Relativistic corrections to the Bethe logarithm for the $2^3S$ and $2^3P$ states of He

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With this work we start a project calculating the QED contribution of order $\alpha^7 m$ to the $2^3P-2^3S$ transition energy in helium, aiming for an accurate determination of the nuclear charge radius $r_E$ from measurements of the corresponding transition frequency. Together with the complementary determination of $r_E$ from muonic helium, this project will provide a stringent test of universality of electromagnetic interactions of leptons in the Standard Model. We report a calculation of the relativistic corrections to the Bethe logarithm for the $2^3S$ and $2^3P$ states, which is the most numerically demanding part of the project.

I. INTRODUCTION

One of the prominent low-energy tests of the Standard Model (SM) with a possible signature of new physics is based on a comparison of the Lamb shift in muonic hydrogen $\mu H$ and electronic hydrogen $H$. The lepton universality of SM implies that the same physical laws and physical constants define the energy levels in $H$ and $\mu H$. However, it has been found that the proton root-mean-square charge radius, extracted from the comparison of theory and experiment for the Lamb shift, turned out to be significantly different for the electronic [1] and muonic [2, 3] hydrogen,

$$r_p(H) = 0.8759(77) \text{ fm},$$
$$r_p(\mu H) = 0.84087(39) \text{ fm}.$$  

This $4.5\sigma$ discrepancy, known as the proton radius puzzle, may signal the existence of interactions that are not accounted for in the Standard Model. Several experiments aiming to resolve the puzzle have been accomplished recently, namely the measurement of the $2S-4P$ transition energy in Garching [4], $2S-2P$ Lamb shift in Toronto [5], and two measurements of the $1S-3S$ transition energy performed in Paris [6] and in Garching [7]. These experiments yield conflicting results for the proton charge radius, which does not solve the puzzle but suggests the presence of unknown systematic effects in hydrogen measurements. Further experiments directed to clarify the proton radius puzzle are currently being pursued, notably, measurements of the $1S-2S$ transition energy in He$^+$ [8, 9], transitions between circular Rydberg states in H-like ions [10], and the direct comparison of the cross sections of the $e-p$ versus $\mu-p$ elastic scattering [11].

An alternative way to solve the proton charge radius puzzle can be gained through spectroscopy of the helium atom. Specifically, a comparison of the nuclear charge radius from the helium spectroscopy with the radius from muonic helium, expected soon from the CREMA collaboration [12], would provide an independent test of the lepton universality in atomic systems. On the experimental side, several transition energies in the helium atom are already known with an accuracy sufficient for determining the nuclear charge radius on a $10^{-3}$ fractional level [13–19]. In order to achieve a similar level of accuracy in theoretical predictions, one needs to improve the previous helium calculations [20, 21] by completing the next-order term of the NRQED expansion, namely the $\alpha^7 m$ correction. This is a very challenging theoretical problem. Among few-electron atoms, it has so far been solved only for the helium fine structure [22–24].

With this paper, we start a project calculating the complete $\alpha^7 m$ correction for energy levels of two-electron atoms. At present, we restrict ourselves to the triplet states, for which the nonrelativistic wave function $\phi(\vec{r}_1, \vec{r}_2)$ vanishes at $\vec{r}_1 = \vec{r}_2$. As a result, the whole class of the so-called contact operators does not contribute, thus making the derivation of $\alpha^7 m$ operators more tractable. An improved theory of the triplet states will allow the determination of the nuclear charge radius from the $2^3S-2^3P$ transition in $^4$He, which was accurately measured by the Hefei group [18].

The present status of theory of helium energy levels complete up to order $\alpha^6 m$ is described in our recent review [25]. The next-order $\alpha^7 m$ contribution can be represented as a sum of three parts,

$$E^{(7)} = \left\langle H^{(7)} \right\rangle + 2 \left\langle H^{(4)} \frac{1}{E-H} H^{(5)} \right\rangle + E_L,$$  

where $H^{(4)}$, $H^{(5)}$, and $H^{(7)}$ are the effective Hamiltonians of order $\alpha^4 m$, $\alpha^5 m$, and $\alpha^7 m$, respectively; $H$ and $E$ are the nonrelativistic Hamiltonian and its eigenvalue, respectively; and $E_L$ is the low-energy contribution, also known as the relativistic correction to the Bethe logarithm, which is the main subject of this work.

Out of the three terms contributing to $E^{(7)}$, the relativistic correction to the Bethe logarithm is numerically the most demanding one and thus is the crucial part of the whole $\alpha^7 m$ project. The calculation of (the spin-dependent part of) such a correction was first performed in Ref. [26] for the fine structure of helium and later improved in Refs. [23, 24]. For the Coulomb two-center sys-
tems (H$_2^+$, HD$, \text{ etc.}$), the relativistic corrections to the Bethe logarithm were calculated by Korobov et al. [27]. The goal of the present work is to calculate the spin-independent low-energy correction $E_L$ for the 2$^3S$ and 2$^3P$ states of helium.

**II. NONRELATIVISTIC LOW-ENERGY CONTRIBUTION**

The leading nonrelativistic (dipole) low-energy contribution of order $\alpha^5 m$ is given by

$$E_{L0}(\Lambda) = \frac{e^2}{m^2} \int_{k<\Lambda} \frac{d^3k}{(2\pi)^3 2k} \left( \delta^{ij} - \frac{k^i k^j}{k^2} \right) \times \left\langle P^i \frac{1}{E - H - k} P^j \right\rangle,$$

where $\vec{P} = \vec{p}_1 + \vec{p}_2$ and $\Lambda$ is the high-momentum cutoff. $E_{L0}(\Lambda)$ diverges when $\Lambda \to \infty$ and requires subtraction of the leading terms in the large-$\Lambda$ asymptotics. Performing the angular integration and dropping the overall prefactor $\alpha^5 m$, one obtains

$$E_{L0}(\Lambda) = \frac{2}{3\pi} \int_0^\Lambda k \, dk \, P(k),$$

where

$$P(k) = \left\langle \frac{\vec{P}}{E - H - k} \right\rangle.$$

The large-$k$ expansion of $P(k)$ is

$$k \, P(k) = -\langle P^2 \rangle + \frac{D}{k} + \ldots,$$

where $D = 2\pi Z (\delta^3(r_1) + \delta^3(r_2))$. The finite part of the low-energy contribution is then defined by dropping terms proportional to $\Lambda$ and $\ln(2\Lambda)$ as

$$E_{L0} = -\frac{2}{3\pi} D \ln k_0,$$

where $\ln k_0$ is the standard Bethe logarithm.

$$\ln k_0 = -\frac{1}{D} \int_0^\infty dk \left[ k \, P(k) + \langle P^2 \rangle - \frac{D}{k} \theta(2k - 1) \right] = \frac{\langle \vec{P} \, (H - E) \, \ln \left[ 2(\Lambda - E) \right] \rangle}{2\pi Z \left( \sum_a \delta^3(r_a) \right)} ,$$

and $\theta(x)$ is the Heaviside step function.

We construct the finite part of the Breit correction as

$$E_{L1} = \frac{2}{3\pi} \int_0^\infty dk \left[ kP_{L1}(k) - A_1 - \frac{B_1}{\sqrt{k}} - \left( \frac{C_1 \ln k}{k} + \frac{D_1}{k} \right) \theta(k - 1) \right].$$

The numerical calculation of the Bethe logarithm for the helium atom remained for a long time a very difficult problem [28, 29], which has been successfully solved only relatively recently [30–32].

