Relativistic Bethe logarithm for triplet states of helium-like ions

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Abstract. We report a calculation of relativistic corrections of order \( m\alpha^7 \) to the Bethe logarithm for the \( ^23S \) and \( ^23P \) states of helium-like ions. The calculation is required for improving the accuracy of theoretical energies of helium-like ions and for checking the evaluation of the \( m\alpha^7 \) effects in helium performed in Patkóš et al. (Phys Rev A 103:042809, 2021), where a significant discrepancy with experimental results was found. The large-\( Z \) limit of the relativistic Bethe logarithm is determined numerically, in excellent agreement with the analytical results obtained from the hydrogen theory.

1 Introduction

The dominant contribution to the Lamb shift of an atomic energy level is induced by the electron self-energy. The nonrelativistic part of it was first described by Bethe [1] in terms of the logarithm of the mean excitation energy, which is nowadays called the Bethe logarithm. The Bethe logarithm involves a summation over the complete spectrum of the Schrödinger equation, which is nearly divergent because of large contributions from high-energy continuum states. The calculation of the Bethe logarithm is a relatively straightforward task in the case of hydrogen, because the electron propagator is known analytically. For atoms with more than one electron, the task becomes more challenging. Accurate calculations of the Bethe logarithm for the helium atom have long been considered to be a difficult problem but are presently well established [2,3]. The most accurate results for helium were obtained in Ref. [4] and for helium-like ions in Refs. [2,5].

The Bethe logarithm is a part of the leading QED correction that is of order \( m\alpha^5 \) for light atoms (where \( m \) is the electron mass and \( \alpha \) is the fine-structure constant). At the present level of experimental and theoretical interest, QED effects of higher orders in \( \alpha \) need to be accounted for. One of the dominant effects of order \( m\alpha^7 \) is the relativistic correction to the Bethe logarithm. It appeared first in the hydrogen theory, where it was evaluated in Refs. [6–8]. Later these calculations were extended to the two-center problem [9]. For the helium atom, the relativistic Bethe logarithm was calculated for the fine structure [10–14] and recently for the \( ^23S \) and \( ^23P \) states [15,16]. In the present work, we improve the numerical accuracy for the helium atom and extend calculations to helium-like ions.

This work is in part motivated by the recent observation of a significant discrepancy between theoretical predictions and experimental results for the ionization energies of the triplet \( n = 2 \) states in the helium atom [17,18]. In view of this discrepancy, it is important to cross-check the calculations of the \( m\alpha^7 \) effects reported in Refs. [15–17,19,20]. A way to check calculations for helium is to perform analogous computations for helium-like ions with different values of the nuclear charge number \( Z \) and, by fitting the \( 1/Z \) expansion, determine the large-\( Z \) limit of the corresponding corrections. This limit should agree with analytical results obtained from the hydrogen theory.

The goal of the present work is to compute the relativistic correction to the Bethe logarithm for the \( ^23S \) and \( ^23P \) states of helium-like atoms with \( Z = 2 – 12 \). By studying the \( Z \) dependence of the numerical results, we will determine their high-\( Z \) limit and compare it with the values obtained from the hydrogen theory. This cross-check will test the consistency of the helium calculations with the more established calculations for hydrogen. In addition, the obtained results for the relativistic Bethe logarithm will be later used to improve the accuracy of theoretical predictions for the energy levels of helium-like ions.

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2 Basic formulas

2.1 Nonrelativistic Bethe logarithm

The starting point of the theoretical description is the nonrelativistic Hamiltonian for an atom in the presence of external electromagnetic fields,

\[ \mathcal{H} = \sum_a \frac{\vec{p}_a^2}{2m} + V + e \sum_a \phi(\vec{r}_a) \]  

where \( \vec{p}_a = \vec{p}_a - e \vec{A}(\vec{r}_a) \), \( \phi(\vec{r}_a) \) and \( \vec{A}(\vec{r}_a) \) are the external scalar and vector potentials, respectively,

\[ V = -\sum_a \frac{Z\alpha}{r_a} + \sum_{a<b} \frac{\alpha}{r_{ab}} \]  

and the summation indices \( a \) and \( b \) run over the electrons in the atom.

The nonrelativistic low-energy part of the one-loop electron self-energy is obtained from the Hamiltonian (1) and has the form

\[ E_L(\Lambda) = \frac{e^2}{m^2} \int_{k<\Lambda} \frac{d^3k}{(2\pi)^3/2k} \left( \delta^{ij} - \vec{k}^i \vec{k}^j \right) \times \sum_{ab} \langle \psi | p_a^i e^{ik \cdot r_a} \frac{1}{E - H - k} p_b^j e^{-ik \cdot r_b} | \psi \rangle, \]

where \( \vec{k} = k/k, \Lambda \) is the high-momentum cutoff parameter, and \( H \) and \( E \) are the nonrelativistic Hamiltonian (without the external electromagnetic field) and its eigenvalue, respectively. To the leading order in \( \alpha \), the exponential factors \( e^{ik \cdot r} \) can be neglected. Performing the integration over \( \vec{k} \), we arrive at known formulas for the low-energy contribution of order \( m\alpha^5 \),

\[ E_L^{(5)}(\Lambda) = \frac{2\alpha}{3\pi m^2} \int_0^\Lambda dk P_{nd}(k), \]

\[ P_{nd}(k) = \left\langle \vec{P} \frac{1}{E - H - k} \vec{P} \right\rangle, \]

where \( \vec{P} = \sum_a \vec{p}_a \).

