty is the order $m\alpha^6$ correction, included in (3) only partially.

The present work is the first of two, which are devoted to the calculation of $\nu_{\rm th}(1^1S)$ with $\mathcal{O}(m\alpha^6)$ accuracy. It contains the analytic part of the calculation, and its main result is comprised by the set of the effective operators which produce the $\mathcal{O}(m\alpha^6)$ shift of the energy. The second paper [4] describes the numerical evaluation of the average values of those operators, as well as the contributions to all previous orders.

2 Framework of the calculation

In the present work we closely follow the scheme of calculation, applied in [5] to the similar problem in positronium. Namely, we employ the dimensionally regularized nonrelativistic QED (NRQED). In this approach, separation of contributions to the energy coming from the hard ($\sim m$) and soft ($\sim m\alpha$) scales is governed by the regularization parameter $\varepsilon = (3-d)/2$, d being the number of spatial dimensions. The shift of d from three gives control over both ultraviolet and infrared divergences appearing in the soft and hard scale contributions, respectively.

The new feature of the helium as compared to the positronium is that the wave function of the former is not available in the analytic form even in three dimensions. Therefore, the problem of control over divergences (the terms which are singular for $\varepsilon \to 0$) arising in NRQED calculations, becomes more involved. In fact, average values of effective NRQED operators over the ground state can be calculated only numerically, by integration with the wave function computed, for example, by the variational method. As already noted, those operators appear either from the hard or from the soft scale. In the former case the effective operators are contact, i.e. $\delta(\boldsymbol{r})$-like ($|\boldsymbol{r}|$ is the distance between a pair of interacting particles). Corresponding Wilson coefficients can be found from the matching of a NRQED scattering amplitude with its QED counterpart and generally are divergent. On the other hand, the soft scale effective operators have finite Wilson coefficients, while divergences arise only when one calculates average values of some of those operators which prove to be sufficiently singular. Hence, in the latter case an extraction of divergences seems to be a notably more complex problem. Recall that the divergences mutually cancel only in the sum of the hard and soft scale contributions.

To keep track of this cancellation we choose the following strategy. The main idea of the approach is to extract divergent pieces of all soft scale contributions on the *analytic* level. Performing such an extraction we manage to demonstrate straightforwardly that the divergences coming from both scales cancel each other *before* any numerical calculation. As the result, the total $\mathcal{O}(m\alpha^6)$ correction to the ground state energy is represented as a sum of the apparently finite average values of the regularization-independent operators. These average values can be immediately calculated using a numerically built wave function.

It is worthy to note that the main idea of the above approach has a simple physical ground. In fact, the soft scale divergences in a bound state energy are of the ultraviolet origin. They hence should be proportional to a value of the corresponding wave function at zeroth separation between interacting particles. In terms of the effective theory it means that by virtue of the Schrödinger equation one can rewrite the singular soft scale contributions in such a way that the corresponding divergences will be shifted to the Wilson coefficients of the contact operators. After the perturbation theory is reformulated in such a manner, and if an underlying theory is renormalizable, all divergences that enter an individual Wilson coefficient have to cancel each other.

In the rest of the paper, we list the individual contributions. Sections 3 and 4 are devoted to the soft scale and hard scale ones, respectively. The final result of this paper is presented in the last Section. Notations used throughout the paper are collected in Appendix. In order to make the formulae more transparent, we write the nonsingular soft scale operators with coefficients taken at $d = 3$.

3 Soft Scale Contributions

3.1 Irreducible corrections

There are several sources of such corrections. The list of expressions for the corresponding average values which arise when the Schrödinger equation for the wave function is extensively employed (for notations see Appendix) includes

- the dispersion correction,

$$\begin{aligned} \Delta_{\mathrm{disp}}E = & -5\frac{E^3}{2m^2} + \frac{3E^2\left\langle c\right\rangle}{8m^2} + \frac{3E}{2m^2}\left\langle C^2 - \frac{Cc}{2} - \frac{p_1^2p_2^2}{4m^2}\right\rangle \\ & + \left\langle \frac{3p_1^2C_{\mathrm{N}}p_2^2}{8m^4} - 3\frac{[\boldsymbol{P}\boldsymbol{p},[\boldsymbol{P}\boldsymbol{p},c]]}{16m^4} - 3\frac{(\boldsymbol{P}\boldsymbol{p})c(\boldsymbol{P}\boldsymbol{p})}{8m^4} - \frac{9C_{\mathrm{N}}^2c}{8m^2}\right. \\ & \left. -\frac{3C_{\mathrm{N}}c^2}{4m^2} + \frac{5(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2)\boldsymbol{e}}{16m^3} - \frac{C_{\mathrm{N}}^3}{2m^2} - \frac{c^3}{8m^2} + \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2}{4m^3} + \frac{e^2}{8m^3}\right\rangle; \end{aligned} \tag{4}$$