**III. RELATIVISTIC LOW-ENERGY CORRECTIONS**

There are three types of relativistic corrections of order $\alpha^7 m$ to the low-energy contribution (2),

$$E_L = E_{L1} + E_{L2} + E_{L3}. \quad (8)$$

The first part $E_{L1}$ is a perturbation of the nonrelativistic low-energy contribution $E_{L0}$ in Eq. (2) by the Breit Hamiltonian $H^{(4)}$, the second part $E_{L2}$ is induced by the relativistic correction to the current operator $\vec{P}$, whereas the third term $E_{L3}$ is the retardation correction. All of these corrections are defined as remainders after dropping divergent in $\Lambda$ terms, such as $\Lambda$ and $\ln \Lambda$.

**A. Breit correction $E_{L1}$**

The low-energy contribution perturbed by the (spin-independent part of the) Breit Hamiltonian $H^{(4)}$ is

$$E_{L1}(\Lambda) = \frac{2}{3\pi} \int_0^\Lambda k \, dk \, P_{L1}(k),$$

where

$$P_{L1}(k) = 2 \left\langle \frac{1}{E - H + k} \vec{P} \vec{P} \frac{1}{E - H - k} \vec{P} \right\rangle + \left\langle \frac{\vec{P}}{E - H - k} \left[ H^{(4)} - \langle H^{(4)} \rangle \right] \frac{1}{E - H - k} \vec{P} \right\rangle ,$$

where (with $r \equiv r_{12}$)

$$H^{(4)} = -\frac{1}{8} (p_1^4 + p_2^4) + \frac{Z\pi}{2} \left[ \delta^3(r_1) + \delta^3(r_2) \right] + \pi \delta^3(r) - \frac{1}{2} p_1^i \left( \frac{\delta^3(r)}{r} + \frac{r^3 r^3}{r^5} \right) p_2^j . \quad (11)$$

The large-$k$ expansion of $P_{L1}(k)$ is given by

$$kP_{L1}(k) = A_1 + \frac{B_1}{\sqrt{k}} + \frac{C_1 \ln k}{k} + \frac{D_1}{k} + \ldots , \quad (12)$$

where the asymptotic constants are derived in Appendix A.
where \( K \geq 1 \) is a free parameter.

### B. Current correction \( E_{L_2} \)

The second low-energy contribution of order \( \alpha^7 m \) is induced by a correction to the current operator in Eq. (2), \( \vec{P} \rightarrow \vec{P} + \delta \vec{j} \), with

\[
\delta j^i = i \left[ H^{(4)}, r_1^i + r_2^i \right] 
= -\frac{1}{2} \left( p_1^i p_1^2 + p_2^i p_2^2 \right) - \frac{1}{2} \left( \frac{\delta j^i}{r} + \frac{r^i r^j}{r^3} \right) \left( p_1^j + p_2^j \right),
\]

where \([ , ]\) denotes a commutator. The corresponding low-energy correction is

\[
E_{L_2}(\Lambda) = \frac{4}{3\pi} \int_{0}^{\Lambda} kdk P_{L_2}(k), \tag{16}
\]

The finite part of the low-energy correction is constructed as

\[
E_{L_2} = \frac{4}{3\pi} \int_{0}^{\infty} dk \left[ k P_{L_2}(k) - A_2 - B_2 \frac{2}{\sqrt{k}} \left( \frac{C_2 \ln k}{k} + \frac{D_2}{k^2} \right) \theta(k - 1) \right] \tag{19}
\]

\[
= \frac{4}{3\pi} \left\{ \int_{0}^{K} kdk P_{L_2}(k) + \int_{K}^{\infty} kdk \left[ P_{L_2}(k) - A_2 \frac{2}{k} - B_2 \frac{C_2 \ln k}{k^2} - D_2 \frac{2}{k^2} \right] \right\}, \tag{20}
\]

where \( K \geq 1 \) is a free parameter.

### C. Retardation correction \( E_{L_3} \)

A retardation correction to the low energy contribution is

\[
E_{L_3}(\Lambda) = \frac{2}{3\pi} \int_{0}^{\Lambda} kdk P_{L_3}(k), \tag{21}
\]

where

\[
P_{L_3}(k) = \frac{3}{8\pi} \int d\Omega_k \left( \delta^{ij} - \frac{k^i k^j}{k^2} \right) \sum_{a,b=1,2} \delta k^2 \left( \frac{p_a^i e^{i\vec{k} \cdot \vec{r}_a} - \frac{1}{E - H - k} p_b^i e^{-i\vec{k} \cdot \vec{r}_a}}{E - H - k} \right), \tag{22}
\]

where \( \delta_{k^2}(\ldots) \) denotes the quadratic in \( k \) term of the small-\( k \) expansion of the exponential functions in the matrix element \( \langle \ldots \rangle \). Performing the expansion and integrating over angular variables, we obtain

\[
P_{L_3}(k) = \frac{3}{8\pi} \int \Omega_k \left( \delta^{ij} - \frac{k^i k^j}{k^2} \right) \sum_{a,b=1,2} \left< p_a^i (\vec{k} \cdot \vec{r}_a) \frac{1}{E - H - k} (\vec{k} \cdot \vec{r}_b) p_b^j - p_a^i (\vec{k} \cdot \vec{r}_a)^2 \frac{1}{E - H - k} p_b^j \right> \]

\[
= \frac{k^2}{10} \left[ 3 \left< (p_1^i r_1^j + p_2^i r_2^j)^2 \right> \frac{1}{E - H - k} (r_1^i p_1^j + r_2^i p_2^j)^2 \right] - \frac{5}{2k} \left< \vec{L}^2 \right>, \tag{23}
\]
where $(a^i b^j)^{(2)} = (a^i b^j + a^j b^i)/2 - \vec{a} \cdot \vec{b} \delta^{ij}/3$ and $\vec{L} = \vec{r}_1 \times \vec{r}_2 + \vec{r}_2 \times \vec{r}_1$. The large-$k$ expansion of $P_{L3}(k)$ is of the form

$$k P_{L3}(k) = G_3 k^2 + F_3 k + A_3 + \frac{B_3}{\sqrt{k}} + \frac{C_3 \ln k}{k} + \frac{D_3}{k} + \ldots,$$

where the asymptotic constants are derived in Appendix C.

We construct the finite part of the retardation correction as

$$E_{L3} = \frac{2}{3\pi} \int_0^\infty dk \left\{ k P_{L3}(k) - k^2 G_3 - k F_3 - A_3 - \frac{B_3}{\sqrt{k}} - \left[ C_3 \ln k + D_3 \right] \theta(k - 1) \right\},$$

$$= \frac{2}{3\pi} \left\{ \int_0^K dk k P_{L3}(k) + \int_K^\infty dk \left[ k P_{L3}(k) - G_3 k^2 - F_3 k - A_3 - \frac{B_3}{\sqrt{k}} - \frac{C_3 \ln k}{k} - \frac{D_3}{k} \right] \right\},$$

where $K \geq 1$ is a free parameter.

