

# QED corrections to singlet levels of the helium atom: A complete set of effective operators to $m\alpha^6$

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Using singlet  $S$  states of the helium atom as an example, precise calculation of energy levels in few-electron atoms is described. In particular, a complete set of effective operators is derived, which generates  $O(m\alpha^6)$  relativistic and radiative corrections to the Schrödinger energy. Average values of these operators can be calculated using a variational Schrödinger wave function.

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## I. INTRODUCTION

Singlet states of the helium atom, especially its ground state, are best suited 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 in helium reached the precision of about 10 ppb. Helium ground-state ionization potential (the difference between ground-state energies of the singly charged ion and of the atom) extracted from those measurements constitutes

$$\nu_{\text{expt}}^{1S-2P}(1^1S) = 5\,945\,204\,238 \text{ (45) MHz}, \quad (1)$$

and

$$\nu_{\text{expt}}^{1S-2S}(1^1S) = 5\,945\,204\,356 \text{ (48) MHz}, \quad (2)$$

respectively.

Theoretically, the ionization potential can be calculated as a power series in the fine-structure constant  $\alpha$ . Leading  $O(m\alpha^2)$  contribution to the ground-state energy<sup>1</sup> is the lowest eigenvalue  $E$  of the nonrelativistic Hamiltonian

$$H = \sum_a \frac{p_a^2}{2m_a} + \alpha \sum_{b>a} \frac{z_a z_b}{r_{ab}}, \quad (3)$$

entering into the Schrödinger equation  $H\psi = E\psi$ . Here and below I use the following notations:  $\mathbf{r}_a$  and  $\mathbf{p}_a$  are the position and momentum operators for the particle  $a$  with mass  $m_a$  and electric charge  $z_a$  (in units of the proton charge). The relative position of two particles is  $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$ ; for any vector  $\mathbf{v}$ ,  $v$  denotes  $|\mathbf{v}|$ . The helium atom consists of two electrons with masses  $m_1 = m_2 = m$  and charges  $z_1 = z_2 = -1$ , and the nucleus with mass  $m_3 = M$  and charge  $z_3 = 2$ . A general case of  $z_3 = Z$  takes into consideration heliumlike ions with  $Z \ll 1/\alpha$ . In the center-of-mass frame, total momentum of the atom vanishes,  $\sum_a \mathbf{p}_a = \mathbf{0}$  so that only two of three position vectors are independent:  $\sum_a m_a \mathbf{r}_a = \mathbf{0}$ . In singlet states, spins of the electrons sum up to zero while the orbital

part of the wave function is symmetric with respect to permutation of the electrons positions,  $\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_2, \mathbf{r}_1)$ .

Relativistic and radiative effects shift the Schrödinger value of the energy by corrections of higher orders in  $\alpha$ . In particular, the leading correction

$$\delta^{(2)}E = \left\langle -\sum_a \frac{p_a^4}{8m_a^3} + \pi Z \alpha \frac{\delta(\mathbf{r}_{13}) + \delta(\mathbf{r}_{23})}{2m^2} + \frac{\pi \alpha \delta(\mathbf{r}_{12})}{m^2} - \frac{\alpha}{2} \sum_{b>a} \frac{z_a z_b}{m_a m_b} \left[ \mathbf{p}_a \frac{1}{r_{ab}} \mathbf{p}_b + (\mathbf{p}_a \mathbf{r}_{ab}) \frac{1}{r_{ab}^3} (\mathbf{r}_{ab} \mathbf{p}_b) \right] \right\rangle, \quad (4)$$

arises as the average value of the Breit perturbation (see, e.g., [3]) over the nonrelativistic wave function and is of the order  $\alpha^2$  relative to the Schrödinger energy. It is taken into account in Eq. (4) that the total spin of electrons and the spin of the nucleus are both equal to zero.

A particular class of corrections appears due to the nucleus structure. There, the most important (and sufficient to be included at the present level of accuracy) is the effect of the nucleus charge radius  $R_N$ ,

$$\delta_{\text{chr}} E = \frac{2\pi Z \alpha}{3} R_N^2 \sum_a \langle \delta(\mathbf{r}_{aN}) \rangle. \quad (5)$$

Here  $\mathbf{r}_{aN}$  denotes the position of the  $a$ th electron with respect to the nucleus.

The most recent theoretical result for the helium ionization potential

$$\nu_{\text{th}}(1^1S) = 5\,945\,204\,226 \text{ (91) MHz}, \quad (6)$$

obtained in Ref. [4] includes along with Eqs. (4) and (5) the  $m\alpha^5$  order, the leading part of the  $m\alpha^6$  order, and some estimates of higher-order contributions. Its uncertainty is twice as large as that of the experimental data (1) and (2). The main source of the uncertainty in Eq. (6) is the yet uncalculated part of the  $O(m\alpha^6)$  correction.

The present work is the first of two devoted to the calculation of the helium ionization potential with  $O(m\alpha^6)$  accuracy. It contains the analytic part of the calculation and its

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<sup>1</sup>The units  $\hbar = 1$ ,  $c = 1$  are used throughout this paper.

main result is a set of effective operators that produce all  $O(m\alpha^6)$  corrections to singlet  $S$  levels of helium atom and low- $Z$  heliumlike ions. To make the presentation self-contained, I also briefly outline how the lower-order correction can be obtained by the same method. The second paper [5] contains numerical results for the average values of the derived effective operators as well as all other known contributions to the helium ionization potential.

The rest of this paper is organized as follows. Section II describes general features of the approach. Order  $m\alpha^5$  effective operators are derived in Sec. III. Sections IV and V are devoted to the  $O(m\alpha^6)$  effective operators appearing from hard and soft scales, respectively. The final result of this paper is presented in the Conclusion.

## II. FRAMEWORK OF THE CALCULATION

Since the early days of quantum electrodynamics (QED), the nonrelativistic expansion of an atom's ground-state energy is known to break down at the  $m\alpha^5$  order [6]. In contrast to the  $O(m\alpha^4)$  effective operators whose average values (4) are completely determined by the soft ( $p \sim 1/r \sim m\alpha$ ) scale, the operators of the next order in momentum-to-mass ratio are too singular to ensure finiteness of their average values over the ground state described by the wave function  $\psi$ .<sup>2</sup> It means that those operators become sensitive also to the hard ( $p \sim m$ ) scale, which is beyond the scope of the nonrelativistic expansion. Another important feature of the  $O(m\alpha^5)$  contribution to the energy is that the very picture of interaction between particles through a potential fails: virtual transitions from the atom's ground state to excited states and a photon become relevant. Thus, one more scale comes into play — this intermediate ultrasoft photon has an order  $m\alpha^2$  energy. The most natural way to calculate such a multiscale shift of the energy is to divide it into several pieces each originating from its own scale and then use simplifying approximations suitable to that scale. For example, the nonrelativistic expansion is applicable at the soft scale. Alternatively, one can neglect bound-state effects at the hard scale. If all relevant contributions are included, their sum is independent of the details of the division. Applied to bound-state problems in QED, this idea was first formulated in Ref. [7] as the nonrelativistic quantum electrodynamics (NRQED).

Traditionally, in atomic calculations involving several scales, some auxiliary parameter is introduced to separate a contribution of the given scale from the others (see, e.g., Ref. [8] where such a scheme is applied to the helium problem). For example, to divide soft and hard-scale contributions one introduces  $\lambda$  satisfying  $m\alpha \ll \lambda \ll m$  and gets a final  $\lambda$ -independent energy shift as a result of cancellation between two  $\lambda$ -dependent contributions. The soft scale one includes  $\lambda$  as the ultraviolet cutoff that makes average values of singular operators finite. Simultaneously,  $\lambda$  cuts off otherwise infrared divergent on-shell scattering amplitudes that represent a hard-scale contribution. The higher is the order of

$\alpha$ , the more severe are singularities of both contributions and the larger is a number of  $\lambda$ -dependent terms to be canceled in order to get a final result. The problem seems even less tractable when the wave function is known only numerically.

Precise calculations of the positronium spectrum [9–12] have shown that contributions from various scales can be separated much more effectively by shifting the number of spatial dimensions  $d$  from three,  $d \rightarrow 3 - 2\epsilon$ . For consistency, the number of space-time dimensions in hard-scale calculations should be shifted from four to  $4 - 2\epsilon$ . This shift implies essentially that all objects defined originally for  $d=3$  are analytically continued to the complex plane of  $d$ . The main advantage of the dimensional regularization over the traditional scheme is that due to the analytic continuation all power divergences automatically drop out of calculations and one only has to keep track of logarithmic divergences that show up as inverse powers of  $\epsilon$ .

Recall that there are two kinds of effective operators in NRQED. Operators coming from the hard scale are contact, i.e., they are proportional to delta functions of distances between particles. Infrared divergences typical in hard-scale contributions manifest themselves as inverse powers of  $\epsilon$  in coefficients of those delta functions. On the other hand, the soft-scale effective operators have finite coefficients at  $d \rightarrow 3$ . Ultraviolet divergences inherent to soft-scale contributions show up as inverse powers of  $\epsilon$  only when one evaluates average values of those operators over a solution of the Schrödinger equation in  $d=3-2\epsilon$  dimensions. The crucial observation made in Refs. [11,12] for the  $O(m\alpha^6)$  corrections to positronium levels is that even without knowing an explicit form of this solution but using only the Schrödinger equation itself, one can extract all the divergent pieces in the form of  $\langle \delta(\mathbf{r}) \rangle / \epsilon$ , where  $r$  is a distance between the electron and the positron while the average value is calculated over the  $d$ -dimensional wave function. Since after such an extraction the divergences contained in both hard and soft-scale contributions have exactly the same form, it is easy to check that they cancel each other so that a finite remainder can be safely calculated in three dimensions.