- relativistic corrections to the Coulomb exchange,

$$\begin{aligned} \Delta_C E = & \frac{E\pi\alpha}{4m^3}\left\langle 4\delta(\boldsymbol{r}) - 3Z\left[\delta(\boldsymbol{r}_1) + \delta(\boldsymbol{r}_2)\right]\right\rangle + \left\langle 3\frac{[\boldsymbol{P}\boldsymbol{p},[\boldsymbol{P}\boldsymbol{p},c]]}{32m^4}\right. \\ & + \frac{3\pi\alpha Z}{4m^3}\left[\delta(\boldsymbol{r}_1)\left(\frac{p_2^2}{2m} + C_2 + c\right) + (1\leftrightarrow 2)\right] \\ & \left. -\frac{\pi\alpha\delta(\boldsymbol{r})}{m^3}\left(\frac{3P^2}{32m} + C_{\mathrm{N}}\right) + \frac{(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2)\boldsymbol{e}}{32m^3} - \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2}{32m^3} + \frac{e^2}{8m^3}\right\rangle; \end{aligned} \tag{5}$$

- relativistic corrections to the instantaneous magnetic exchange,

$$\begin{aligned} \Delta_M E = & \frac{E}{m}\left\langle \frac{\boldsymbol{p}_1 c\boldsymbol{p}_2 + (\boldsymbol{p}_1\boldsymbol{n})c(\boldsymbol{n}\boldsymbol{p}_2)}{2m^2} - \frac{2\pi\alpha\delta(\boldsymbol{r})}{m^2}\right\rangle \\ & + \left\langle \frac{2\boldsymbol{p}i\alpha\delta(\boldsymbol{r})}{m^3}C_{\mathrm{N}} - \left\{\frac{C}{4m^2}, \frac{\boldsymbol{p}_1 c\boldsymbol{p}_2 + (\boldsymbol{p}_1\boldsymbol{n})c(\boldsymbol{n}\boldsymbol{p}_2)}{m}\right\}\right. \\ & \left. -\frac{[\boldsymbol{P}\boldsymbol{p},[\boldsymbol{P}\boldsymbol{p},c]]}{8m^4} - 3\frac{(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2)\boldsymbol{e}}{8m^3} - 3\frac{d-1}{8}\frac{e^2}{m^3}\right\rangle; \end{aligned} \tag{6}$$

- retardation corrections induced by zero-, single-, and double-Coulomb exchanges,

$$\begin{aligned} \Delta_{\mathrm{ret}}^0 E = & -\frac{E^2\left\langle c\right\rangle}{8m^2} + \frac{E\left\langle Cc\right\rangle}{4m^2} + \left\langle -\frac{C_{\mathrm{N}}^2c}{8m^2} - \frac{C_{\mathrm{N}}c^2}{4m^2} + \frac{\pi\alpha\delta(\boldsymbol{r})}{2m^4}P^2 + \frac{\boldsymbol{p}c\boldsymbol{p}}{4m^4}P^2\right. \\ & -\frac{p_1^2c(\boldsymbol{n}\boldsymbol{p}_2)^2 + (\boldsymbol{p}_1\boldsymbol{n})^2cp_2^2 - 3(\boldsymbol{p}_1\boldsymbol{n})^2c(\boldsymbol{n}\boldsymbol{p}_2)^2 + (1\leftrightarrow 2)}{16m^4} \\ & \left. -\frac{(\boldsymbol{P}\boldsymbol{p})c(\boldsymbol{P}\boldsymbol{p})}{8m^4} + \frac{(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2)\boldsymbol{e}}{8m^3} - \frac{c^3}{8m^2} + \frac{d-1}{8}\frac{e^2}{m^3}\right\rangle, \end{aligned} \tag{7}$$