### IV. NUMERICAL EVALUATION

#### A. Transformation to a regularized form

The Breit Hamiltonian $H^{(4)}$ [Eq. (11)] contains singular operators $(\delta(r_a), \phi^k_a)$ which complicates numerical evaluations of the Breit correction $E_{L1}$. In order to achieve high numerical accuracy, we transform Eq. (10) to a more regular form. Specifically, by using the identity

$$H^{(4)}|\phi\rangle = H^{(4)}_A|\phi\rangle + \{H - E, Q\}|\phi\rangle,$$

where $|\phi\rangle$ is the eigenfunction $H$ with energy $E$,

$$Q = -\frac{1}{4} \left( \frac{Z}{r_1} + \frac{Z}{r_2} - \frac{2}{r} \right)$$

and

$$H^{(4)}_A|\phi\rangle = \left[ -\frac{1}{2} (E - V)^2 + \frac{1}{4} \nabla_1^2 \nabla_2^2 - \frac{Z}{4} \frac{\vec{r}_1}{r_1^2} \cdot \nabla_1 - \frac{Z}{4} \frac{\vec{r}_2}{r_2^2} \cdot \nabla_2 - \frac{1}{2} \frac{p_1^i}{r} \left( \delta^{ij} + \frac{r^i r^j}{r^2} \right) p_2^j \right]|\phi\rangle,$$

$$H^{(4)}_B = \frac{1}{2} (E - V) \left( E - \frac{1}{r} \right) + \frac{1}{4} \nabla_1^2 \nabla_2^2 - \frac{Z}{4} \frac{\vec{p}_1}{r_1^2} \cdot \nabla_1 - \frac{Z}{4} \frac{\vec{p}_2}{r_2^2} \cdot \nabla_2 - \frac{1}{2} \frac{p_1^i}{r} \left( \delta^{ij} + \frac{r^i r^j}{r^2} \right) p_2^j,$$

we transform the second term in the right-hand-side of Eq. (10) to the regularized form,

$$P_{\text{ret}}(k) = \left\langle \vec{P} \left| \frac{1}{E - H - k} \left[ H^{(4)}_B - 2k Q_B - \frac{k^2}{2} - \left( H^{(4)}_B \right) \right] \right| \frac{1}{E - H - k} \right\rangle - \left\langle \left( 2 \vec{P} Q_B + k \vec{P} \right) \left| \frac{1}{E - H - k} \right\rangle - \frac{1}{2} \left\langle \vec{P}^2 \right\rangle. \right\}$$

#### B. Angular decomposition

In our approach, we express all wave functions and perform the angular momentum algebra in Cartesian co-
and $3P^o$ symmetry are represented as
\[ \phi (3S) = F(r_1, r_2, r) - (1 \leftrightarrow 2), \]
\[ \phi^i (3P^o) = r_1^i F(r_1, r_2, r) - (1 \leftrightarrow 2), \]
where the scalar functions $F$ are linear combinations of exponential functions,
\[ F(r_1, r_2, r) = \sum_i c_i \exp \left( -\alpha_i r_1 - \beta_i r_2 - \gamma_i r \right). \]

The wave functions are normalized by $\langle \phi | \phi \rangle = 1$ and $\langle \phi^i | \phi^i \rangle = 1$.

The angular decomposition of formulas in Sec. III is
\[ \text{performed by using the identity for the angular decomposition for the } \{3P^o \text{ intermediate states, respectively,} \]
\[ P(k) = \sum_n \frac{\phi_n^i (3P^o)}{E_n - E - k} \langle \phi_n^k (3P^o) | P^k | \phi (3S) \rangle. \]

The angular decomposition for the $3P^o$ reference state is performed by using the identity
\[ P^i(k) = \sum_n \frac{\phi_n^i (3P^o)}{E_n - E} \langle \phi_n^k (3P^o) | P^k | \phi (3S) \rangle. \]

The three terms in the right-hand-side of the above expression give rise to contributions from the $3S$, $3P^o$, and $3D^e$ intermediate states, respectively,
\[ P(k) = P_{L=0}(k) + P_{L=1}(k) + P_{L=2}(k) \]
\[ = \frac{1}{3} \left( \Psi_0 \left| \frac{1}{E - H - k} \right| \frac{1}{3P^o} \right) \langle \Psi_0 | \phi (3S) \rangle \]
\[ + \frac{1}{2} \left( \Psi_1 \left| \frac{1}{E - H - k} \right| \frac{1}{3P^o} \right) \langle \Psi_1 | \phi (3S) \rangle \]
\[ + \frac{1}{4} \left( \Psi_2 \left| \frac{1}{E - H - k} \right| \frac{1}{3P^o} \right) \langle \Psi_2 | \phi (3S) \rangle, \]
where $\Psi_0 = \tilde{j} \cdot \tilde{\phi}$, $\Psi_1 = \tilde{j} \times \tilde{\phi}$, and $\Psi_2 = j^i \phi^k + j^k \phi^i - \frac{2}{3} \delta^{ik} \tilde{j} \cdot \tilde{\phi}$.

A more complicated situation arises in the evaluation of the symmetric part of the $E_{L3}$ contribution for the $3P^o$ reference state [the first term in brackets in Eq. (24), $P_{L3}^{sym}$]. In order to perform the angular decomposition in this case, we use the following identity,
\[ \frac{1}{2} \sum_{a=1, 2} (r_a^i p_a^j + r_a^j p_a^i) \phi^k = T^{ijk} + e^{ijkl} T^{ij} + e^{ijkl} T^{ik}, \]
where $T^{ijk}$, $T^{ij}$, and $T^i$ are the components of the (symmetric and traceless) irreducible tensors of the first, second, and third rank, respectively,
\[ T^{ijk} = \sum_a (r_a^i p_a^j \phi^k)^{(3)}, \]
\[ T^{ij} = \frac{1}{12} \sum_a \left[ e^{ilm} (r_a^l p_a^i + r_a^i p_a^l) \phi^m \right. \]
\[ + e^{ilm} (r_a^l p_a^i + r_a^i p_a^l) \phi^m \left. \right], \]
\[ T^i = \frac{1}{20} \sum_a \left[ 3 (r_a^i p_a^j + r_a^j p_a^i) \phi^j - 2 r_a^i p_a^j \phi^j \right], \]
\[ T^{ik} = \frac{1}{10} \sum_a \left[ 4 r_a^j p_a^j - r_a^j p_a^j \phi^j - r_a^j p_a^j \phi^j \right]. \]

Using this identity, we express $P_{L3}^{sym}$ as a sum of the $L = 1$, $L = 2$, and $L = 3$ parts,
\[ P_{L3}^{sym}(k) = P_{L3,1}^{sym}(k) + P_{L3,2}^{sym}(k) + P_{L3,3}^{sym}(k), \]
where
\[ P_{L3,1}^{sym}(k) = \frac{3k^2}{2} \frac{4}{3} \left( T^{ij} \left| \frac{1}{E - H - k} \right| \frac{1}{3P^o} \right) \langle T^{ij} \rangle, \]
\[ P_{L3,2}^{sym}(k) = \frac{3k^2}{2} \frac{6}{5} \left( T^{ijk} \left| \frac{1}{E - H - k} \right| \frac{1}{3P^o} \right) \langle T^{ijk} \rangle, \]
\[ P_{L3,3}^{sym}(k) = \frac{3k^2}{2} \frac{1}{5} \left( T^{ijk} \left| \frac{1}{E - H - k} \right| \frac{1}{3P^o} \right) \langle T^{ijk} \rangle. \]

Wave functions of the different symmetries in Cartesian coordinates required in this work are summarised in Appendix D.

C. Numerical details

Numerical evaluation of the relativistic corrections to the Bethe logarithm was performed according to Eqs. (14), (20), and (27). The general scheme of the computation was similar to the one developed in our previous calculation of the helium fine structure [23] (as described in Sec. V.E of that work). Numerical cancelations, however, were much larger in the present work, because of a greater number of asymptotic expansion terms that needed to be separated out.