I employ the same idea for the helium atom, where an analytic form of the wave function is not available even in three dimensions. Nevertheless, in perfect analogy to the positronium case, the use of the Schrödinger equation alone makes it possible to extract the divergent pieces of all soft-scale contributions on the *operator* level. Performing such an extraction I manage to demonstrate straightforwardly that the divergences coming from both scales cancel each other *before* any numerical calculation. As the result, the total  $O(m\alpha^6)$  correction to a singlet  $S$  level is represented as a sum of apparently finite average values of the regularization-independent operators. These average values can be calculated using a wave function of the helium atom, built as a numerical solution of the Schrödinger equation [5].

It is worth mentioning that the idea of the approach has a simple physical reason. In fact, soft-scale divergences in bound-state energy are of the ultraviolet origin. Hence they 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

<sup>2</sup>See Sec. III for details.

Schrödinger equation one should be able to rewrite the singular soft-scale contributions in such a way that corresponding divergences are moved to the Wilson coefficients of the contact operators. After the perturbation theory is reformulated in such a manner, and if the underlying theory is renormalizable, all divergences that appear in any given Wilson coefficient have to cancel each other.

Validity of the results obtained below for the helium can be checked in two limiting cases. The first,  $\alpha \rightarrow 0$  at finite  $Z\alpha$  describes heliumlike ion with the electron-electron interaction switched off. The second,  $Z \rightarrow 0$  at  $z_2 \rightarrow 1$  describes parapositronium. Since in both cases three-dimensional wave functions of all  $S$  states are available in an analytic form, the average values of effective operators can be calculated explicitly [modulo  $\langle \delta(\mathbf{r}) \rangle / \epsilon$  terms]. Comparison with the known results shows complete agreement for all contributions.

In order to make the formulas more transparent, I write the nonsingular soft-scale operators with coefficients taken at  $d=3$ .

### III. ORDER $m\alpha^5$ EFFECTIVE OPERATORS

This section illustrates the general scheme by the calculation of effective operators in the first nontrivial order. As previously mentioned, at  $O(m\alpha^5)$  the relevant contributions to the energy come from three scales: ultrasoft, soft, and hard. Below we will calculate corresponding effective operators.

#### A. Hard-scale contribution

Hard-scale effects in the interaction between nonrelativistic particles  $a$  and  $b$  give rise to the contact operators that show up as  $c_{ab}\delta(\mathbf{r}_{ab})$  in the spatial representation and, therefore, as  $c_{ab}$  in the momentum one. In the NRQED approach,  $c_{ab}$  is extracted through the matching procedure, namely, equating the  $ab \rightarrow ab$  scattering amplitude calculated in the full QED to that in the effective theory approach. Dimensional regularization is best suited to this procedure:  $c_{ab}$  equals minus QED scattering amplitude for the particles  $a$  and  $b$  taken on their mass shells and at rest. In this manner the hard one-loop vertex correction to the single Coulomb exchange between the spin-1/2 point particle  $a$  and a particle  $b$  induces the effective potential<sup>3</sup>

$$V_{hc}(\mathbf{r}_{ab}) = \frac{2\alpha^2}{3} \frac{z_a^3 z_b}{m_a^2} \left( \frac{1}{\epsilon} - 2 \ln m_a \right) \delta(\mathbf{r}_{ab}). \quad (7)$$

The electron's anomalous magnetic moment taken in the leading one-loop approximation gives rise to the potential between electrons  $a$  and  $b$ ,

<sup>3</sup>To simplify the presentation, I omit the factor  $(4\pi)^d \Gamma(1+\epsilon)$  from the final expressions for all operators in Sec. III. This factor does not contribute to the finite total  $O(m\alpha^5)$  energy correction.

$$V_{hm}(\mathbf{r}_{ab}) = -\frac{8\alpha^2}{3m^2} s_a s_b \delta(\mathbf{r}_{ab}), \quad (8)$$

where  $s_a$  is the spin operator of the  $a$ th particle. If the nucleus spin is zero, the corresponding electron-nucleus potential vanishes. The next effective potential is generated by the hard one-loop box diagrams. For two spin-1/2 particles such a potential reads [13]

$$V_{\text{box}}(\mathbf{r}_{ab}) = \frac{(\alpha z_a z_b)^2}{m_a m_b} \left( \frac{1}{\epsilon} - \ln(m_a m_b) - \frac{1}{3} + \frac{m_a + m_b - 2\mu_{ab}(1 + 4s_a s_b)}{m_a - m_b} \ln \frac{m_a}{m_b} \right) \delta(\mathbf{r}_{ab}), \quad (9)$$

where  $\mu_{ab} = m_a m_b / (m_a + m_b)$  is the reduced mass of the pair. With the  $O(m/M)$  precision, the corresponding electron-nucleus effective potential is

$$V_{\text{box}}(\mathbf{r}_{eN}) = \frac{(Z\alpha)^2}{mM} \left( \frac{1}{\epsilon} - 2 \ln m - \frac{1}{3} \right) \delta(\mathbf{r}_{eN}). \quad (10)$$

The last  $O(m\alpha^5)$  contribution coming from the hard scale appears due to vacuum polarization. In ordinary few-electron atoms, an account of the electron vacuum polarization is sufficient for the present-day accuracy,

$$V_{\text{vp}}(\mathbf{r}_{ab}) = \frac{4\alpha^2}{15} \frac{z_a z_b}{m^2} \delta(\mathbf{r}_{ab}). \quad (11)$$

The hard-scale contribution to the energy equals the average value of  $V_{hc} + V_{hm} + V_{\text{box}} + V_{\text{vp}}$  summed over all pairs of particles.

#### B. Ultrasoft-scale contribution

According to the standard rules of the perturbation theory, virtual transition of the atom into an excited state induced by the emission and subsequent absorption of a photon is described by the following effective operator:

$$\int \frac{d^d q}{(2\pi)^d} \frac{4\pi\alpha}{2q} \sum_a j_{ai} \exp(-i\mathbf{q}\cdot\mathbf{r}_a) \delta_{ij} \frac{q_i q_j}{q^2} \sum_b j_{bj} \exp(i\mathbf{q}\cdot\mathbf{r}_b), \quad (12)$$

where  $H$  is the  $d$ -dimensional Schrödinger Hamiltonian,  $E$  is its lowest eigenvalue,  $\mathbf{q}$  is the photon momentum,  $q = |\mathbf{q}|$ . Assuming that  $q \sim m\alpha^2$ , we can restrict our attention to the electric dipole transitions, i.e., replace the exponents  $\exp(\pm\mathbf{q}\cdot\mathbf{r}_a)$  by 1 and the current density operators  $\mathbf{j}_a$  by their orbital counterparts taken in the leading nonrelativistic ap-

proximation,  $\mathbf{j}_a \rightarrow z_a \mathbf{p}_a / m_a$ , in Eq. (12). Integration over directions of  $\mathbf{q}$  then gives for the ultrasoft-scale effective operator

$$V_{\text{us}} = \frac{\alpha \Omega_d}{(2\pi)^{d-1}} \frac{d-1}{d} \mathbf{J} \int_0^\infty \frac{dq q^{d-2}}{E-H-q} \mathbf{J}, \quad (13)$$

where the operator  $\mathbf{J}$  is defined as  $\sum_a z_a \mathbf{p}_a / m_a$  and  $\Omega_d = 2\pi^{d/2} / \Gamma(d/2)$  is the  $d$ -dimensional solid angle. Analytic continuation of the integral over  $q$  from the stripe  $1 < \text{Re}(d) < 2$  reads

$$\int_0^\infty \frac{dq q^{d-2}}{E-H-q} = \frac{\pi(H-E)^{d-2}}{\sin(\pi d)}. \quad (14)$$

Expanding now the right-hand side (rhs) of Eq. (13) in  $\epsilon = (3-d)/2$ , we get with the  $O(\epsilon^0)$  accuracy

$$V_{\text{us}} \rightarrow \frac{2\alpha}{3\pi} \mathbf{J}(H-E) \left( \frac{1}{2\epsilon} + \frac{5}{6} - \ln 2(H-E) \right) \mathbf{J}. \quad (15)$$

As previously mentioned, the  $1/\epsilon$  term is due to the divergence of  $V_{\text{us}}$  in three dimensions. The  $O(m\alpha^5)$  ultrasoft-scale contribution to the energy is the average value of the operator (15) over the  $d$ -dimensional wave function,

$$\delta_{\text{us}}^{(3)} E = \frac{2\alpha}{3\pi} \left\langle \left( \frac{1}{2\epsilon} + \frac{5}{6} - \ln(m\alpha^2) \right) \frac{[\mathbf{J}, [H, \mathbf{J}]]}{2} - \mathbf{J}(H-E) \ln \frac{H-E}{R_\infty} \mathbf{J} \right\rangle. \quad (16)$$

Here I used the Schrödinger equation and also the standard notation for the Rydberg constant  $R_\infty = m\alpha^2/2$ . Since the Poisson equation  $[\mathbf{p}_a, [p_a, C_{ab}]] = 4\pi\alpha z_a z_b \delta(\mathbf{r}_a - \mathbf{r}_b)$  for the Coulomb potential  $C_{ab}$  between two particles holds in any dimensions, we have

$$[\mathbf{J}, [H, \mathbf{J}]] = -4\pi\alpha \sum_a z_a \sum_{b>a} z_b \left( \frac{z_a}{m_a} - \frac{z_b}{m_b} \right)^2 \delta(\mathbf{r}_{ab}). \quad (17)$$

The ultrasoft correction (16) in helium then reads

$$\delta_{\text{us}}^{(3)} E = \frac{4Z\alpha^2}{3} \left( \frac{1}{m} + \frac{Z}{M} \right)^2 \left( \frac{1}{2\epsilon} + \frac{5}{6} - \ln(m\alpha^2) - \ln \frac{k_0}{R_\infty} \right) \times \langle \delta(\mathbf{r}_{23}) + \delta(\mathbf{r}_{31}) \rangle, \quad (18)$$

where the helium Bethe logarithm [14] is defined as

$$\ln \frac{k_0}{R_\infty} = \frac{\left\langle (\mathbf{p}_1 + \mathbf{p}_2)(H-E) \ln \frac{H-E}{R_\infty} (\mathbf{p}_1 + \mathbf{p}_2) \right\rangle}{\langle (\mathbf{p}_1 + \mathbf{p}_2)(H-E)(\mathbf{p}_1 + \mathbf{p}_2) \rangle}, \quad (19)$$

and can be safely calculated in three dimensions.