$$\Delta_{\mathrm{ret}}^1 E = \frac{E\left\langle c^2\right\rangle}{4m^2} + \left\langle -cr\frac{2(\boldsymbol{n}\boldsymbol{p}_2)(\boldsymbol{\mathcal{E}}_1\boldsymbol{p}_2) + (\boldsymbol{n}\boldsymbol{\mathcal{E}}_1)\left[(\boldsymbol{n}\boldsymbol{p}_2)^2 - p_2^2\right]}{8m^3} - \frac{C_{\mathrm{N}}c^2}{4m^2}\right. \tag{8}$$

$$-3\frac{(\boldsymbol{p}_1\boldsymbol{n})^2c^2+c^2(\boldsymbol{n}\boldsymbol{p}_1)^2+(1\leftrightarrow 2)}{16m^3}-\frac{d-2}{4}\frac{c^3}{m^2}+\frac{d-1}{4}\frac{e^2}{m^3}\Big\rangle,$$

$$\Delta^2_{\text{ret}}E=\Big\langle cr^2\frac{3\boldsymbol{\mathcal{E}}_1\boldsymbol{\mathcal{E}}_2-(\boldsymbol{n}\boldsymbol{\mathcal{E}}_1)(\boldsymbol{n}\boldsymbol{\mathcal{E}}_2)-2(\boldsymbol{\mathcal{E}}_1-\boldsymbol{\mathcal{E}}_2)\boldsymbol{e}}{8m^2}-\frac{(d-1)(d-2)^2}{8(4-d)}\frac{c^3}{m^2}\Big\rangle;$$

- and finally, the seagull correction,

$$\Delta_{\text{seag}}E=\Big\langle\frac{\boldsymbol{p}_1c^2\boldsymbol{p}_1+3(\boldsymbol{p}_1\boldsymbol{n})c^2(\boldsymbol{n}\boldsymbol{p}_1)}{8m^3}+(1\leftrightarrow 2)+\frac{d-1}{4}\frac{e^2}{m^3}\Big\rangle. \qquad (9)$$

3.2 Reducible Corrections

Breit Hamiltonian for the helium singlet states,

$$U=U_S+U_P, \qquad (10)$$

consists of two parts, U_S and U_P, with the selection rules $|\Delta\mathcal{S}|=0$ and $|\Delta\mathcal{S}|=1$, respectively. The second order iteration of the P-wave part, which mixes singlet S and triplet P states, is saturated by the soft scale and therefore we can take corresponding perturbation in three dimensions:

$$U_P=\frac{Z\alpha}{4m^2}\frac{\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2}{2}\left(\frac{\boldsymbol{l}_1}{r_1^3}-\frac{\boldsymbol{l}_2}{r_2^3}\right)+\frac{\alpha}{4m^2}\frac{\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2}{2}\frac{\boldsymbol{r}\times\boldsymbol{P}}{r^3}. \qquad (11)$$

The S-wave part should be considered in d dimensions,

$$\begin{aligned}U_S=&-\frac{p_1^4+p_2^4}{8m^3}+\frac{\pi Z\alpha}{2m^2}\left(\delta(\boldsymbol{r}_1)+\delta(\boldsymbol{r}_2)\right)\\&+\frac{(d-2)\pi\alpha}{m^2}\delta(\boldsymbol{r})-\frac{\boldsymbol{p}_1c\boldsymbol{p}_2+(d-2)(\boldsymbol{p}_1\boldsymbol{n})c(\boldsymbol{n}\boldsymbol{p}_2)}{2m^2},\end{aligned} \qquad (12)$$

since its second order iteration contains divergences. After some manipulations corresponding correction to the energy can be represented as