The low-energy part of the $k$ integral, $k \in (0, K)$ with $K = 10–100$, was evaluated analytically after diagonalizing the matrix representation of the Schrödinger Hamiltonian. In order to perform the high-energy part of the integral, $k \in (K, \infty)$, we calculated the integrand for several hundreds different values of $k \in (5, 10000)$, subtracted the contributions of the known asymptotic expansion coefficients, fitted the residual, and calculated
the integral analytically. For fitting of the subtracted integrands \( w_L \),

\[
  w_{L1}(k) = k P_{L1}(k) - A_1 - \frac{B_1}{\sqrt{k}} - \frac{C_1 \ln k}{k} - \frac{D_1}{k},
\]

\[
  w_{L2}(k) = k P_{L2}(k) - A_2 - \frac{B_2}{\sqrt{k}} - \frac{C_2 \ln k}{k} - \frac{D_2}{k},
\]

\[
  w_{L3}(k) = k P_{L3}(k) - G_3 k^2 - F_3 k
\]

\[
- A_3 - \frac{B_3}{\sqrt{k}} - \frac{C_3 \ln k}{k} - \frac{D_3}{k},
\]

we assumed the following functional forms of their large-\( k \) expansion [27],

\[
  w_{L1}(k) = \frac{1}{k} \sum_{m=1}^M \sum_{n=0}^m c_{m,n} \ln^n k, 
\]

\[
  w_{L2,3}(k) = \frac{1}{k} \sum_{m=1}^M d_{m,2} \sqrt{k} + d_{m,1} \ln k + d_{m,0},
\]

where \( c_{i,j} \) and \( d_{i,j} \) are fitting coefficients. In order to ensure the stability of the fitting, high numerical accuracy of the integrand \( P_{L}(k) \) was required, typically 10-12 significant digits.

Such accuracy turned out to be difficult to reach for the perturbed wave function part of the Breit correction for the \( 2^1P \) state. The reason for this is the logarithmic singularity [27] of the perturbed wave function \( \delta \phi \) for the \( 2^1S \) state. The reason for this is the logarithmic singularity present in the integral analytically. For fitting of the subtracted integrands \( w_L \),

\[
  \delta \phi = \frac{1}{(E - H)} H_A^{(4)} \phi.
\]

In order to ensure good convergence of numerical results for \( \delta \phi \) we had to choose the basis for the propagator very carefully. It was constructed as follows. We start by variationally optimizing two symmetric second-order corrections,

\[
  \delta_1 E = \left\langle H_A^{(4)} \frac{1}{(E - H)} H_A^{(4)} \right\rangle,
\]

\[
  \delta_2 E = \left\langle P^2 \frac{1}{(E - H)} P^2 \right\rangle.
\]

The form of \( \delta_2 E \) is suggested by the expression for the leading asymptotic constant \( A_1 \), Eq. (A2). In order to account for the logarithmic singularity present in \( \delta_1 E \), we exploit the flexibility of our exponential basis functions (38) and emulate the singularity by allowing the nonlinear parameters to be very large. In order to effectively span large regions of nonlinear parameters, we used a non-uniform distribution of nonlinear parameters \( \alpha_i, \beta_i \), and \( \gamma_i \) introduced in Ref. [33], typically,

\[
  \alpha_i = A_1 + (1/t^3 - 1) A_2,
\]

where the variable \( t_i \) has a uniform quasirandom distribution over the interval (0,1), and \( A_1 \) and \( A_2 \) are the variational optimization parameters. Finally, we merge the optimized basis sets for \( \delta_1 E \) and \( \delta_2 E \) and use the result for calculating the perturbed wave function \( \delta \phi \). Nonetheless, a large number of basis functions (\( N = 3000-5000 \)) were required in order to reach the desired accuracy.

### Table I. Numerical results for the relativistic corrections to the Bethe logarithm and asymptotic expansion constants for the \( 2^1S \) and \( 2^3P \) (centroid) states of helium, in atomic units.

| Term       | \( 2^1S \)       | \( 2^3P \)       |
|------------|------------------|------------------|
| \( A_1 \)  | \(-33.989031782 \) (2) | \(-31.9756564 \) |
| \( A_1 \)  | \(-132.15824269 \) (5) | \(-127.4984939 \) (9) |
| \( E_L \)  | \(-45.129135 \) (35) | \(-41.7175 \) (40) |
| \( G_3 \)  | \(0.032569625 \) | \(-0.0650153 \) |
| \( F_3 \)  | \(2.121589 \) | \(2.0798359 \) |
| \( A_3 \)  | \(-49.768158 \) | \(-47.453938 \) (3) |
| \( D_4 \)  | \(1175.043968 \) 722 (4) | \(1121.176717 \) 34 (10) |
| \( E_L \)  | \(-1095.0439 \) (3) | \(-1045.214 \) (6) |

### V. RESULTS

Our numerical results for the asymptotic expansion coefficients and the relativistic corrections to the Bethe logarithm are presented in Table I. For the \( 2^1S-2^3P \) transition energy in helium, the total relativistic correction to the Bethe logarithm, \( E_L = E_{L1} + E_{L2} + E_{L3} \), amounts to \( E_L = -4.97433 \) (13) MHz. This can be compared with the estimate of Ref. [25, 34] obtained from the hydrogenic results by rescaling the electron density at the origin. For the \( 2^1S-2^3P \) transition energy, this approximation yields

\[
  E_L(\text{appr}) = \alpha^7 m Z^3 \left[ L(2s) - \frac{1}{3} L(2p_{1/2}) - \frac{2}{3} L(2p_{3/2}) \right] 
\]

\[
\times \left[ \langle \delta^3(r_1) \rangle_{2S} - \langle \delta^3(r_1) \rangle_{2P} \right].
\]

with \( L(2s) = -28.350 \) 965, \( L(2p_{1/2}) = -0.795 \) 650, and \( L(2p_{3/2}) = -0.584517 \) [35, 36]. The corresponding numerical value is \( E_L(\text{appr}) = -3.7 \) (0.9) MHz, where we assumed a 25\% uncertainty, like in Ref. [25].

A complete treatment of the \( \alpha^7 m \) correction requires calculations of the two remaining terms in Eq. (1), which will be addressed to in our future investigations. The numerical contribution of these terms is expected to be comparable to that of \( E_L \). In particular, for the \( 2^1S-2^3P \) transition energy in helium, the hydrogenic approximation for the remaining contribution yields \(-4.3 \) (1.1) MHz.