### C. Soft-scale contribution

At the soft scale, momenta of all particles (electrons, nucleus, and virtual photons) are of the order  $m\alpha$ . Therefore, the  $O(m\alpha^5)$  soft-scale effective operators are generated by transverse photon exchange(s), since only such scattering amplitudes can contain odd powers of photon momentum.

#### I. Retardation

Let us again start with the single transverse photon exchange described by the effective operator (12) but now assuming that  $q \sim m\alpha$ . Since  $H-E \ll m\alpha$ , we can expand the integrand in  $(H-E)/q$ . Zeroth order term of this expansion describes the magnetic interaction in instantaneous approximation and is included (modulo relativistic corrections) into the Breit perturbation [see Eq. (4)]. The first-order retardation effect is represented by the operator

$$V_{\text{ret}} = 4\pi\alpha \int \frac{d^d q}{(2\pi)^d} \frac{\delta_{ij} - \frac{q_i q_j}{q^2}}{2q^3} \sum_a j_{ai} \exp(-i\mathbf{q} \cdot \mathbf{r}_a) \times (H-E) \sum_b j_{bj} \exp(i\mathbf{q} \cdot \mathbf{r}_b). \quad (20)$$

Using again the Schrödinger equation, we get

$$\delta_{\text{ret}} E = \pi\alpha \int \frac{d^d q}{(2\pi)^d} \frac{\delta_{ij} - \frac{q_i q_j}{q^2}}{q^3} \left\langle \left[ \sum_a j_{ai} \times \exp(-i\mathbf{q} \cdot \mathbf{r}_a), \left[ H, \sum_b j_{bj} \exp(i\mathbf{q} \cdot \mathbf{r}_b) \right] \right] \right\rangle. \quad (21)$$

The order  $m\alpha^5$  correction arises due to the nonrelativistic current densities.

$$\mathbf{j}_a(\mathbf{p}', \mathbf{p}) \rightarrow z_a \frac{\mathbf{p}' + \mathbf{p} + 2[(\mathbf{p}' - \mathbf{p})s_a, s_a]}{2m}. \quad (22)$$

We then see that in Eq. (21) only the exchange between different particles ( $a \neq b$ ) can give a nonzero contribution. In fact, the integral over  $q$  in the ‘‘diagonal’’ terms ( $a = b$ ) is scaleless and hence vanishes. The expression (21) simplifies to

$$\delta_{\text{ret}}^{(3)} E = -2\pi\alpha \sum_a \sum_{b>a} \frac{z_a z_b}{m_a m_b} \langle U_{ij}(\mathbf{r}_{ab}) \times [p_{ai}, [p_{bj}, C_{ab}(\mathbf{r}_{ab})]] \rangle, \quad (23)$$

and reproduces the result obtained in Ref. [15] for positronium. Here

$$\begin{aligned}
 U_{ij}(\mathbf{r}) &= \int \frac{d^d q}{(2\pi)^d} \frac{\delta_{ij} - \frac{q_i q_j}{q^2}}{q^3} \exp(i\mathbf{q} \cdot \mathbf{r}) \\
 &= \frac{\Gamma\left(\frac{d-3}{2}\right) r^{3-d}}{6\pi^{(d+1)/2}} \left( \delta_{ij} + \frac{d-3}{2} n_i n_j \right), \quad (24)
 \end{aligned}$$

$C_{ab}(\mathbf{r}) = \alpha z_a z_b \Gamma(d/2-1) r^{2-d} / \pi^{d/2-1}$  is the Coulomb potential in  $d$  dimensions and  $\mathbf{n} = \mathbf{r}/r$ . Thus we get

$$\delta_{\text{ret}}^{(3)} E = -\frac{4\alpha^2}{3} \frac{\Gamma\left(\frac{d+1}{2}\right) \Gamma\left(\frac{d}{2}\right)}{\pi^{d-3/2}} \sum_a \sum_{b>a} \frac{z_a^2 z_b^2}{m_a m_b} \langle r_{ab}^{3-2d} \rangle. \quad (25)$$

Here we cannot take the limit  $d \rightarrow 3$  since the average value of  $r^{-3}$  diverges logarithmically. However, we can extract the divergence in the following way. By definition, we have

$$\langle r_{ab}^{3-2d} \rangle = a_{ab}^{4\epsilon} \int d\mathbf{r}' \int d\mathbf{n}_{ab} \int_0^\infty \frac{d\rho}{\rho^{1-2\epsilon}} \psi^2(a_{ab} \rho \mathbf{n}_{ab}, \mathbf{r}'). \quad (26)$$

Here  $a_{ab} = |z_a z_b \mu_{ab} \alpha|^{-1}$  is the Bohr radius for a given pair of particles,  $\mathbf{r}_{ab} = a_{ab} \rho \mathbf{n}_{ab}$  being their relative position. The remaining independent variables are denoted by  $\mathbf{r}'$ . Integrating by parts in the last integral, we get

$$\begin{aligned}
 &\int_0^\infty \frac{d\rho}{\rho^{1-2\epsilon}} \psi^2(a_{ab} \rho \mathbf{n}_{ab}, \mathbf{r}') \\
 &= -\frac{1}{2\epsilon} \int_0^\infty d\rho \rho^{2\epsilon} \frac{\partial}{\partial \rho} \psi^2(a_{ab} \rho \mathbf{n}_{ab}, \mathbf{r}'). \quad (27)
 \end{aligned}$$

Here I took into account that  $\lim_{\rho \rightarrow 0} \rho^{2\epsilon}$  being written as the integral over momentum has no scale and hence vanishes. Substituting  $\rho^{2\epsilon} \rightarrow 1 + 2\epsilon \ln \rho + O(\epsilon^2)$  into the rhs of Eq. (27) gives for the retardation correction (25)

$$\begin{aligned}
 \delta_{\text{ret}}^{(3)} E \rightarrow &-\frac{4\alpha^2}{3} \sum_a \sum_{b>a} \frac{z_a^2 z_b^2}{m_a m_b} \left\{ \left( \frac{1}{\epsilon} - 2 \ln \frac{4}{a_{ab}} - 1 \right) \langle \delta(\mathbf{r}_{ab}) \rangle \right. \\
 &\left. - \left\langle \frac{\gamma + \ln \frac{2r_{ab}}{a_{ab}}}{\pi r_{ab}^2} \mathbf{n}_{ab} \cdot \nabla_{ab} \right\rangle \right\}, \quad (28)
 \end{aligned}$$

where  $\nabla_{ab} = \partial/\partial \mathbf{r}_{ab}$  and  $\gamma = 0.5772 \dots$  is the Euler constant. The gradient acts on the right wave function. Thus we have managed to extract the divergences in the form of average values of the contact operators  $\delta(\mathbf{r}_{ab})$  divided by  $\epsilon$ . Since  $\psi$

and its first derivatives are finite<sup>4</sup> for  $\mathbf{r}_{ab} \rightarrow 0$ , the noncontact average values in Eq. (28) are finite in three dimensions.

## 2. Double seagull

One more soft-scale contribution of the order  $m\alpha^5$  appears due to the double transverse exchange between two particles when both photons are emitted and reabsorbed in the seagull vertices. The corresponding effective potential derived in Ref. [15] for the positronium can be easily generalized to a more complex atom

$$\begin{aligned}
 V_{\text{ds}} &= -2\alpha^2 \frac{\Gamma(1-\epsilon)^2}{(4\pi)^{1-2\epsilon}} \left[ 1 - \epsilon \frac{17-8 \ln 2}{3} \right. \\
 &\left. + O(\epsilon^2) \right] \sum_a \sum_{b>a} \frac{z_a^2 z_b^2}{m_a m_b} \langle r_{ab}^{3-2d} \rangle. \quad (29)
 \end{aligned}$$

Exploiting the same trick as above to extract the divergences we get the double seagull contribution to the energy

$$\begin{aligned}
 \delta_{\text{ds}}^{(3)} E \rightarrow &-\alpha^2 \sum_a \sum_{b>a} \frac{z_a^2 z_b^2}{m_a m_b} \left\{ \left( \frac{1}{\epsilon} + 2 \ln a_{ab} - \frac{11-2 \ln 2}{3} \right) \right. \\
 &\left. \times \langle \delta(\mathbf{r}_{ab}) \rangle - \left\langle \frac{\gamma + \ln \frac{2r_{ab}}{a_{ab}}}{\pi r_{ab}^2} \mathbf{n}_{ab} \cdot \nabla_{ab} \right\rangle \right\}. \quad (30)
 \end{aligned}$$

## D. Total $m\alpha^5$ correction

The  $\epsilon^{-1}$  terms cancel out in the sum of all  $O(m\alpha^5)$  corrections to the energy. Hence we can take the limit  $d \rightarrow 3$  in this sum. With the  $O(m^2/M^2)$  precision, the result for the helium ground state reads

$$\begin{aligned}
 \delta^{(3)} E = &-\frac{2Z\alpha^2}{3m^2} \left( 4 \ln(Z\alpha) + 2 \ln \frac{k_0}{Z^2 R_\infty} - \frac{19}{15} \right) \langle \delta(\mathbf{r}_1) \\
 &+ \delta(\mathbf{r}_2) \rangle + \frac{2\alpha^2}{3m^2} \left( 7 \ln \alpha + \frac{82}{5} \right) \langle \delta(\mathbf{r}) \rangle \\
 &+ \frac{7\alpha^2}{3\pi m^2} \left\langle \frac{\gamma + \ln(m\alpha r)}{r^2} \mathbf{n} \cdot \nabla \right\rangle - \frac{2(Z\alpha)^2}{3mM} \\
 &\times \left( \ln(Z\alpha) + 4 \ln \frac{k_0}{Z^2 R_\infty} - \frac{31}{3} \right) \langle \delta(\mathbf{r}_1) + \delta(\mathbf{r}_2) \rangle \\
 &+ \frac{7(Z\alpha)^2}{3\pi m M} \left\langle \frac{\gamma + \ln(Zm\alpha r_1)}{r_1^2} \mathbf{n}_1 \cdot \nabla_1 + (1 \rightarrow 2) \right\rangle. \quad (31)
 \end{aligned}$$

<sup>4</sup>It follows from the Schrödinger equation in  $d$  dimensions.