$$\begin{aligned}\Delta_S E=&-\frac{E^3}{m^2}-\frac{E^2\langle c\rangle}{m^2}+\frac{E}{m}\left(4B+\frac{\langle p_1^2p_2^2\rangle}{4m^3}-\frac{\langle C^2\rangle}{2m}+\frac{\langle cC\rangle}{2m}\right)+\Big\langle\mathcal{O}_2^\dagger G\mathcal{O}_2\Big\rangle\\&+\frac{B\langle c\rangle}{2m}-\frac{\pi\alpha(Z-2)}{4m^3}\langle\delta(\boldsymbol{r}_1)C_2+\delta(\boldsymbol{r}_2)C_1\rangle+\Big\langle\frac{3CcC_{\text{N}}}{4m^2}-\frac{p_1^2C_{\text{N}}p_2^2}{8m^4}\\&-\frac{\pi\alpha\delta(\boldsymbol{r})}{2m^3}C_{\text{N}}+\frac{[\boldsymbol{P}\boldsymbol{p},[\boldsymbol{P}\boldsymbol{p},c]]+2(\boldsymbol{P}\boldsymbol{p})c(\boldsymbol{P}\boldsymbol{p})}{8m^4}\\&+\left\{\frac{C+(d-2)c}{8m^2},\frac{\boldsymbol{p}_1c\boldsymbol{p}_2+(\boldsymbol{p}_1\boldsymbol{n})c(\boldsymbol{n}\boldsymbol{p}_2)}{m}\right\}\\&-\frac{(\boldsymbol{\mathcal{E}}_1-\boldsymbol{\mathcal{E}}_2)\boldsymbol{e}}{8m^3}-\frac{(d-1)(3-d)e^2}{16m^3}-3\frac{\mathcal{E}_1^2+\mathcal{E}_2^2}{32m^3}+\frac{C_{\text{N}}^3}{4m^2}+\frac{d-1}{8m^2}c^3\Big\rangle,\end{aligned} \qquad (13)$$

where

$$\mathcal{O}_2 = \frac{p_1^2 p_2^2}{4m^3} + \left[\frac{p_1^2+p_2^2}{8m^2}, c\right] - \frac{C^2}{2m} + \sum_{i=1}^{2} \frac{\boldsymbol{\mathcal{E}}_\alpha \boldsymbol{\nabla}_\alpha}{4m^2} - \frac{\boldsymbol{e}\boldsymbol{\nabla}}{2m^2} \\ - \frac{\boldsymbol{p}_1 c \boldsymbol{p}_2 + (d-2)(\boldsymbol{p}_1\boldsymbol{n})c(\boldsymbol{n}\boldsymbol{p}_2)}{2m^2}, \tag{14}$$

G is the reduced Green function of the Schrödinger equation and $B = \langle U_S \rangle$. Action of the operator $\mathcal{O}_2$ on the wave function can be checked not to produce functions more singular than C_α^2 or c^2. Therefore, in contrast to the second iteration of the original perturbation, Eq.(12), that of the operator $\mathcal{O}_2$ delivers a result which is finite in three dimensions.

3.3 Total soft scale contribution

Summing up all soft scale contributions, we get:

$$\begin{aligned}
\Delta_{\rm soft} E = & -\frac{2E^3}{m^2} - \frac{3E^2\langle c\rangle}{4m^2} + \frac{3EB}{m} + \frac{B\langle c\rangle}{2m} + \langle U_P G U_P\rangle + \left\langle \mathcal{O}_2^\dagger G \mathcal{O}_2 \right\rangle \\
& + \frac{E}{m}\left\langle \frac{2C^2+c^2}{4m} + \frac{p_1^2p_2^2}{8m^3} - \frac{\pi\alpha Z}{4m^2}\left[\delta(\boldsymbol{r}_1)+\delta(\boldsymbol{r}_2)\right] \right\rangle \\
& + \left\langle -\frac{cC_{\rm N}C}{2m^2} - \left\{ \frac{C_{\rm N}}{8m^3}, \frac{\boldsymbol{p}_1 c\boldsymbol{p}_2 + (\boldsymbol{p}_1\boldsymbol{n})c(\boldsymbol{n}\boldsymbol{p}_2)}{m} \right\} + \frac{p_1^2 C_{\rm N} p_2^2}{4m^4} \right. \\
& + \frac{\boldsymbol{p}_1 c^2 \boldsymbol{p}_1 + \boldsymbol{p}_2 c^2 \boldsymbol{p}_2}{8m^3} + \frac{\boldsymbol{p} c \boldsymbol{p} P^2 - (\boldsymbol{P}\boldsymbol{p})c(\boldsymbol{P}\boldsymbol{p})}{4m^4} \\
& - \frac{p_1^2 c(\boldsymbol{n}\boldsymbol{p}_2)^2 + (\boldsymbol{p}_1\boldsymbol{n})^2 c p_2^2 - 3(\boldsymbol{p}_1\boldsymbol{n})^2 c(\boldsymbol{n}\boldsymbol{p}_2)^2 + (1\leftrightarrow 2)}{16m^4} \\
& - \frac{cr}{16m^3}\left(2(\boldsymbol{n}\boldsymbol{p}_2)(\boldsymbol{\mathcal{E}}_1\boldsymbol{p}_2) + (\boldsymbol{n}\boldsymbol{\mathcal{E}}_1)\left[(\boldsymbol{n}\boldsymbol{p}_2)^2 - p_2^2\right] + (1\leftrightarrow 2) + \mathrm{H.c.}\right) \\
& + \frac{cr^2}{8m^2}\left(3\boldsymbol{\mathcal{E}}_1\boldsymbol{\mathcal{E}}_2 - (\boldsymbol{n}\boldsymbol{\mathcal{E}}_1)(\boldsymbol{n}\boldsymbol{\mathcal{E}}_2) - 2(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2)\boldsymbol{e}\right) \\
& - \frac{3\left[\boldsymbol{P}\boldsymbol{p}, [\boldsymbol{P}\boldsymbol{p}, c]\right]}{32m^4} + \frac{\pi\alpha\delta(\boldsymbol{r})}{2m^3}\left(\frac{13P^2}{16m} + C_{\rm N}\right) \\
& + \frac{\pi\alpha Z}{4m^3}\left[\delta(\boldsymbol{r}_1)\left(\frac{3p_2^2}{2m} + 2C_2 + c\right) + (1\leftrightarrow 2)\right] - \frac{(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2)\boldsymbol{e}}{32m^3} \\
& \left. - \frac{C_{\rm N}^3}{4m^2} + \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2}{8m^3} - \frac{d^3 - 4d^2 - d + 16}{8(4-d)m^2}c^3 + \frac{d^3 - 2d^2 + 9d - 24}{16(d-2)m^3}e^2 \right\rangle .
\end{aligned} \tag{15}$$