In summary, in this work we report calculations of the relativistic corrections to the Bethe logarithm for the \( 2^1S \) and \( 2^3P \) states of helium. This is the first step on the path to calculating the complete QED contribution of order \( \alpha^7 m \) to the triplet states of helium. Being the most numerically demanding part, the calculation of the relativistic corrections to the Bethe logarithm indicates the feasibility of the whole \( \alpha^7 m \) project.
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Appendix A: Asymptotic coefficients of $P_{L,1}$

Here we derive the coefficients $A_1$, $B_1$, $C_1$, and $D_1$ of the large-$k$ expansion of $P_{L,1}$ given by Eq. (12). There are contributions coming from both the low-energy and the high-energy regions of the virtual photon momenta. Individually, the low- and the high-energy parts may contain divergences, which are regularized by working in $d$ dimensions and are canceled when both parts are added together.

\[
D^L_{1a} = -2 Z \left\langle H_A^{(4)} \frac{1}{(E-H)^2} \left( \frac{Z}{r_1} \frac{\nabla_1}{r_1} + \frac{Z}{r_2} \frac{\nabla_2}{r_2} \right) \right\rangle + E^{(4)} \left( \frac{2}{r} \right) - 4E \]

\[
+ \left\langle \left( \frac{Z}{r_1} \right) \left( E + \left[ \frac{Z}{r_1} + \frac{Z}{r_2} \right] - \frac{1}{r} \right)^2 + \frac{1}{4} \left[ \frac{Z^2}{r_1^2} \right] - \frac{1}{2} \frac{p_1^2}{r_1} \frac{Z}{r_1} p_2^2 \right. \]

\[
\left. + \left( 2E - \frac{2}{r_2} + \left( \frac{1}{r} \right) \right) \pi Z \delta^{(3)}(r_1) + p_1 \left( \frac{Z}{r_1} \left( \frac{\delta^{(3)}(r_1)}{r} + \frac{p_1^2}{r^3} \right) + (1 \leftrightarrow 2) \right) \right\rangle. \tag{A4}
\]

Here, $[Z/r_1]_e$ is the $d$-dimensional form of the Coulomb potential (for details see [20]). The terms $[(Z/r_1)^3]_e$ and $[Z^2/r_1^4]_e$ contain singularities which will be canceled when combined with corresponding terms coming from the high-energy part. Term $D^L_{1b}$ is evaluated as

\[
D^L_{1b} = \left\langle - \left( E + \frac{Z^2 - 1}{r_2} - \frac{p_2^2}{2} \right) \pi Z \delta^{(3)}(r_1) \right. \]

\[
\left. + \frac{Z}{2} \frac{p_1}{p_2} \pi \delta^{(3)}(r_1) p_1 + (1 \leftrightarrow 2) \right\rangle. \tag{A5}
\]

The low-energy part can be derived by performing a direct large-$k$ expansion of the expression

\[
\delta \left\langle P_i \frac{k}{E-H-k} P^j \right\rangle, \tag{A1}
\]

where $\delta$ denotes the first-order perturbation of the matrix element by Breit Hamiltonian $H^{(4)}$. The coefficient $A_1$ from Eq. (12) comes from the perturbation of the reference-state wave function,

\[
A_1 = -2 \left\langle H^{(4)} \frac{1}{(E-H)^2} P^2 \right\rangle \tag{A2}
\]

\[
= -2 \left\langle H^{(4)} \frac{1}{(E-H)^2} P^2 \right\rangle + 2 \left\langle [Q - \langle Q \rangle] P^2 \right\rangle.
\]

The low-energy part of the coefficient $D_1$ is

\[
D^L_1 = \delta \left\langle P^i (H - E) P^j \right\rangle
\]

\[
= \left\langle H^{(4)} \frac{1}{(E-H)^2} [P^i, [V, P^j]] \right\rangle + \frac{1}{2} \left\langle [P^i, [H^{(4)}, P^j]] \right\rangle
\]

\[
= D^{L1a} + D^{L1b}. \tag{A3}
\]

The second-order term $D^{L1a}$ is singular. We employ the regularized form of the Breit Hamiltonian $H_A^{(4)}$, Eq. (28), in order to move singularities into first-order terms and use the dimensional regularization in order to handle the remaining divergences. The result is

\[
D^{L1a} = \sqrt{2} Z^2 \left\langle \pi \left[ \delta^{(3)}(r_1) + \delta^{(3)}(r_2) \right] \right\rangle. \tag{A6}
\]

The Breit correction to the forward-scattering three-photon exchange diagram contains both the coefficient $C_1$ and the high-energy part of the coefficient $D_1$.

\[
C_1 = Z^3 \left\langle \pi \left[ \delta^{(3)}(r_1) + \delta^{(3)}(r_2) \right] \right\rangle, \tag{A7}
\]
and
\[ D^H_1 = Z^3 \langle \pi [\delta^{(d)}(r_1) + \delta^{(d)}(r_2)] \rangle \left(-8 - \frac{1}{2\epsilon} + 9 \ln 2\right). \]  
(A8)

Finally, the coefficient \(D_1\) is the sum of the low-energy part \(D_1^L\) and the high-energy part \(D_1^H\). Making use of the identity
\[
\left[ Z^2 \frac{r_1^2}{r_1^4} \right] = -2 \left[ Z^3 \frac{r_1^2}{r_1^4} \right] + \frac{Z^2}{r_1} \frac{p_1^2}{r_1^3} \frac{p_1}{r_1} + \frac{Z^2}{r_1} \frac{r_1}{r_1^3},
\]
(A9)
we write the result as
\[
D_1 = -2 Z \left\langle \frac{H^{(4)}}{E - H} \right\rangle \left( \frac{\hat{r}_1}{r_1^3} + \frac{\hat{r}_2}{r_2^3} \cdot \nabla \right) + E^{(4)} \left( \frac{\dot{\theta}}{r} \right) - 4E
\]
\[
+ \left( \frac{Z}{2} \frac{p_1}{p_1^2} \pi \delta^{(3)}(r_1) \hat{p}_1 + \frac{Z}{r_1} (E - V)^2 - \frac{X_1}{2} - \frac{1}{2} \frac{p_1^2}{r_1^2} \frac{Z}{r_1^3} + \frac{p_1}{r_1} \left( \frac{\delta_{ij}}{r} + \frac{r_{ij}}{r^3} \right) \right) \hat{p}_2
\]
\[
+ \left[ E - \frac{Z + \frac{1}{r_2} + \frac{p_2^2}{2}}{r} + \frac{1}{r} \right] Z^2 \left(-7 + 9 \ln 2\right) \pi Z \delta^{(3)}(r_1) + (1 \leftrightarrow 2) \right\rangle,
\]
(A10)

where
\[
\left\langle \left[ \frac{Z^3}{r_1^2} \right] \right\rangle = \left\langle \frac{1}{r_1^2} \right\rangle + Z^3 \langle \pi \delta^{(d)}(r_1) \rangle \left( \frac{1}{r} + 2 \right),
\]
(A11)
\[
\left\langle \frac{1}{r_1^2} \right\rangle = \lim_{\alpha \rightarrow 0} \left\langle \Theta(r_1 - a) \right\rangle + 4 \pi \delta^{(3)}(r_1) \left( \gamma + \ln \alpha \right),
\]
(A12)
\[
X_1 = \frac{Z^2}{r_1^4} \left( E - V - \frac{p_2^2}{2} \right) - \frac{1}{2} \hat{p}_1 Z^2 \frac{r_1}{r_1^3}.
\]
(A13)

Appendix B: Asymptotic coefficients of \(P_{L2}\)

Here we derive the coefficients \(A_2\), \(B_2\), \(C_2\), and \(D_2\) of the large-\(k\) expansion of \(P_{L2}\) given by Eq. (18).