Here and below I use simplified notations:  $\mathbf{r}_1 = r_1 \mathbf{n}_1 = \mathbf{r}_{23}$ ,  $\mathbf{r}_2 = r_2 \mathbf{n}_2 = \mathbf{r}_{31}$ ,  $\mathbf{r} = r \mathbf{n} = \mathbf{r}_{12}$ , the gradients are taken over the corresponding position vectors,  $\nabla_1 = \partial / \partial \mathbf{r}_1$  and so on. In the limit of no recoil ( $m/M \rightarrow 0$ ), the result (31) agrees with the results of Araki [16] and Sucher [17] after integrating by parts in their average value  $Q$ ,

$$Q = \lim_{\rho \rightarrow 0} \left\langle \frac{\Theta(r-\rho)}{4\pi r^3} + [\gamma + \ln(m\alpha\rho)]\delta(\mathbf{r}) \right\rangle \\ = -\frac{1}{2\pi} \left\langle \frac{\gamma + \ln(m\alpha r)}{r^2} \mathbf{n} \cdot \nabla \right\rangle. \quad (32)$$

The first recoil (linear in  $m/M$ ) correction was previously discussed in Ref. [18].

#### IV. ORDER $m\alpha^6$ HARD-SCALE CONTRIBUTIONS

Similar to what was done in the previous order, one has to consider the hard scale part of a two-particle scattering amplitude but now in two loops. There is no need to consider *three*-particle scattering amplitudes. In fact, the probability density to find three particles forming the helium atom at the same point is of the order  $(m\alpha)^6$ . On the other hand, these particles should exchange at least three photons to form a hard loop. Hence, hard scale effective operators proportional to  $\delta(\mathbf{r}_{ab})\delta(\mathbf{r}_{bc})$  can produce an  $O(m\alpha^9)$  correction only.

The radiative recoil potential appears when we account for the first radiative corrections to the hard one-loop box diagrams (see, e.g., Ref. [12]). The corresponding two-loop diagrams involve only even powers of the electric charges  $z_1$  and  $z_2$ . Hence the radiative recoil effective operator coincides with that for parapositronium [19,12],

$$\delta_{\text{rad rec}} E = \left( \frac{6\zeta(3)}{\pi^2} - \frac{697}{27\pi^2} - 8 \ln 2 + \frac{1099}{72} \right) \frac{\pi\alpha^3}{m^2} \langle \delta(\mathbf{r}) \rangle. \quad (33)$$

The corresponding electron-nucleus operator vanishes in the nonrecoil limit  $m/M \rightarrow 0$  considered from now on.<sup>5</sup> Then, one- [20] and two-loop [21–23] pure radiative corrections to electron-nucleus interaction give rise to the following energy shifts:

$$\delta_{\text{rad11}}^{eN} E = \left( \frac{427}{96} - 2 \ln 2 \right) \frac{\pi\alpha(Z\alpha)^2}{m^2} \langle \delta(\mathbf{r}_1) + \delta(\mathbf{r}_2) \rangle, \quad (34)$$

<sup>5</sup>Order  $m^2\alpha^6/M$  correction is much less than unknown  $m\alpha^7$  corrections.

$$\delta_{\text{rad21}}^{eN} E = \left( -\frac{9\zeta(3)}{4\pi^2} - \frac{2179}{648\pi^2} + \frac{3 \ln 2}{2} \right. \\ \left. - \frac{10}{27} \right) \frac{\pi\alpha^2(Z\alpha)}{m^2} \langle \delta(\mathbf{r}_1) + \delta(\mathbf{r}_2) \rangle. \quad (35)$$

The net effect of two-loop contributions to the slope of the electron Dirac formfactor [21], Pauli formfactor [22], and vacuum polarization [23] reads

$$\delta_{\text{rad}}^{\text{ee}} E = \left( \frac{15\zeta(3)}{2\pi^2} + \frac{631}{54\pi^2} - 5 \ln 2 + \frac{29}{27} \right) \frac{\pi\alpha^3}{m^2} \langle \delta(\mathbf{r}) \rangle. \quad (36)$$

Finally, to get the pure recoil contribution to the electron-electron hard-scale interaction (three-photon exchange) we have to change the sign of the corresponding parapositronium result<sup>6</sup> [12],

$$\delta_{\text{rec}} E = \left( -\frac{1}{\epsilon} + 4 \ln m - \frac{39\zeta(3)}{\pi^2} \right. \\ \left. + \frac{32}{\pi^2} - 6 \ln 2 + \frac{7}{3} \right) \frac{\pi\alpha^3}{4m^2} \langle \delta(\mathbf{r}) \rangle. \quad (37)$$

Among the hard-scale contributions only the last one contains the divergence.

#### V. ORDER $m\alpha^6$ SOFT-SCALE CONTRIBUTIONS

The aim of this section is to demonstrate that in analogy to the previous order the sum of all singular average values reduces to the form

$$\delta_{\text{soft}}^{\text{sing}} E = \frac{1}{\epsilon} \frac{\pi\alpha^3}{4m^2} \langle \delta(\mathbf{r}) \rangle, \quad (38)$$

so that the sum of soft and hard-scale contributions is finite in three dimensions.

There are many soft-scale effective operators with singular average values. One can easily determine whether an average value of a given operator is singular or regular for  $d \rightarrow 3$  using only the fact that the wave function and its first derivatives are finite when positions of two particles coincide.

<sup>6</sup>Recall that it is convenient to omit the overall factor  $(4\pi)^2 \epsilon \Gamma^2(1+\epsilon)$  from the final expressions for all  $O(m\alpha^6)$  operators.

## A. Irreducible corrections

### 1. Dispersion correction

Let us consider details of the singularities extraction procedure using the dispersion correction as an example. Non-relativistic expansion of the electron's dispersion law,  $\omega_p = \sqrt{m^2 + p^2}$ , reads

$$\omega_p = m + \frac{p^2}{2m} - \frac{p^4}{8m^3} + \frac{p^6}{16m^5} + \dots \quad (39)$$

The last written term induces a correction of the appropriate order. Using the Schrödinger equation we get

$$\begin{aligned} \delta_{\text{disp}} E &= \left\langle \frac{p_1^6 + p_2^6}{16m^5} \right\rangle = \frac{1}{2m^2} \left\langle \left( \frac{p_1^2 + p_2^2}{2m} \right)^3 - 3 \frac{p_1^2 p_2^2}{4m^2} \frac{p_1^2 + p_2^2}{2m} \right\rangle \\ &= \frac{1}{2m^2} \left\langle (E-C)(H-C)(E-C) - 3 \left[ \frac{p_1^2 p_2^2}{8m^2}, E-C \right] \right\rangle \\ &= \frac{1}{2m^2} \left\langle (E-C)^3 + \left[ C, \frac{[H,C]}{2} \right] - 3 \frac{p_1^2 p_2^2}{4m^2} E \right. \\ &\quad \left. + \frac{3}{8} \left\langle \frac{p_1^2 p_2^2}{m^2}, C \right\rangle \right\rangle. \end{aligned} \quad (40)$$

Here the total Coulomb potential  $C$  is the sum of the electron-nucleus and electron-electron parts,

$$C = C_N + c = C_1 + C_2 + c, \quad (41)$$

while a pairwise Coulomb potential is defined after Eq.(24). Singular contributions to Eq. (40) are induced by the following operators: (i)  $C^3$ ; (ii) the double commutator

$$\begin{aligned} \frac{1}{2m^2} \left\langle \left[ C, \frac{[H,C]}{2} \right] \right\rangle &= \frac{1}{2m^2} \left\langle \left[ C, \sum_{a=1}^2 \frac{\boldsymbol{\mathcal{E}}_a \cdot \nabla_a}{2m} + \frac{\mathbf{e} \cdot \nabla}{m} \right] \right\rangle \\ &= \left\langle \frac{(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2) \cdot \mathbf{e}}{2m^3} + \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2}{4m^3} + \frac{e^2}{2m^3} \right\rangle, \end{aligned} \quad (42)$$

where

$$\boldsymbol{\mathcal{E}}_a = -[\nabla_a, C_a]; \quad \mathbf{e} = -[\nabla, c], \quad (43)$$

are electric forces exerted on electrons; and (iii) the anticommutator

$$\begin{aligned} &\frac{3}{16m^2} \left\langle \left\langle \frac{p_1^2 p_2^2}{m^2}, c \right\rangle \right\rangle \\ &= \frac{3}{16m^2} \left\langle \left\langle \left( \frac{p_1^2 + p_2^2}{2m} \right)^2 - \left( \frac{p_1^2 - p_2^2}{2m} \right)^2, c \right\rangle \right\rangle \\ &= \frac{3}{16m^2} \left\langle 2c(E-C)^2 - [c, [H, C]] - \left\langle c, \frac{(\mathbf{P} \cdot \mathbf{p})^2}{m^2} \right\rangle \right\rangle, \end{aligned} \quad (44)$$

where  $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$  and  $\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2$ . Double commutator  $[c, [H, C]]$  can be transformed similarly to Eq. (42), the last term from Eq. (44) is conveniently rewritten as

$$\begin{aligned} -\frac{3}{16m^2} \left\langle \left\langle c, \frac{(\mathbf{P} \cdot \mathbf{p})^2}{m^2} \right\rangle \right\rangle &= -\frac{3}{16m^4} \langle [\mathbf{P} \cdot \mathbf{p}, [\mathbf{P} \cdot \mathbf{p}, c]] \rangle \\ &\quad + 2(\mathbf{P} \cdot \mathbf{p})c(\mathbf{P} \cdot \mathbf{p}). \end{aligned} \quad (45)$$

Summing up all of the above contributions and using the virial theorem in three dimensions,  $\langle C \rangle = 2E$ , we get for the dispersion correction

$$\begin{aligned} \delta_{\text{disp}} E &= -\frac{5E^3}{2m^2} + \frac{3E^2 \langle c \rangle}{8m^2} + \frac{3E}{2m^2} \left\langle C^2 - \frac{Cc}{2} - \frac{p_1^2 p_2^2}{4m^2} \right\rangle \\ &\quad + \left\langle \frac{3p_1^2 C_N p_2^2}{8m^4} - 3 \frac{[\mathbf{P} \cdot \mathbf{p}, [\mathbf{P} \cdot \mathbf{p}, c]]}{16m^4} - 3 \frac{(\mathbf{P} \cdot \mathbf{p})c(\mathbf{P} \cdot \mathbf{p})}{8m^4} \right. \\ &\quad \left. - \frac{9C_N^2 c}{8m^2} - \frac{3C_N c^2}{4m^2} + \frac{5(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2) \cdot \mathbf{e}}{16m^3} - \frac{C_N^3}{2m^2} - \frac{c^3}{8m^2} \right. \\ &\quad \left. + \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2}{4m^3} + \frac{e^2}{8m^3} \right\rangle. \end{aligned} \quad (46)$$

One can easily check that only the operators  $C_a^3$ ,  $c^3$ , and  $\mathcal{E}_a^2$ ,  $e^2$  have divergent average values in three dimensions. The following analysis shows that in a similar manner singularities of all soft scale effective operators appear either as the third power of the Coulomb potentials or as the electric forces squared.