For the bulk of the operators above, their average values can be safely evaluated in three dimensions. Special care is needed when one deals with the operator $p_1^2 c(\boldsymbol{n}\boldsymbol{p}_2)^2 + (1 \leftrightarrow 2) + \mathrm{H.c.}$ Although its average value is finite in three dimensions, the $d \to 3$ transition is not smooth:

$$\lim_{d\to 3} \left\langle p_1^2 c(\boldsymbol{n}\boldsymbol{p}_2)^2 \right\rangle = \left\langle p_1^2 c(\boldsymbol{n}\boldsymbol{p}_2)^2 \right\rangle\Big|_{d=3} + \left\langle \pi m^2 \alpha^3 \delta(\boldsymbol{r}) \right\rangle . \tag{16}$$

In order to calculate the divergent average values from the last line of (15), we first consider the Coulomb potential $\mathcal{C}$ between two particles with the charges Z_1 and Z_2. The average value of $\mathcal{C}^3$ is

$$\begin{aligned}\left\langle \mathcal{C}^3 \right\rangle &= (Z_1 Z_2 \alpha)^3 \left(\frac{\Gamma\left(\frac{d}{2}-1\right)}{\pi^{d/2-1}} \right)^3 \left\langle \frac{1}{r^{3d-6}} \right\rangle \\ &= (Z_1 Z_2 \alpha)^3 a^{4\varepsilon} \left(\frac{\Gamma\left(\frac{1}{2}-\varepsilon\right)}{\pi^{1/2-\varepsilon}} \right)^3 \int \mathrm{d}^d r' \int \mathrm{d}\boldsymbol{n} \int_0^\infty \frac{\mathrm{d}\varrho}{\varrho^{1-4\varepsilon}} \psi^2(a\varrho\boldsymbol{n}, \boldsymbol{r}').\end{aligned}$$

Here $a = (|Z_1 Z_2| \mu\alpha)^{-1}$ is the Bohr radius for a given pair of particles, μ being their reduced mass, the vectors $\boldsymbol{r} = a\varrho\boldsymbol{n}$ and $\boldsymbol{r}'$ denote relative position of the constituents and position of the pair center of mass, respectively. Integration by parts in the last integral gives:

$$\int_0^\infty \frac{\mathrm{d}\varrho}{\varrho^{1-4\varepsilon}} \psi^2(a\varrho\boldsymbol{n}, \boldsymbol{r}') = \left(-\frac{1}{4\varepsilon}\right) \int_0^\infty \mathrm{d}\varrho\, \varrho^{4\varepsilon} \frac{\partial}{\partial\varrho} \psi^2(a\varrho\boldsymbol{n}, \boldsymbol{r}'). \tag{17}$$

Here we took into account that $\lim_{\varrho\to 0} \varrho^{4\varepsilon} = 0$ for finite positive ε. Expanding now (17) in powers of ε, we get

$$\left\langle \mathcal{C}^3 \right\rangle = (Z_1 Z_2 \alpha)^3 \left\{ \left(\frac{1}{\varepsilon} - 4\ln\frac{2}{a} + 2 \right) \langle \pi\delta(\boldsymbol{r}) \rangle - 2 \left\langle \frac{\gamma + \ln(2r/a)}{r^2} \frac{\partial}{\partial r} \right\rangle + \mathcal{O}(\varepsilon) \right\},$$

where $\gamma = 0.5772\ldots$ is the Euler constant. As expected, the divergence arises at $r = 0$. The non-contact average value is finite in three dimensions.