Low-energy part

First we examine contributions coming from the region of low virtual photon momenta. The coefficient \(A_2\) is the leading-order term of the direct large-\(k\) expansion of Eq. (17), with the result
\[
A_2 = \frac{1}{2} \left\langle 4 (E - V)^2 - 2 p_1^2 p_2^2 + 2 (E - V) p_1 \cdot p_2 + \frac{\delta_{ij}}{r} + \frac{r_{ij}}{r^3} \right\rangle \left(p_1^2 + p_2^2\right). \tag{B1}
\]

The low-energy part of the coefficient \(D_2\) is
\[ D^L_2 = \langle \phi | \delta_{jj} (H - E) j^j | \phi \rangle \]
\[ = \left\langle \frac{1}{2} \left[ \delta_{ij} \left( -\frac{Z}{r_1} + \frac{Z}{r_2} \right) , j^j \right] \right\rangle = D^L_{2a} + D^L_{2b}. \tag{B2}
\]

Individual terms are
\[ D^L_{2a} = \left\langle \frac{1}{4} \left[ (p_1^2 + p_2^2)^2, \left[ \frac{Z}{r_1} + \frac{Z}{r_2} \right], j^j \right] \right\rangle \]
\[ = \left\langle \left[ -2 \left( E + \frac{Z - 1}{r_2} \right) - p_1^2 \pi Z \delta^{(3)}(r_1) \right] \right\rangle - \frac{1}{2} \hat{p}_1 \frac{Z^2}{r_1} \frac{r_1}{r_1} + \left[ \frac{Z}{r_1} \right] \left( \frac{E + \frac{1}{r} + \frac{Z}{r_1} + \frac{Z}{r_2}}{r} \right) - \frac{1}{2} \frac{p_1^2}{r_1^3} \frac{Z^2}{r_1} + \frac{1}{2} \frac{Z}{r_1^3} \frac{r_1}{r_1} \right\rangle + \frac{1}{4} \frac{Z}{r_2} \delta^{(3)}(r_1) + (1 \leftrightarrow 2) \right\rangle, \tag{B3}
\]
and
\[ D^L_{2b} = \left\langle \frac{1}{3} \left[ \left( \frac{r_{ij}}{r^3} \right) \left( p_1^2 + p_2^2 \right), \left[ \frac{Z}{r_1} + \frac{Z}{r_2} \right], j^j \right] \right\rangle \]
\[ = \left\langle \frac{1}{3} \left( \frac{r_{ij}}{r^3} \right) \left( 3r^2_{ij} + \delta_{ij} r^2 \right) \right\rangle - \frac{4 \pi}{3} \frac{Z}{r_2} \delta^{(3)}(r_1) + (1 \leftrightarrow 2) \right\rangle. \tag{B4}
\]

High-energy part

Now we turn to contributions induced by high momenta of virtual photons. The coefficient \(B_2\) comes from the forward-scattering two-photon exchange perturbed by \(\delta_{ij}\) and can be evaluated to yield
\[ B_2 = -Z^2 \sqrt{2} \left( 4 \pi \left[ \delta^{(3)}(r_1) + \delta^{(3)}(r_2) \right] \right). \tag{B5}
\]

Similarly to the case of \(P_{L1}\), the coefficient \(C_2\) and the high-energy part of \(D_2\) are obtained from the forward scattering three-photon exchange with additional \(\delta_{ij}\) and \(j^j\) vertices,
\[ \delta^2(0) \int \frac{d^4 q_1^2}{(2\pi)^d} \frac{d^4 q_2^2}{(2\pi)^d} \],
\[ \times \left( \frac{-4\pi Z}{q_1^2} \right) \left( \frac{-4\pi Z}{q_2^2} \right) \left( \frac{-4\pi Z}{(q_1 - q_2)^2} \right) \left( \frac{2}{q_1^2} \right) \left( \frac{2}{q_2^2} \right) \]

\[ \times \left[ \left( \frac{-1}{q_1^2 + k} \left( \frac{2}{q_1^2 + k} \right) - \frac{q_2^2}{2} \right) - \frac{q_1^2}{2} \left( \frac{2}{q_1^2 + k} \right) \right]. \quad (B6) \]

From this expression, we derive the following results,

\[ C_2 = \frac{Z^3}{2} \langle \delta^3(r_1) + \delta^3(r_2) \rangle, \quad (B7) \]

and

\[ D_2^H = \langle Z^3 \pi \left[ \delta^3(r_1) + \delta^3(r_2) \right] \rangle \left( 8 - \frac{1}{\epsilon} - 6 \ln 2 \right). \quad (B8) \]

The total coefficient \( D_2 \) is then the sum of the corresponding low-energy and high-energy parts,

\[ D_2 = \left( \frac{Z}{4} \right) \left( \frac{E}{r} + \frac{r^3}{r^3} \right) \left( \frac{3r_1 r_2 - \delta^3(r)}{r^3} \right) \]

\[ + \left( \sqrt{E} + 2Z \frac{5 - 3 \ln 2}{2} - \frac{r^3}{2} \right) 4\pi Z \delta^3(r_1) \]

\[ + X_1 + \frac{Z r_1}{2 r_1} \frac{r}{r^3} + (1 \leftrightarrow 2) \right). \quad (B9) \]

**Appendix C: Asymptotic coefficients of \( P_{L3} \)**

We now turn to the derivation of the coefficients \( G_3 \), \( F_3 \), \( A_3 \), \( B_3 \), \( C_3 \), and \( D_3 \) of the large-\( k \) expansion of \( P_{L3} \) given by Eq. (25), which is the most complicated part.

**Low-energy part**

In order to derive contributions coming from the low photon momenta, we first make a large-\( k \) expansion of the propagator \( 1/(E - H - k) \) in Eq. (22). In the obtained expression, we then make a small-\( k \) expansion and keep the \( k^2 \) contribution.

Using the angular average identity in \( d \) dimensions (with \( \hat{k} = \vec{k} / k \))

\[ \int \frac{d\Omega_k}{4\pi} \hat{k}^m \hat{k}^n (\delta_{ij} - \hat{k}^i \hat{k}^j) \]

\[ = \frac{1}{d(d + 1)} \left[ (d + 1) \delta_{ij} \delta^{mn} - \delta^{im} \delta^{jn} - \delta^{jn} \delta^{im} \right], \quad (C1) \]

we get

\[ G_3 = -\frac{3}{2} \sum_{a,b=1,2} \int \frac{d\Omega_k}{4\pi} \left( \delta_{ij} - \hat{k}^i \hat{k}^j \right) \delta_{k^2} (p^a e^{-i\vec{k} \cdot \vec{r} - \vec{r}^2}) p^b \]

\[ = \frac{1}{5} \left( p^i \left( 2\delta^{ij} r^2 - r^i r^j \right) p^j \right), \quad (C2) \]

where the symbol \( \delta_{k^2} \) stands for performing a small-\( k \) expansion and taking the coefficient at the \( k^2 \) term.