### 2. Coulomb corrections

The order  $p^4/m^4$  correction to the Coulomb potential between electron and nucleus reads

$$V_C^{eN} = \frac{5}{128m^4} [p_1^2, [p_1^2, C_1]] - \frac{3\pi Z\alpha}{16m^4} \{ p_1^2, \delta(\mathbf{r}_1) \} + (1 \rightarrow 2). \quad (47)$$

I drop the spin-orbit term, which vanishes in a state with the

total spin zero. The average value of the double commutator can be conveniently rewritten as

$$\begin{aligned} & \langle [p_1^2, [p_1^2, C_1]] + (1 \leftrightarrow 2) \rangle \\ &= 2m \langle [H - C, [p_1^2, C_1]] + (1 \leftrightarrow 2) \rangle \\ &= -4m \langle \mathcal{E}_1^2 + \mathcal{E}_2^2 + (\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e} \rangle. \end{aligned} \quad (48)$$

For the anticommutator in Eq. (47), it should be taken into account that the average value of the operator  $\delta(\mathbf{r}_a)C_a$  is a scaleless integral over  $\mathbf{r}_a$  and hence vanishes in the dimensional regularization

$$\begin{aligned} \langle \{p_1^2, \delta(\mathbf{r}_1)\} + \{p_2^2, \delta(\mathbf{r}_2)\} \rangle &= \langle \delta(\mathbf{r}_1) \{4m(E - C_2 - c) - 2p_2^2\} \\ &+ (1 \leftrightarrow 2) \rangle. \end{aligned} \quad (49)$$

The energy shift induced by Eq. (47) is

$$\begin{aligned} \delta_C^{eN} E &= \left\langle \frac{3\pi Z\alpha}{4m^3} \delta(\mathbf{r}_1) \left( \frac{p_2^2}{2m} + C_2 + c - E \right) - \frac{5\mathcal{E}_1(\mathcal{E}_1 + \mathbf{e})}{32m^3} \right\rangle \\ &+ (1 \leftrightarrow 2). \end{aligned} \quad (50)$$

Note that  $\mathbf{e}$  changes its sign under the permutation  $(1 \leftrightarrow 2)$ .

Similar analysis for the correction to the electron-electron Coulomb interaction,

$$\begin{aligned} V_C^{ee} &= \frac{5}{128m^4} [p_1^2, [p_1^2, c]] + \frac{7\pi\alpha}{32m^4} \{p_1^2, \delta(\mathbf{r})\} + (1 \leftrightarrow 2) \\ &+ \frac{(\mathbf{p}_1 \cdot \mathbf{p}_2)c(\mathbf{p}_1 \cdot \mathbf{p}_2) - p_{1i}p_{2j}c p_{1j}p_{2i}}{16m^4}, \end{aligned} \quad (51)$$

gives

$$\begin{aligned} \delta_C^{ee} E &= \left\langle 3 \frac{[\mathbf{P} \cdot \mathbf{p}, [\mathbf{P} \cdot \mathbf{p}, c]]}{32m^4} + \frac{\pi\alpha\delta(\mathbf{r})}{m^3} \left( E - C_N - \frac{3P^2}{32m} \right) \right. \\ &\left. - \frac{(\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e}}{16m^3} - \frac{e^2}{8m^3} \right\rangle. \end{aligned} \quad (52)$$

Virtual transitions of electrons to negative-energy states induced by the Coulomb exchanges generate the energy shift

$$\delta_C^- E = \left\langle \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2 + 2(\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e} + 2e^2}{8m^3} \right\rangle. \quad (53)$$

The total irreducible Coulomb correction is the sum of Eqs. (50), (52), and (53),

$$\begin{aligned} \delta_C E &= \frac{E\pi\alpha}{4m^3} \langle 4\delta(\mathbf{r}) - 3Z[\delta(\mathbf{r}_1) + \delta(\mathbf{r}_2)] \rangle + \left\langle \frac{3\pi\alpha Z}{4m^3} \left[ \delta(\mathbf{r}_1) \right. \right. \\ &\times \left( \frac{p_2^2}{2m} + C_2 + c \right) + (1 \leftrightarrow 2) \left. \right] - \frac{\pi\alpha\delta(\mathbf{r})}{m^3} \left( \frac{3P^2}{32m} + C_N \right) \\ &\left. + 3 \frac{[\mathbf{P} \cdot \mathbf{p}, [\mathbf{P} \cdot \mathbf{p}, c]]}{32m^4} + \frac{(\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e}}{32m^3} - \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2}{32m^3} + \frac{e^2}{8m^3} \right\rangle. \end{aligned} \quad (54)$$

### 3. Magnetic corrections

These corrections originate from single magnetic exchanges between particles in instantaneous approximation. There are two sources of such effects. Relativistic corrections to the instantaneous interaction of the Pauli currents of the electrons induce the following contribution to the energy:

$$\begin{aligned} \delta_M^{ee} E &= \left\langle \left\{ \frac{p_1^2 + p_2^2}{2m}, \frac{\mathbf{p}_1 \cdot c\mathbf{p}_2 + (d-2)(\mathbf{p}_1 \cdot \mathbf{n})c(\mathbf{n} \cdot \mathbf{p}_2)}{4m^3} \right. \right. \\ &\left. \left. - \frac{\pi\alpha\delta(\mathbf{r})}{m^3} \right\} - \frac{d-1}{32m^4} ([p_1^2, [p_1^2, c]] + [p_2^2, [p_2^2, c]]) \right\rangle, \end{aligned} \quad (55)$$

which can be transformed to

$$\begin{aligned} \delta_M^{ee} E &= \frac{E}{m} \left\langle \frac{\mathbf{p}_1 \cdot c\mathbf{p}_2 + (\mathbf{p}_1 \cdot \mathbf{n})c(\mathbf{n} \cdot \mathbf{p}_2)}{2m^2} - \frac{2\pi\alpha\delta(\mathbf{r})}{m^2} \right\rangle \\ &+ \left\langle \frac{2\pi\alpha\delta(\mathbf{r})}{m^3} C_N \right. \\ &\left. - \left\{ \frac{C}{4m^2}, \frac{\mathbf{p}_1 \cdot c\mathbf{p}_2 + (d-2)(\mathbf{p}_1 \cdot \mathbf{n})c(\mathbf{n} \cdot \mathbf{p}_2)}{m} \right\} \right. \\ &\left. - \frac{[\mathbf{P} \cdot \mathbf{p}, [\mathbf{P} \cdot \mathbf{p}, c]]}{8m^4} + \frac{(\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e}}{8m^3} + \frac{d-1}{8} \frac{e^2}{m^3} \right\rangle. \end{aligned} \quad (56)$$

Then, virtual transitions to negative-energy states of one electron induced by a single magnetic exchange with the other and a single Coulomb exchange with both other particles, shift the energy by

$$\delta_M^- E = \left\langle -\frac{(\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e}}{2m^3} - \frac{d-1}{2} \frac{e^2}{m^3} \right\rangle. \quad (57)$$

**4. Retardation corrections**

The effect of retardation on a single magnetic exchange between the electrons is described in the appropriate order by the following average value:

$$\delta_R E = \left\langle \int \frac{d^d q}{(2\pi)^d} \frac{2\pi\alpha}{q^4} \left[ H, e^{-iq \cdot r_1} \frac{\mathbf{p}_1^q + [s_1 \cdot \mathbf{q}, s_1]}{m} \right] \right. \\ \left. \times \left[ H, e^{iq \cdot r_2} \frac{\mathbf{p}_2^q - [s_2 \cdot \mathbf{q}, s_2]}{m} \right] + \text{H.c.} \right\rangle, \quad (58)$$

where  $\mathbf{q}$  is the magnetic photon's momentum and  $\mathbf{p}_a^q = \mathbf{p}_a - \mathbf{q}(\mathbf{p}_a \cdot \mathbf{q})/q^2$ . The correction (58) consists of zero-, single-, and double-Coulomb parts:

$$\delta_R E = \Delta_0 + \Delta_1 + \Delta_2, \quad (59)$$

$$\Delta_0 = \left\langle \int \frac{d^d q}{(2\pi)^d} \frac{\pi\alpha}{m^4} \left[ p_1^2, \left[ p_2^2, \frac{\mathbf{p}_1^q \cdot \mathbf{p}_2 - \frac{d-1}{4} q^2}{q^4} e^{iq \cdot r} \right] \right] \right\rangle, \quad (60)$$

$$\Delta_1 = \left\langle \int \frac{d^d q}{(2\pi)^d} \frac{2\pi\alpha}{m^3} [C, \mathbf{p}_1] \left[ p_2^2, \frac{\mathbf{p}_2^q}{q^4} e^{iq \cdot r} \right] + (1 \leftrightarrow 2) \right\rangle, \quad (61)$$

$$\Delta_2 = \left\langle \int \frac{d^d q}{(2\pi)^d} \frac{4\pi\alpha}{m^2} [C, \mathbf{p}_1] \frac{e^{iq \cdot r}}{q^4} [C, \mathbf{p}_2] \right\rangle. \quad (62)$$