The second singular operator, $\mathcal{E}^2$, can be averaged in the following way:

$$\left\langle \mathcal{E}^2 \right\rangle = \left\langle [\boldsymbol{\nabla}, \mathcal{C}]^2 \right\rangle = \langle [\boldsymbol{\nabla}, \mathcal{C}[\boldsymbol{\nabla}, \mathcal{C}]] - \mathcal{C}\Delta\mathcal{C} \rangle = -2 \langle \mathcal{C}[\boldsymbol{\nabla}, \mathcal{C}]\boldsymbol{\nabla} \rangle . \tag{18}$$

At the last step, we use equation $\langle \mathcal{C}\Delta\mathcal{C} \rangle = 0$, valid in the dimensional regularization. In order to express the average value

$$\left\langle \mathcal{E}^2 \right\rangle = 2(d-2)(Z_1 Z_2 \alpha)^2 \left(\frac{\Gamma\left(\frac{d}{2}-1\right)}{\pi^{d/2-1}} \right)^2 \left\langle \frac{1}{r^{2d-3}} \frac{\partial}{\partial r} \right\rangle \tag{19}$$

through $\left\langle \mathcal{C}^3 \right\rangle$, we subtract from $\partial/\partial r$ and add to it the operator $\mu r \mathcal{C}$:

$$\left\langle \mathcal{E}^2 \right\rangle = 2\mu(d-2) \left\langle \mathcal{C}^3 \right\rangle + 2(Z_1 Z_2 \alpha)^2 \left\langle \frac{1}{r^3} \left(\frac{\partial}{\partial r} - \mu Z_1 Z_2 \alpha \right) \right\rangle . \tag{20}$$

Extracting from (15) all divergent pieces, we find:

$$\Delta^{\mathrm{div}}_{\mathrm{soft}} E = \frac{1}{\varepsilon} \left\langle \frac{\pi\alpha^3 \delta(\boldsymbol{r})}{4m^2} \right\rangle . \tag{21}$$

4 Hard Scale Contributions

4.1 Radiative Recoil Correction

Effective operator coincides with that for parapositronium [5]:

$$\Delta_{\text{rad rec}} E = \left\langle \left(\frac{6\zeta(3)}{\pi^2} - \frac{697}{27\pi^2} - 8\ln 2 + \frac{1099}{72} \right) \frac{\pi\alpha^3 \delta(\boldsymbol{r})}{m^2} \right\rangle .$$

4.2 Radiative Corrections

eN Interaction

One- [6] and two-loop [7,8,9] radiative corrections to electron–nucleus interaction give rise to the following energy shifts, respectively:

$$\Delta^{\text{eN}}_{\text{rad1l}} E = \left\langle \left(\frac{427}{96} - 2\ln 2 \right) \frac{\pi\alpha(Z\alpha)^2}{m^2} \left(\delta(\boldsymbol{r}_1) + \delta(\boldsymbol{r}_2)\right) \right\rangle ,$$

$$\Delta^{\text{eN}}_{\text{rad2l}} E = \left\langle \left(-\frac{9\zeta(3)}{4\pi^2} - \frac{2179}{648\pi^2} + \frac{3\ln 2}{2} - \frac{10}{27} \right) \frac{\pi\alpha^2(Z\alpha)}{m^2} \left(\delta(\boldsymbol{r}_1) + \delta(\boldsymbol{r}_2)\right) \right\rangle .$$

ee Interaction

Net effect of two-loop contributions to the slope of Dirac formfactor [7], Pauli formfactor [8], and vacuum polarization [9] reads:

$$\Delta^{\text{ee}}_{\text{rad}} E = \left\langle \left(\frac{15\zeta(3)}{2\pi^2} + \frac{631}{54\pi^2} - 5\ln 2 + \frac{29}{27} \right) \frac{\pi\alpha^3 \delta(\boldsymbol{r})}{m^2} \right\rangle .$$