Analogously, the next coefficient \( F_3 \) is obtained as

\[ F_3 = \frac{3}{2} \sum_{a,b=1,2} \int \frac{d\Omega_k}{4\pi} (\delta_{ij} - \hat{k}^i \hat{k}^j) \]

\[ \times \delta_{k^2} (p^a e^{-i\vec{k} \cdot \vec{r} - \vec{r}^2}) \left( H - E \right) p^b e^{-i\vec{k} \cdot \vec{r}} \]

\[ = \left( E - V - \frac{1}{5r} \right). \quad (C3) \]

Furthermore,

\[ A_3 = -\frac{3}{2} \sum_{a,b=1,2} \int \frac{d\Omega_k}{4\pi} (\delta_{ij} - \hat{k}^i \hat{k}^j) \]

\[ \times \delta_{k^2} (p^a e^{-i\vec{k} \cdot \vec{r} - \vec{r}^2}) \left( H - E \right)^2 p^b e^{-i\vec{k} \cdot \vec{r}} \]

\[ = \frac{1}{10} \left( \frac{Z}{2} \right) \left( \frac{r_1 \cdot r_2}{r_1^2 r_2^2} \right) \left( \frac{E - V}{r_1^2 r_2^2} \right) - \frac{2}{r^2} \]

\[ - \frac{5}{4} \left( E - V \right) - 6 \left( p_1 \cdot p_2 \right)^2 + 6 p_1^2 p_2^2 \]

\[ + \left( p_1^2 \left( \frac{Z r_1}{r_1} - \frac{r_1^3}{r^3} \right) (3 \delta^{ik} r^k + 3 \delta^{ij} r^k - 2 \delta^{jk} r^k) p_2^2 \right) \]

\[ + 2 \frac{Z r_1}{r_1} \frac{r^3}{r^3} - 2 \pi Z \delta^3(r_1) + (1 \leftrightarrow 2) \right). \quad (C4) \]

The low-energy part of the coefficient \( D_3 \) is the most complicated term and thus will be discussed in some detail. The starting expression is

\[ D_3^L = \frac{3}{2} \sum_{a,b=1,2} \int \frac{d\Omega_k}{4\pi} (\delta_{ij} - \hat{k}^i \hat{k}^j) \]

\[ \times \delta_{k^2} (p^a e^{-i\vec{k} \cdot \vec{r} - \vec{r}^2}) \left( H - E \right) \left( H - E \right) p^b e^{-i\vec{k} \cdot \vec{r}} \]. \quad (C5) \]

It is convenient to split the above expression into two parts, with \( a = b \) and \( a \neq b \). The first part can be evaluated with help of the identity

\[ e^{-i\vec{k} \cdot \vec{r}} f(p) e^{i\vec{k} \cdot \vec{r}} = f(p + k). \quad (C6) \]

We obtain

\[ D_3^{L_{ab}} = \frac{3}{2} \sum_{a=1,2} \int \frac{d\Omega_k}{4\pi} (\delta_{ij} - \hat{k}^i \hat{k}^j) \]

\[ \times \delta_{k^2} (p^a \left( H - E \right) \left( H - E \right)^3 p^b \]. \quad (C7) \]

After straightforward but tedious manipulations that involve expanding the matrix element in small \( k \) and retaining the coefficient in front of \( k^2 \) and using identities

\[ \left[ \frac{Z^2}{r_1^2} \right] = \frac{Z r_1}{r_1^2} = \frac{Z r_1}{r_1^2} + \frac{Z r_1}{r_1^2} \]

\[ + \frac{1}{2} \frac{Z r_1}{r_1^2} \]

\[ = \frac{Z^2}{r_1^2} - 3 \frac{Z r_1}{r_1^3} + \frac{1}{2} \frac{Z r_1}{r_1^2} \]

\[ + \frac{3}{2} \frac{Z r_1}{r_1^2} \]

\[ = \frac{Z^2}{r_1^2} - 3 \frac{Z r_1}{r_1^3} + \frac{1}{2} \frac{Z r_1}{r_1^2} \]

\[ + \frac{3}{2} \frac{Z r_1}{r_1^2} \]
\[ + \frac{1}{4} P^i P^j \frac{3 \delta_{ij} r^2 - \delta_{ij} r^2}{r^5} + \frac{1}{2} p_i^l [p_i^l, [V, p_i^l]] p_i = \left( E + \frac{Z}{r_2} - \frac{p_2^l}{2} \right) 4\pi Z \delta^{(3)}(r_1), \tag{C8} \]

as well as Eq. (A9), we arrive at

\[ D_{3a}^L = \frac{3}{2} \sum \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \delta_{\vec{k}\vec{k}} \left\langle \left[ p_1^i e^{-i\vec{k}\cdot\vec{r}}, \left( H - E \right)^3 \left( p_2^i e^{i\vec{k}\cdot\vec{r}} \right) \right] \right\rangle + (1 \leftrightarrow 2) \]

\[ = \frac{3}{4} \sum \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, H - E], \left[ H - E, \left[ H - E, p_2^i e^{i\vec{k}\cdot\vec{r}} \right] \right] \right] \right\rangle + (1 \leftrightarrow 2) = \frac{3}{4} \sum_{m=1.8} T_m. \tag{C10} \]

The second term in Eq. (C5) with \( a \neq b \) is evaluated as

\[ D_{3b}^L = \frac{3}{2} \sum \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \delta_{\vec{k}\vec{k}} \left\langle \left[ p_1^i e^{-i\vec{k}\cdot\vec{r}}, V, \left[ [V, p_2^i e^{i\vec{k}\cdot\vec{r}}] \right] \right] \right\rangle + (1 \leftrightarrow 2) \]

\[ = \frac{3}{4} \sum \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, H - E], \left[ H - E, \left[ H - E, p_2^i e^{i\vec{k}\cdot\vec{r}} \right] \right] \right] \right\rangle + (1 \leftrightarrow 2) = \frac{3}{4} \sum_{m=1.8} T_m. \tag{C10} \]

The individual terms \( T_i \) are calculated as follows:

\[ T_1 = \int \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \times \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, V], \left[ [V, p_2^i e^{i\vec{k}\cdot\vec{r}}] \right] \right] \right\rangle + (1 \leftrightarrow 2) = 0, \tag{C11} \]

\[ T_2 = \int \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \times \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, V], \left[ [V, p_2^i e^{i\vec{k}\cdot\vec{r}}] \right] \right] \right\rangle + (1 \leftrightarrow 2) \]

\[ = \frac{2}{15} \left( \frac{Z r_1^2}{r_1^2} - \frac{Z r_2^2}{r_2^2} \right) \frac{r}{r^3} \left( \frac{r^2}{r^2} \right), \tag{C12} \]

\[ T_3 = \int \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \times \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, V], \left[ [V, p_2^i e^{i\vec{k}\cdot\vec{r}}] \right] \right] \right\rangle + (1 \leftrightarrow 2) = 0, \tag{C13} \]

\[ T_4 = \int \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \times \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, V], \left[ [V, p_2^i e^{i\vec{k}\cdot\vec{r}}] \right] \right] \right\rangle + (1 \leftrightarrow 2) \]

\[ = \frac{4}{15} \left( \frac{Z r_1^2}{r^2} - \frac{Z r_2^2}{r^2} \right) \frac{r^2}{r^2} \left( \frac{r^2}{r^2} \right) + 3 \left( \frac{Z r_1^2}{r^2} \right) \frac{r}{r^3}, \tag{C14} \]

\[ T_5 = \int \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \times \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, V], \left[ [V, p_2^i e^{i\vec{k}\cdot\vec{r}}] \right] \right] \right\rangle + (1 \leftrightarrow 2) \]

\[ = -\frac{16}{45} \frac{\vec{p}}{4\pi} \delta^{(3)}(r) \vec{b} + \frac{2 \pi^P P_j}{15} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \]

\[ = -\frac{4}{15} \vec{p} \left( \frac{r^2}{r^3} - \frac{3 r^2}{r^2} \right) \vec{p}^j, \tag{C15} \]

where \( p^i = \frac{1}{2} (p_i^1 - p_i^2) \),

\[ T_6 = \int \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \times \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, V], \left[ [V, p_2^i e^{i\vec{k}\cdot\vec{r}}] \right] \right] \right\rangle + (1 \leftrightarrow 2) \]

\[ = -\frac{4}{45} \vec{p} \delta^{(3)}(r) \vec{b} + \frac{2 \pi^P P_j}{15} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \]