Integrating over  $\mathbf{q}$  and using the Schrödinger equation we transform these expressions to the following ones:

$$\Delta_0 = -\frac{E^2 \langle c \rangle}{8m^2} + \frac{E \langle Cc \rangle}{4m^2} + \left\langle -\frac{C_N^2 c}{8m^2} - \frac{C_N c^2}{4m^2} + \frac{\pi\alpha \delta(\mathbf{r})}{2m^4} P^2 + \frac{\mathbf{p} \cdot c\mathbf{p}}{4m^4} P^2 - \frac{(\mathbf{P} \cdot \mathbf{p})c(\mathbf{P} \cdot \mathbf{p})}{8m^4} \right. \\ \left. - \frac{p_1^2 c (\mathbf{n} \cdot \mathbf{p}_2)^2 + (\mathbf{p}_1 \cdot \mathbf{n})^2 c p_2^2 - 3(\mathbf{p}_1 \cdot \mathbf{n})^2 c (\mathbf{n} \cdot \mathbf{p}_2)^2 + (1 \leftrightarrow 2)}{16m^4} + \frac{(\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e}}{8m^3} - \frac{c^3}{8m^2} + \frac{d-1}{8} \frac{e^2}{m^3} \right\rangle, \quad (63)$$

$$\Delta_1 = \frac{E \langle c^2 \rangle}{4m^2} + \left\langle -cr \frac{2(\mathbf{n} \cdot \mathbf{p}_2)(\mathcal{E}_1 \cdot \mathbf{p}_2) + (\mathbf{n} \cdot \mathcal{E}_1)[(\mathbf{n} \cdot \mathbf{p}_2)^2 - p_2^2]}{16m^3} + \text{H.c.} - 3 \frac{(\mathbf{p}_1 \cdot \mathbf{n})^2 c^2 + c^2 (\mathbf{n} \cdot \mathbf{p}_1)^2}{16m^3} \right. \\ \left. + (1 \leftrightarrow 2) - \frac{C_N c^2}{4m^2} - \frac{d-2}{4} \frac{c^3}{m^2} + \frac{d-1}{4} \frac{e^2}{m^3} \right\rangle, \quad (64)$$

$$\Delta_2 = \left\langle cr^2 \frac{3\mathcal{E}_1 \cdot \mathcal{E}_2 - (\mathbf{n} \cdot \mathcal{E}_1)(\mathbf{n} \cdot \mathcal{E}_2) - 2(\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e}}{8m^2} - \frac{(d-1)(d-2)^2 c^3}{8(4-d) m^2} \right\rangle. \quad (65)$$

Here and below I use shorthand notations  $(\mathbf{n} \cdot \mathbf{p}_a)^2$  and  $(\mathbf{p}_a \cdot \mathbf{n})^2$  for the operator  $n_i(\mathbf{n} \cdot \mathbf{p}_a)p_{ai}$  and its hermitean conjugate, respectively.

**5. Seagull correction**

Double magnetic exchange between the two electrons one of which goes over into negative-energy intermediate states gives rise to the energy shift

$$\delta_{\text{seag}} E = \left\langle \frac{\mathbf{p}_1 \cdot c^2 \mathbf{p}_1 + 3(\mathbf{p}_1 \cdot \mathbf{n})c^2(\mathbf{n} \cdot \mathbf{p}_1)}{8m^3} + (1 \leftrightarrow 2) \right. \\ \left. + \frac{d-1}{4} \frac{e^2}{m^3} \right\rangle. \quad (66)$$

This correction completes the list of the  $O(m\alpha^6)$  irreducible contributions to the helium energy.

## B. Reducible corrections

### 1. Breit Hamiltonian

Breit Hamiltonian for the helium singlet states

$$U = U_S + U_P, \quad (67)$$

consists of two parts,  $U_S$  and  $U_P$ , with the selection rules  $|\Delta S| = 0$  and  $|\Delta S| = 1$ , respectively.<sup>7</sup> Just like in the positronium case (see Ref. [12]), the second-order iteration of the  $S$ -wave Breit perturbation diverges in three dimensions. That is why this perturbation should be considered in  $d$  dimensions,

$$U_S = -\frac{p_1^4 + p_2^4}{8m^3} + \frac{\pi Z\alpha}{2m^2} [\delta(\mathbf{r}_1) + \delta(\mathbf{r}_2)] + \frac{(d-2)\pi\alpha}{m^2} \delta(\mathbf{r}) - \frac{\mathbf{p}_1 \cdot c\mathbf{p}_2 + (d-2)(\mathbf{p}_1 \cdot \mathbf{n})c(\mathbf{n} \cdot \mathbf{p}_2)}{2m^2}. \quad (68)$$

As for the  $P$ -wave part, which mixes singlet  $S$  and triplet  $P$  states, the corresponding second-order iteration is saturated by the soft scale and, therefore, we can take this perturbation in the limit of  $d = 3$ ,

$$U_P = \alpha \frac{s_1 - s_2}{4m^2} \left( \frac{Z\mathbf{l}_1}{r_1^3} - \frac{Z\mathbf{l}_2}{r_2^3} + \frac{\mathbf{r} \times \mathbf{P}}{r^3} \right). \quad (69)$$

Here  $\mathbf{l}_a = \mathbf{r}_a \times \mathbf{p}_a$ . Below I consider energy shifts arising in second order in  $U_P$  and  $U_S$ .

### 2. Second iteration of the Breit Hamiltonian: $P$ wave

To find the singlet  $S$  level shift induced by an admixture of triplet  $P$  states,

$$\delta_P E = \langle U_P G U_P \rangle, \quad (70)$$

where  $G$  is the (reduced) Green function of the Schrödinger equation, consider first the action of  $U_P$  on the ground-state wave function. As far as the latter depends on the absolute values of  $\mathbf{r}_1$ ,  $\mathbf{r}_2$ , and  $\mathbf{r}$ ,  $\psi = \psi(r_1, r_2, r)$ , we can substitute

$$\mathbf{l}_1 = \mathbf{r}_1 \times \mathbf{p}_1 \rightarrow -i\mathbf{r}_1 \times (\mathbf{n}_1 \partial_1 + \mathbf{n} \partial) = i \frac{\mathbf{r}_1 \times \mathbf{r}_2}{r} \partial,$$

$$\mathbf{l}_2 \rightarrow -i \frac{\mathbf{r}_1 \times \mathbf{r}_2}{r} \partial,$$

$$\mathbf{r} \times \mathbf{P} \rightarrow -i\mathbf{r}_1 \times \mathbf{r}_2 \left( \frac{1}{r_1} \partial_1 + \frac{1}{r_2} \partial_2 \right),$$

$$U_P \rightarrow i\alpha \frac{\mathbf{A} \cdot (\mathbf{s}_1 - \mathbf{s}_2)}{2m^2} \left( \frac{Z}{r_1^3 r} \partial - \frac{1}{r^3 r_1} \partial_1 + (1 \leftrightarrow 2) \right), \quad (71)$$

where  $\partial_a = \partial / \partial r_a$ ,  $\partial = \partial / \partial r$ , while the vector

$$\mathbf{A} = \frac{\mathbf{r}_1 \times \mathbf{r}_2}{2} = \frac{\mathbf{r} \times \mathbf{r}_1}{2} = \frac{\mathbf{r} \times \mathbf{r}_2}{2}, \quad (72)$$

is perpendicular to the triangle composed by  $\mathbf{r}_1$ ,  $\mathbf{r}_2$ , and  $\mathbf{r}$ , while its norm equals this triangle's area. The  $P$ -wave admixture to the  $S$ -state wave function

$$\delta_P \psi = G U_P \psi, \quad (73)$$

has the same angular dependence as the perturbation

$$\delta_P \psi = i\alpha \frac{\mathbf{A} \cdot (\mathbf{s}_1 - \mathbf{s}_2)}{2m^2} \frac{\phi_P(r_1, r_2, r)}{r_1 r_2 r}. \quad (74)$$

Function  $\phi_P(r_1, r_2, r)$  is introduced in such a way in order to make it finite at coalescence points:  $\phi_P(r_1, r_2, r) < \infty$  when  $r_a \rightarrow 0$  or  $r \rightarrow 0$ . Substituting the rhs of Eq. (74) into the inhomogeneous equation

$$(E - H) \delta_P \psi = U_P \psi, \quad (75)$$

we can cancel the spin- and angular-dependent factor using the following relations:

$$[H, s_1 - s_2] = 0;$$

$$[H, \mathbf{r}_1 \times \mathbf{r}_2] = \left[ \frac{p_1^2}{2m}, \mathbf{r}_1 \right] \times \mathbf{r}_2 + \mathbf{r}_1 \times \left[ \frac{p_2^2}{2m}, \mathbf{r}_2 \right] \rightarrow -\frac{\mathbf{r}_1 \times \mathbf{r}_2}{m} \left( \frac{1}{r_1} \partial_1 + \frac{1}{r_2} \partial_2 + \frac{2}{r} \partial \right).$$

At the last step I took into account that the operator acts on the function depending only on  $r_1, r_2$ , and  $r$ . The resulting equation for  $\phi_P$  reads

$$\left\{ H' - \frac{1}{m} \left( \partial_1 \frac{1}{r_1} + \partial_2 \frac{1}{r_2} + \partial \frac{2}{r} \right) - E \right\} \phi_P = \left\{ \frac{r_1}{r^2} \partial_2 - \frac{Zr_1}{r_2^2} \partial + (1 \leftrightarrow 2) \right\} \psi. \quad (76)$$

Here  $H'$  is obtained from  $H$  by the substitutions  $\partial \rightarrow \partial - 1/r$ ,  $\partial_1 \rightarrow \partial_1 - 1/r_1$ ,  $\partial_2 \rightarrow \partial_2 - 1/r_2$ .