4.3 Pure Recoil Correction

Changing sign of the corresponding result for parapositronium [5], we get

$$\Delta_{\text{rec}} E = \left\langle \left(-\frac{1}{\varepsilon} + 4\ln m - \frac{39\zeta(3)}{\pi^2} + \frac{32}{\pi^2} - 6\ln 2 + \frac{7}{3} \right) \frac{\pi\alpha^3 \delta(\boldsymbol{r})}{4m^2} \right\rangle .$$

Among the hard scale contributions only this one contains the divergence,

$$\Delta^{\text{div}}_{\text{hard}} E = -\frac{1}{\varepsilon} \left\langle \frac{\pi\alpha^3 \delta(\boldsymbol{r})}{4m^2} \right\rangle . \tag{22}$$

5 Conclusion

The divergent contributions from the soft (21) and hard (22) scales cancel each other, so that in the sum of all contributions we can put $d = 3$. We thus get the final expression for the $\mathcal{O}(m\alpha^6)$ correction to a singlet S-state energy of the helium atom (all average values below are over the three-dimensional wave function):

$$
\begin{aligned}
\Delta_{m\alpha^6} E = & -\frac{2E^3}{m^2} - \frac{3E^2\langle c\rangle}{4m^2} + \frac{3EB}{m} + \frac{B\langle c\rangle}{2m} + \langle U_P G U_P\rangle + \left\langle \mathcal{O}_2^\dagger G \mathcal{O}_2\right\rangle \\
& +\frac{E}{m}\left\langle \frac{2C^2+c^2}{4m} + \frac{p_1^2 p_2^2}{8m^3} - \frac{\pi\alpha Z}{4m^2}\left[\delta(\boldsymbol{r}_1)+\delta(\boldsymbol{r}_2)\right]\right\rangle \\
& +\pi\alpha^3 m^2 \left\langle k_{\mathrm{eN}}\left(\delta(\boldsymbol{r}_1)+\delta(\boldsymbol{r}_2)\right) + k_{\mathrm{ee}}\delta(\boldsymbol{r})\right\rangle \\
& +\Big\langle -\frac{3C_1C_2C_{\mathrm{N}}}{4m^2} - \frac{cC_{\mathrm{N}}C}{2m^2} - \left\{\frac{C_{\mathrm{N}}}{8m^3}, \frac{\boldsymbol{p}_1 c \boldsymbol{p}_2 + (\boldsymbol{p}_1\boldsymbol{n})c(\boldsymbol{n}\boldsymbol{p}_2)}{m}\right\} \\
& +\frac{p_1^2 C_{\mathrm{N}} p_2^2}{4m^4} + \frac{\boldsymbol{p}_1 c^2 \boldsymbol{p}_1 + \boldsymbol{p}_2 c^2 \boldsymbol{p}_2}{8m^3} + \frac{(\boldsymbol{p}_1\times \boldsymbol{p}_2)c(\boldsymbol{p}_1\times \boldsymbol{p}_2)}{4m^4} \\
& -\frac{p_1^2 c(\boldsymbol{n}\boldsymbol{p}_2)^2 + (\boldsymbol{p}_1\boldsymbol{n})^2 c p_2^2 - 3(\boldsymbol{p}_1\boldsymbol{n})^2 c(\boldsymbol{n}\boldsymbol{p}_2)^2 + (1\leftrightarrow 2)}{16m^4} \qquad (23) \\
& -\frac{\alpha}{16m^3}\left(2(\boldsymbol{n}\boldsymbol{p}_2)(\boldsymbol{\mathcal{E}}_1\boldsymbol{p}_2) + (\boldsymbol{n}\boldsymbol{\mathcal{E}}_1)\left[(\boldsymbol{n}\boldsymbol{p}_2)^2 - p_2^2\right] + (1\leftrightarrow 2) + \mathrm{H.c.}\right) \\
& +\frac{\alpha r}{8m^2}\left(3\boldsymbol{\mathcal{E}}_1\boldsymbol{\mathcal{E}}_2 - (\boldsymbol{n}\boldsymbol{\mathcal{E}}_1)(\boldsymbol{n}\boldsymbol{\mathcal{E}}_2) - 2(\boldsymbol{\mathcal{E}}_1-\boldsymbol{\mathcal{E}}_2)\boldsymbol{e}\right) \\
& -\frac{3\alpha}{32m^4}\frac{P^2-3(\boldsymbol{n}\boldsymbol{P})^2}{r^3} + \frac{\pi\alpha\delta(\boldsymbol{r})}{2m^3}\left(\frac{9P^2}{16m}+C_{\mathrm{N}}\right) - \frac{(\boldsymbol{\mathcal{E}}_1-\boldsymbol{\mathcal{E}}_2)\boldsymbol{e}}{32m^3} \\
& +\frac{\pi\alpha Z}{4m^3}\left[\delta(\boldsymbol{r}_1)\left(\frac{3p_2^2}{2m} - \frac{(2Z-1)\alpha}{r_2}\right) + (1\leftrightarrow 2)\right] - \alpha^3\frac{\ln(m\alpha r)+\gamma}{2m^2r^2}\partial \\
& +\frac{(Z\alpha)^2}{4m^3}\left[\frac{1}{r_1^3}\left(\partial_1 + mZ\alpha\right) + (1\leftrightarrow 2)\right] + \frac{3\alpha^2}{2m^3}\frac{1}{r^3}\left(\partial - \frac{m\alpha}{2}\right)\Big\rangle .
\end{aligned}
$$