\[ = \frac{8}{15} \vec{p} \left( \frac{r^2}{r^3} - \frac{3 r^2}{r^2} \right) \vec{p}^j, \tag{C16} \]

\[ T_7 = \int \frac{d\Omega_k}{4\pi} \left( \delta^{ij} - \delta^{ij}_{\vec{k}\vec{k}} \right) \times \delta_{\vec{k}\vec{k}} \left\langle \left[ [p_1^i e^{-i\vec{k}\cdot\vec{r}}, p_2^j e^{i\vec{k}\cdot\vec{r}}], \left[ [V, p_2^i e^{i\vec{k}\cdot\vec{r}}] \right] \right] \right\rangle + (1 \leftrightarrow 2) \]
\[ D^L_3 = 3 \left\langle \frac{1}{3} p^i \left( \frac{\delta^{ij}}{r^3} - 3 \frac{r^i r^j}{r^5} \right) p^j - \frac{23}{90} \tilde{p}^i 4\pi \delta^{(3)}(r) \tilde{p}^j + \frac{37}{30} \frac{1}{r^4} \delta^{ij} \right\rangle \]

\[ + \frac{1}{10} \tilde{p}^i 4\pi Z \delta^{(3)}(r_1) \tilde{p}^j - \frac{61}{30} \frac{Z r_1 \cdot \vec{F}}{r_1^3} + \frac{4}{3} \frac{p_1^2 Z^2}{r_1^2} + \frac{4}{15} Z \left( \frac{\delta^{ij}}{r_1^3} - 3 \frac{r^i r^j}{r_1^5} \right) \]

\[ + \left[ \frac{7}{15} \left( E + \frac{Z}{r_2} - \frac{p_2^2}{2} \right) - \frac{23}{45} Z \right] \left( \frac{2}{3} \frac{\pi Z}{90} + 103 \right) \right\rangle . \]

\[ \text{High-energy part} \]

The coefficient \( B_3 \) comes from the corresponding forward-scattering two-photon exchange diagram,

\[ B_3 = \frac{3k \sqrt{k}}{2} \int \frac{d^4 \Omega_k}{4\pi} \delta_{k^2} \phi^2(0) \int \frac{d^4 p}{(2\pi)^4} \left[ -4\pi Z \alpha \right]^2 \left( \frac{2}{p^2} \right)^2 \]

\[ \times p^i \left( \frac{r^3}{p^2} - 3 \frac{r^i r^j}{p^4} \right) p^j = 2 \sqrt{Z^2} \left( 4\pi \left[ \delta^3(r_1) + \delta^3(r_2) \right] \right) . \]

Similarly, the analogous forward-scattering three-photon exchange diagram gives rise to the coefficient \( C_3 \),

\[ C_3 = -2 Z^3 \left( 4\pi \left[ \delta^3(r_1) + \delta^3(r_2) \right] \right) , \]

and the high-energy part of the coefficient \( D_3 \),

\[ D^H_3 = Z^3 \left( 4\pi \left[ \delta^3(r_1) + \delta^3(r_2) \right] \right) \]

we express the final result for \( D_3 \) as

\[ D_3 = \frac{1}{5} \left\langle -3 \tilde{p}^i 4\pi \delta^{(3)}(r) \tilde{p}^j + \frac{16}{r^4} + 2 Z \left( \frac{\delta^{ij}}{r^3} - 3 \frac{r^i r^j}{r^5} \right) \frac{r^i r^j}{r_1^3} - 20 X_1 + \frac{3}{4} \tilde{p}^i 4\pi Z \delta^{(3)}(r_1) \tilde{p}^j - 14 \frac{Z r_1}{r_1^3} \cdot \vec{r} \]

\[ + \left( 7E \right) \left( \frac{2}{2} + \frac{7Z}{6} \right) - 23 \frac{1}{6} \frac{r_2}{r_2} - \frac{7}{4} \frac{p_2^2}{Z^2} - 83 Z^2 \frac{\ln 2}{4} \right\rangle \]

\[ \left( 4\pi Z \delta^{(3)}(r_1) + (1 \leftrightarrow 2) \right) . \]

The operator \( \tilde{p}_1 4\pi Z \delta^{(3)}(r_1) \tilde{p}_1 \) requires some clarifications, because its expectation value is conditionally converging. It should be calculated with the implicit projection into the \( L = 0 \) state between \( \tilde{p}_1 \) operators and this requirement comes from the dimensional regularization.

\[ \text{Appendix D: Wave functions in Cartesian coordinates} \]

Following Schwartz [28], we use the following representations of the wave functions, with \( F = F(r_1, r_2, r) \),
\( G \equiv G(r_1, r_2, r) \), and the upper sign corresponding to the singlet function and the lower sign, to the triplet function,

\[
\phi \left( \frac{1}{3}S^\alpha \right) = F \pm (1 \leftrightarrow 2),
\]

\[
\bar{\phi} \left( \frac{1}{3}P^\alpha \right) = \bar{r}_1 F \pm (1 \leftrightarrow 2),
\]

\[
\bar{\phi} \left( \frac{1}{3}P^\alpha \right) = \bar{r}_1 \times \bar{r}_2 F \pm (1 \leftrightarrow 2),
\]

\[
\phi^{ij} \left( \frac{1}{3}D^\alpha \right) = \left( e^{iab} r_{12}^a r_{12}^b \bar{r}_1 + e^{iab} a b \bar{r}_1 \right) F \pm (1 \leftrightarrow 2),
\]

\[
\phi^{ij} \left( \frac{1}{3}D^\alpha \right) = \left( r_{12}^i r_{12}^j - \frac{1}{3} \delta^{ij} r_{12} \bar{r}_1 \right) G \pm (1 \leftrightarrow 2),
\]

\[
\phi^{ijk} \left( \frac{1}{3}F^\alpha \right) = \left[ r_{12}^i r_{12}^j \bar{r}_1 - \frac{1}{5} r_{12}^2 \left( \delta^{ij} r_{12}^k + \delta^{ik} r_{12}^j + \delta^{jk} r_{12}^i \right) \right] F
\]

\[
+ \frac{1}{3} \left[ r_{12}^i r_{12}^j + r_{12}^j r_{12}^i + \frac{2}{3} \delta^{ij} \bar{r}_1 \bar{r}_2 \right] - \frac{1}{5} \delta^{ij} \left( r_{12}^2 \bar{r}_1 + 2 r_{12} \bar{r}_2 \right)
\]

\[
- \frac{1}{5} \delta^{ik} \left( r_{12}^i \bar{r}_2 + 2 r_{12} \bar{r}_1 \right)
\]

and

\[
\phi^{ijk} \left( \frac{1}{3}F^\alpha \right) = \left[ r_{12}^i r_{12}^j \bar{r}_1 - \frac{1}{5} r_{12}^2 \left( \delta^{ij} r_{12}^k + \delta^{ik} r_{12}^j + \delta^{jk} r_{12}^i \right) \right] F
\]

\[
+ \frac{1}{3} \left[ r_{12}^i r_{12}^j + r_{12}^j r_{12}^i + \frac{2}{3} \delta^{ij} \bar{r}_1 \bar{r}_2 \right] - \frac{1}{5} \delta^{ij} \left( r_{12}^2 \bar{r}_1 + 2 r_{12} \bar{r}_2 \right)
\]

\[
- \frac{1}{5} \delta^{ik} \left( r_{12}^i \bar{r}_2 + 2 r_{12} \bar{r}_1 \right)
\]