The final expression for the energy shift (70) then reads

$$\delta_P E = \frac{\alpha^2}{4m^4} \left\langle \phi_P \left| \frac{A^2}{r^2 r_1^2 r_2^2} \left\{ \frac{r_1}{r^2} \partial_2 - \frac{Zr_1}{r_2^2} \partial + (1 \leftrightarrow 2) \right\} \right| \psi \right\rangle. \quad (77)$$

<sup>7</sup> $S = s_1 + s_2$ .

**3. Second iteration of the Breit Hamiltonian:  $S$  wave**

In order to extract divergences from the second-order correction induced by the  $S$ -wave part of the Breit Hamiltonian, Eq. (68), it is convenient to rewrite the latter in the form

$$U_S = -\frac{H^2}{2m} + \{H, u\} - 2Eu + O_d, \quad (78)$$

where

$$u = \frac{C_N + (d-1)c}{4m}, \quad (79)$$

$$O_d = E \frac{C_N + (d-1)c}{2m} + \frac{1}{8m} \left\{ \frac{p_1^2}{m} + c, \frac{p_2^2}{m} + c \right\} - \frac{C_N c}{2m} - \frac{2d-3}{4m} c^2 + \frac{\mathbf{p}_1 \cdot [C_N - (d-2)c] \mathbf{p}_1 + (1 \leftrightarrow 2)}{4m^2} - \frac{\mathbf{p}_1 \cdot c \mathbf{p}_2 + (d-2)(\mathbf{p}_1 \cdot \mathbf{n})c(\mathbf{n} \cdot \mathbf{p}_2)}{2m^2}. \quad (80)$$

Inserting Eq. (78) into equation

$$\delta_S E = \langle U_S G U_S \rangle, \quad (81)$$

and using the Schrödinger equation for the reduced Green function,  $(H-E)G(R, R') = \psi(R)\psi(R') - \delta(R-R')$ , where  $R$  denotes the vector  $(r_1, r_2, r)$ , we get

$$\delta_S E = 2\langle U_S \rangle \langle u \rangle - \left\langle \frac{1}{2} [[H, u], u] + \{U_S, u\} \right\rangle + \langle O_3 G O_3 \rangle. \quad (82)$$

Note that we can take the limit  $d \rightarrow 3$  in the last term since in contrast to  $U_S$  the perturbation  $O_3$  does not contain operators more singular than  $C_a^2$  and  $c^2$ . In other words, all the divergences in Eq. (82) are moved to the average values of local operators.

The first term from Eq. (82) is most easy to calculate,

$$2\langle U_S \rangle \langle u \rangle = B \frac{2E + \langle c \rangle}{2m}. \quad (83)$$

Here  $B = \langle U_S \rangle$  is the nonrecoil limit of the first-order Breit correction (4). For the second term from Eq. (82) we have

$$-\left\langle \frac{1}{2} [[H, u], u] \right\rangle = \left\langle \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2}{32m^3} + \frac{(\mathcal{E}_1 - \mathcal{E}_2)\mathbf{e}}{8m^3} + \frac{(d-1)^2 e^2}{16m^3} \right\rangle. \quad (84)$$

Then, the third term from Eq. (82) can be rewritten as

---


$$-\langle \{U_S, u\} \rangle = \frac{E^3}{2m^2} - \frac{E\langle C^2 \rangle}{2m^2} - \frac{\pi\alpha(Z-2)}{4m^3} \langle \delta(\mathbf{r}_1)C_2 + \delta(\mathbf{r}_2)C_1 \rangle + \left\langle \frac{3CcC_N}{4m^2} - \frac{p_1^2 C_N p_2^2}{8m^4} + \frac{[\mathbf{P} \cdot \mathbf{p}, [\mathbf{P} \cdot \mathbf{p}, c]] + 2(\mathbf{P} \cdot \mathbf{p})c(\mathbf{P} \cdot \mathbf{p})}{8m^4} - \frac{\pi\alpha\delta(\mathbf{r})}{2m^3} C_N + \left\{ \frac{C_N + (d-1)c}{8m^2}, \frac{\mathbf{p}_1 c \cdot \mathbf{p}_2 + (d-2)(\mathbf{p}_1 \cdot \mathbf{n})c(\mathbf{n} \cdot \mathbf{p}_2)}{m} \right\} - \frac{(\mathcal{E}_1 - \mathcal{E}_2) \cdot \mathbf{e}}{4m^3} + \frac{C_N^3}{4m^2} + \frac{d-1}{8m^2} c^3 - \frac{\mathcal{E}_1^2 + \mathcal{E}_2^2}{8m^3} - \frac{(d-1)e^2}{8m^3} \right\rangle. \quad (85)$$

Finally, the fourth term from Eq. (82) can be calculated in a way similar to that used above for the  $P$ -wave contribution. Namely, we first find the solution for the inhomogeneous equation

$$(E-H)\delta_S \psi = (O_3 - \langle O_3 \rangle)\psi,$$

orthogonal to the ground state,  $\langle \delta_S \psi | \psi \rangle = 0$ , and then evaluate the matrix element of  $O_3$  between  $\delta_S \psi$  and  $\psi$ ,

$$\langle O_3 G O_3 \rangle = \langle \delta_S \psi | O_3 | \psi \rangle. \quad (86)$$

An alternative way to calculate Eq. (86) is to include the operator  $O_3$  directly into the Hamiltonian,

$$(H + O_3)\psi' = E'\psi'. \quad (87)$$

Then, with the  $O(\alpha^2)$  precision,

$$\langle O_3 G O_3 \rangle = E' - E - \langle O_3 \rangle. \quad (88)$$

**C. Total soft-scale contribution**

Summing up all soft-scale contributions, given by Eqs. (46), (54), (56), (57), (63–66), (77), and (83–86), we get

$$\begin{aligned}
\delta_{\text{soft}}E = & -\frac{E^3}{2m^2} + \frac{E^2\langle c \rangle}{4m^2} + \frac{E}{m} \left\langle \frac{2C_N C + c^2}{4m} - \frac{p_1^2 p_2^2}{8m^3} - \frac{\pi\alpha Z}{4m^2} [\delta(\mathbf{r}_1) + \delta(\mathbf{r}_2)] \right\rangle + \frac{B\langle c \rangle}{2m} + \delta_P E + \langle O_3 G O_3 \rangle + \left\langle -\frac{c C_N C}{2m^2} \right. \\
& - \left\langle \frac{C_N}{8m^3}, \frac{\mathbf{p}_1 \cdot c \mathbf{p}_2 + (\mathbf{p}_1 \cdot \mathbf{n}) c (\mathbf{n} \cdot \mathbf{p}_2)}{m} \right\rangle + \frac{p_1^2 C_N p_2^2}{4m^4} + \frac{\mathbf{p}_1 \cdot c^2 \mathbf{p}_1 + \mathbf{p}_2 \cdot c^2 \mathbf{p}_2}{8m^3} + \frac{\mathbf{p} \cdot c \mathbf{p} \cdot P^2 - (\mathbf{P} \cdot \mathbf{p}) c (\mathbf{P} \cdot \mathbf{p})}{4m^4} \\
& - \frac{p_1^2 c (\mathbf{n} \cdot \mathbf{p}_2)^2 + (\mathbf{p}_1 \cdot \mathbf{n})^2 c p_2^2 - 3(\mathbf{p}_1 \cdot \mathbf{n})^2 c (\mathbf{n} \cdot \mathbf{p}_2)^2 + (1 \leftrightarrow 2)}{16m^4} - \frac{cr}{16m^3} [2(\mathbf{n} \cdot \mathbf{p}_2)(\boldsymbol{\mathcal{E}}_1 \cdot \mathbf{p}_2) + (\mathbf{n} \cdot \boldsymbol{\mathcal{E}}_1)[(\mathbf{n} \cdot \mathbf{p}_2)^2 - p_2^2] \\
& + (1 \leftrightarrow 2) + \text{H.c.}] + \frac{cr^2}{8m^2} [3\boldsymbol{\mathcal{E}}_1 \cdot \boldsymbol{\mathcal{E}}_2 - (\mathbf{n} \cdot \boldsymbol{\mathcal{E}}_1)(\mathbf{n} \cdot \boldsymbol{\mathcal{E}}_2) - 2(\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_2) \cdot \mathbf{e}] - \frac{3[\mathbf{P} \cdot \mathbf{p}, [\mathbf{P} \cdot \mathbf{p}, c]]}{32m^4} + \frac{\pi\alpha\delta(\mathbf{r})}{2m^3} \left( \frac{13P^2}{16m} + C_N \right) \\
& + \frac{\pi\alpha Z}{4m^3} \left[ \delta(\mathbf{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) \mathbf{e}}{32m^3} \frac{C_N^3}{4m^2} + \frac{\boldsymbol{\mathcal{E}}_1^2 + \boldsymbol{\mathcal{E}}_2^2}{8m^3} - \frac{1-3\epsilon}{2m^2} c^3 + \frac{3-6\epsilon}{4m^3} e^2 \Bigg\rangle. \quad (89)
\end{aligned}$$

Order  $\epsilon$  coefficients are kept in Eq. (89) only if they multiply the operators whose average values contain  $1/\epsilon$  singularities. In Eq. (89), the following relations are taken into account:

$$\begin{aligned}
[p_i, [p_j, c^2 n_i n_j]] &= \frac{3-d}{d-2} e^2, \\
(d-3) \left\langle \left\{ c, \frac{\mathbf{p}_1 \cdot c \mathbf{p}_2 + (\mathbf{p}_1 \cdot \mathbf{n}) c (\mathbf{n} \cdot \mathbf{p}_2)}{m} \right\} \right\rangle & \\
&= (d-3) \langle c^3 \rangle + O(\epsilon). \quad (90)
\end{aligned}$$

For the bulk of the operators in Eq. (89), their average values can be safely evaluated at  $d \rightarrow 3$ . Special care is needed when one deals with the operator  $p_1^2 c (\mathbf{n} \cdot \mathbf{p}_2)^2 + (1 \leftrightarrow 2) + \text{H.c.}$ , which is not well defined in three dimensions. We can take the limit  $d \rightarrow 3$  having previously determined what the momenta operators are acting on

$$\begin{aligned}
\lim_{d \rightarrow 3} \langle p_1^2 c (\mathbf{n} \cdot \mathbf{p}_2)^2 + (1 \leftrightarrow 2) + \text{H.c.} \rangle & \\
&= \langle \overline{p_1^2 c (\mathbf{n} \cdot \mathbf{p}_2)^2} + (1 \leftrightarrow 2) + \text{H.c.} + 4\pi m^2 \alpha^3 \delta(\mathbf{r}) \rangle|_{d=3}. \quad (91)
\end{aligned}$$

In order to be certain that this relation holds, it is sufficient to consider the two-body problem, where both sides of Eq. (91) can be calculated analytically.