Although d-dimensional notations are pertained here, the immediate three-dimensional counterparts are implied for all the operators. The contact terms enter into (23) with the coefficients

$$k_{\mathrm{eN}} = \frac{Z^3}{2} + \frac{427Z^2}{96} - \frac{10Z}{27} - \frac{9Z\zeta(3)}{4\pi^2} - \frac{2179Z}{648\pi^2} + \frac{3Z-4Z^2}{2}\ln 2, \qquad (24)$$

$$k_{\mathrm{ee}} = -\ln\alpha + \frac{3385}{216} - \frac{331}{54\pi^2} - \frac{29\ln 2}{2} + \frac{15\zeta(3)}{4\pi^2}. \qquad (25)$$

Equations (23-25) constitute the principal result of the present work. Its application to the ground state of helium atom is considered elsewhere [4].

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Appendix

Throughout the paper we use the following notations. The electrons are located at points $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$; $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ are the operators of their momenta. Then,

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2; \quad \boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2 = -\mathrm{i}\,(\boldsymbol{\nabla}_1 + \boldsymbol{\nabla}_2)\,; \quad \boldsymbol{p} = \frac{\boldsymbol{p}_1 - \boldsymbol{p}_2}{2} = -\mathrm{i}\boldsymbol{\nabla}; \tag{26}$$

$$\boldsymbol{n}_\alpha = \frac{\boldsymbol{r}_\alpha}{r_\alpha}, \quad \boldsymbol{n} = \frac{\boldsymbol{r}}{r}. \tag{27}$$

Greek indices equal to 1 or 2 and enumerate the electrons, Latin ones correspond to the Descartes components. We use the short-hand notations for the derivatives:

$$\partial_1 = \frac{\partial}{\partial r_1}, \quad \partial_2 = \frac{\partial}{\partial r_2}, \quad \partial = \frac{\partial}{\partial r}. \tag{28}$$

Nonrelativistic Hamiltonian of the helium atom in the non-recoil limit ($m/m_{\mathrm{N}} \to 0$) is

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + C, \tag{29}$$

where the total Coulomb potential is the sum of the electron-nucleus and electron-electron parts:

$$C = C_{\mathrm{N}} + c; \tag{30}$$

$$C_{\mathrm{N}} = C_1 + C_2 = -\frac{\Gamma(\frac{d}{2}-1)}{\pi^{d/2-1}}\left(\frac{Z\alpha}{r_1^{d-2}} + \frac{Z\alpha}{r_2^{d-2}}\right); \tag{31}$$

$$c = \frac{\Gamma(\frac{d}{2}-1)}{\pi^{d/2-1}}\,\frac{\alpha}{r^{d-2}}. \tag{32}$$

The electric forces exerted on electrons are

$$\boldsymbol{\mathcal{E}}_\alpha = -\left[\boldsymbol{\nabla}_\alpha, C_\alpha\right]; \qquad \boldsymbol{e} = -\left[\boldsymbol{\nabla}, c\right]. \tag{33}$$

Unless otherwise specified, $\langle \ldots \rangle$ denotes the average value over a singlet S-state of the helium atom in d dimensions.

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