In order to calculate singular average values entering into Eq. (89), consider the Coulomb potential  $C_{ab}$  between two particles with charges  $z_a$  and  $z_b$ . The average value of  $C_{ab}^3$  is

$$\langle C_{ab}^3 \rangle = (z_a z_b \alpha)^3 \left( \frac{\Gamma\left(\frac{d}{2} - 1\right)}{\pi^{d/2-1}} \right)^3 \langle r_{ab}^{6-3d} \rangle. \quad (92)$$

Repeating the procedure used in Sec. III we get

$$\begin{aligned}
\langle C_{ab}^3 \rangle &= (z_a z_b \alpha)^3 \left\{ \left( \frac{1}{\epsilon} - 4 \ln \frac{2}{a_{ab}} + 2 \right) \langle \pi \delta(\mathbf{r}_{ab}) \rangle \right. \\
&\quad \left. - 2 \left\langle \frac{\gamma + \ln \frac{2r_{ab}}{a_{ab}}}{r_{ab}^2} \mathbf{n}_{ab} \cdot \nabla_{ab} \right\rangle \right\}. \quad (93)
\end{aligned}$$

Recall that  $a_{ab} = |z_a z_b \mu_{ab} \alpha|^{-1}$ . Average value of the second singular operator,  $\mathcal{E}_{ab}^2$ , can be found in the following way:

$$\begin{aligned}
\langle \mathcal{E}_{ab}^2 \rangle &= \langle [\nabla_a, C_{ab}]^2 \rangle \\
&= \langle [\nabla_a, C_{ab} [\nabla_a, C_{ab}]] - C_{ab} [\nabla_a, [\nabla_a, C_{ab}]] \rangle \\
&= -2 \langle C_{ab} [\nabla_a, C_{ab}] \nabla_a \rangle. \quad (94)
\end{aligned}$$

At the last step, I again have used the equation  $\langle C_{ab} \delta(\mathbf{r}_{ab}) \rangle = 0$  valid in the dimensional regularization. In order to express the average value

$$\langle \mathcal{E}_{ab}^2 \rangle = 2(d-2)(z_a z_b \alpha)^2 \left( \frac{\Gamma\left(\frac{d}{2} - 1\right)}{\pi^{d/2-1}} \right)^2 \langle r^{3-2d} \mathbf{n}_{ab} \cdot \nabla_{ab} \rangle, \quad (95)$$

in terms of  $\langle C_{ab}^3 \rangle$ , the known derivative of the wave function at  $\mathbf{r}_{ab} \rightarrow 0$  can<sup>8</sup> be added to and subtracted from  $\mathbf{n}_{ab} \cdot \nabla_{ab}$ ,

<sup>8</sup>Strictly speaking, with a coefficient  $1 + O(\epsilon)$ . Inspection of the known two-body average values, however, shows that the coefficient is in fact equal to 1.

$$\langle \mathcal{E}_{ab}^2 \rangle = 2\mu_{ab}(d-2)\langle C_{ab}^3 \rangle + 2(z_a z_b \alpha)^2 \left\langle \frac{1}{r_{ab}^3} (\mathbf{n}_{ab} \cdot \nabla_{ab} - \mu_{ab} z_a z_b \alpha) \right\rangle. \quad (96)$$

Since the last average value in the rhs of Eq. (96) is finite, it

can be considered in three dimensions. Now, extracting all divergent pieces from Eq. (89) we get Eq. (38).

## VI. CONCLUSION

The divergences contained in the hard (37) and soft scale (38) contributions cancel each other so that in the sum of all contributions, Eqs. (33)–(37), (89), we can put  $d=3$ . Taking into account Eqs. (91),(93),(96), the final expression for the  $O(m\alpha^6)$  correction to a singlet  $S$ -state energy of the helium atom can be written as

$$\begin{aligned} \delta^{(4)}E = & -\frac{E^3}{2m^2} + \frac{E^2\langle c \rangle}{4m^2} + \frac{E}{m} \left\langle \frac{2C_N C + c^2}{4m} - \frac{p_1^2 p_2^2}{8m^3} - \frac{\pi\alpha Z}{4m^2} [\delta(\mathbf{r}_1) + \delta(\mathbf{r}_2)] \right\rangle + \frac{B\langle c \rangle}{2m} + \delta_P E + \langle O_3 G O_3 \rangle \\ & + \pi\alpha^3 m^2 \langle k_{eN} [\delta(\mathbf{r}_1) + \delta(\mathbf{r}_2)] + k_{ee} \delta(\mathbf{r}) \rangle + \left\langle -\frac{3C_1 C_2 C_N}{4m^2} - \frac{c C_N C}{2m^2} - \frac{C_N c [\mathbf{p}_1 \mathbf{p}_2 + \mathbf{n}(\mathbf{n} \mathbf{p}_1) \mathbf{p}_2]}{8m^4} + \text{H.c.} + \frac{p_1^2 C_N p_2^2}{4m^4} \right. \\ & + \frac{\mathbf{p}_1 \cdot c^2 \mathbf{p}_1 + \mathbf{p}_2 \cdot c^2 \mathbf{p}_2}{8m^3} + \frac{(\mathbf{p}_1 \times \mathbf{p}_2) \cdot c(\mathbf{p}_1 \times \mathbf{p}_2)}{4m^4} - \frac{p_1^2 c(\mathbf{n} \cdot \mathbf{p}_2)^2 + (\mathbf{p}_1 \cdot \mathbf{n})^2 c p_2^2 - 3(\mathbf{p}_1 \cdot \mathbf{n})^2 c(\mathbf{n} \cdot \mathbf{p}_2)^2 + (1 \leftrightarrow 2)}{16m^4} \\ & - \alpha \frac{2(\mathbf{n} \cdot \mathbf{p}_2)(\mathcal{E}_1 \cdot \mathbf{p}_2) + (\mathbf{n} \cdot \mathcal{E}_1)[(\mathbf{n} \cdot \mathbf{p}_2)^2 - p_2^2] + (1 \leftrightarrow 2) + \text{H.c.}}{16m^3} + \alpha r \frac{3\mathcal{E}_1 \cdot \mathcal{E}_2 - (\mathbf{n} \cdot \mathcal{E}_1)(\mathbf{n} \cdot \mathcal{E}_2) - 2(\mathcal{E}_1 - \mathcal{E}_2) \cdot \mathbf{e}}{8m^2} \\ & - \frac{3\alpha}{32m^4} \frac{P^2 - 3(\mathbf{n} \cdot \mathbf{P})^2}{r^3} + \frac{\pi\alpha\delta(\mathbf{r})}{2m^3} \left( \frac{9P^2}{16m} + C_N \right) + \frac{\pi\alpha Z}{4m^3} \left[ \delta(\mathbf{r}_1) \left( \frac{3p_2^2}{2m} - \frac{(2Z-1)\alpha}{r_2} \right) + (1 \leftrightarrow 2) \right] - \frac{(\mathcal{E}_1 - \mathcal{E}_2) \cdot \mathbf{e}}{32m^3} \\ & + \frac{(Z\alpha)^2}{4m^3} \left[ \frac{1}{r_1^3} (\mathbf{n}_1 \cdot \nabla_1 + mZ\alpha) + (1 \leftrightarrow 2) \right] - \alpha^3 \frac{\ln(m\alpha r) + \gamma}{2m^2 r^2} \mathbf{n} \cdot \nabla + \frac{3\alpha^2}{2m^3} \frac{1}{r^3} \left( \mathbf{n} \cdot \nabla - \frac{m\alpha}{2} \right) \Bigg\rangle. \quad (97) \end{aligned}$$

Here all momentum operators standing to the right (left) of position-dependent operators are assumed to act on the right (left) wave function. Although  $d$ -dimensional notations for the Coulomb potentials and electric forces are kept in Eq. (97), the immediate three-dimensional counterparts are implied for all operators, e.g.,  $C_1 \rightarrow -Z\alpha/r_1$ ,  $\mathbf{e} \rightarrow \alpha\mathbf{n}/r^2$  and so on. The contact terms enter into Eq.(97) with the coefficients

$$k_{eN} = \frac{Z^3}{2} + \frac{427Z^2}{96} - \frac{10Z}{27} - \frac{9Z\zeta(3)}{4\pi^2} - \frac{2179Z}{648\pi^2} + \frac{3Z-4Z^2}{2} \ln 2, \quad (98)$$

$$k_{ee} = -\ln \alpha + \frac{3385}{216} - \frac{331}{54\pi^2} - \frac{29 \ln 2}{2} + \frac{15\zeta(3)}{4\pi^2}. \quad (99)$$

Equations (97)–(99) are the principal result of the present work. Its application to the ground state of the helium atom is considered elsewhere [5].

The approach elaborated here can be applied to other few-electron atoms as well as to higher-order corrections. The only stumbling block to higher-order calculations is the yet unknown three-loop hard-scale electron-electron potential. Nevertheless, the order  $m\alpha^7$  corrections enhanced by powers of  $\ln \alpha$  can be determined by combination of methods used in Ref. [15] and in the present work.

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