Since \( E_L(\Lambda) \) diverges as \( \Lambda \to \infty \), one obtains the finite result by subtracting the divergent terms of the large-\( \Lambda \) asymptotics and then performing the limit \( \Lambda \to \infty \). The large-\( k \) expansion of \( P_{nd}(k) \) reads as

\[ k P_{nd}(k) = \left\langle \nabla^2 \right\rangle + \frac{1}{k} D + \ldots, \]

where \( \nabla \equiv \sum_a \vec{\nabla}_a \) and \( D = 2\pi Z \left\langle \sum_a \delta^3(r_a) \right\rangle \).

The \( m\alpha^5 \) low-energy contribution is standardly expressed in terms of the Bethe logarithm \( \ln k_0 \), which represents the finite part of Eq. (4) as

\[ \ln k_0 = \left\langle \vec{P} (H - E) \ln[2(H - E)/E_h] \vec{P} \right\rangle - \frac{1}{2D} \int_0^\infty dk \left[ k P_{nd}(k) - \left\langle \nabla^2 \right\rangle - \frac{D}{k} \theta(k - E_h/2) \right], \]

where \( \theta(x) \) is the Heaviside \( \theta \) function, \( \theta(x) = 0 \) for \( x < 0 \) and 1 for \( x \geq 0 \), and \( E_h = m\alpha^2 \) is the Hartree energy.

2.2 Relativistic Bethe logarithm

In the present work, we are interested in the relativistic corrections to the Bethe logarithm. They can be obtained from the Breit Hamiltonian in the presence of external electromagnetic fields. Since we are interested in the center-of-gravity energy levels, it is sufficient to take into account only the spin-independent part of the Breit Hamiltonian. It is given by

\[ \mathcal{H}_{\text{Breit}}^{(4)} = \sum_a \left[ -\frac{\pi_a^4}{8m^3} + \frac{\pi Z\alpha}{2m^2} \delta^3(r_a) \right] + \sum_{a<b} \frac{\pi\alpha}{m^2} \delta^3(r_{ab}) - \frac{\alpha}{2m^2} \pi_a \left( \frac{\delta^{ij}}{r_{ab}} + \frac{r_i^j r_j^i}{r_{ab}^3} \right) \pi_b. \]

From this Hamiltonian, we obtain the relativistic correction to the Bethe logarithm of order \( m\alpha^7 \) as a sum of three parts,

\[ E_L^{(7)}(\Lambda) = E_{L1}(\Lambda) + E_{L2}(\Lambda) + E_{L3}(\Lambda) \]

\[ = \frac{2\alpha}{3\pi m^2} \int_0^\Lambda dk k \left[ P_{L1}(k) + P_{L2}(k) + P_{L3}(k) \right]. \]

The first part is a perturbation of the \( m\alpha^5 \) contribution by the Breit Hamiltonian (without external electromagnetic fields),

\[ P_{L1}(k) = 2 \left\langle \mathcal{H}_{\text{Breit}} \frac{1}{E - H - k} \vec{P} \frac{1}{E - H - k} \vec{P} \right\rangle \]

\[ + \left\langle \vec{P} \frac{1}{E - H - k} \left[ \mathcal{H}_{\text{Breit}} - \langle \mathcal{H}_{\text{Breit}} \rangle \right] \frac{1}{E - H - k} \vec{P} \right\rangle. \]

The second part is induced by the correction to the current,

\[ P_{L2}(k) = 2 \left\langle \delta^j \frac{1}{E - H - k} \vec{P} \right\rangle. \]
The correction to the current \( \delta j^i \) is obtained from the Breit–Pauli Hamiltonian, specifically from the first and fourth terms of Eq. (8), with the result

\[
\delta j^i = -\frac{1}{2m^2} \sum_a p^2_a \sum_a \left( \frac{\delta g^i}{r_{ab}} + r_{ab}^3 \right) p^j_b.
\]

Finally, the third part is the retardation correction induced by the expansion of the exponential functions in Eq. (3),

\[
P_{L3}(k) = \frac{3k^2}{8\pi} \int d\kappa \left( \delta j^i - \kappa^i \kappa^j \right)
\times \left[ \left( \sum_a p^2_a (\kappa \cdot r_a) - \frac{1}{E - H - k} \sum_b (\kappa \cdot r_b) p^j_b \right) - \left( \sum_a p^2_a (\kappa \cdot r_a)^2 - \frac{1}{E - H - k} \sum_b p^j_b \right) \right].
\]

The large-\( k \) expansion of the functions \( P_{Li}(k) \) has the form

\[
k P_{Li}(k) = G_i k^2 + F_i k + A_i + \frac{B_i}{k} + \frac{C_i \ln k}{k} + \frac{D_i}{k} + \ldots,
\]

where the first two coefficients are nonzero only for the \( P_{L3} \) term (i.e., \( G_1 = G_2 = F_1 = F_2 = 0 \)).

The finite parts of the corrections \( E_{Li}(A) \) in Eq. (9) are defined as

\[
E_{Li} = \frac{2\alpha}{3\pi m^2} \int_0^\infty dk \left\{ \frac{k P_{Li}(k) - k^2 G_i - k F_i - A_i}{k} - \frac{B_i}{k} - \left( \frac{C_i \ln k}{k} + \frac{D_i}{k} \right) \theta(k - E_h) \right\}.
\]

For the numerical evaluation, it is convenient to transform the above expression to an equivalent form,

\[
E_{Li} = \frac{2\alpha}{3\pi m^2} \left\{ \int_0^K dk k P_{Li}(k) + \int_K^\infty dk \left[ k P_{Li}(k) - G_i k^2 - F_i k - A_i - \frac{B_i}{k \sqrt{k}} - \frac{C_i \ln k}{k} + D_i \right] - G_i \frac{K^3}{3} - F_i \frac{K^2}{2} - A_i K - 2B \sqrt{K_i}
- \frac{C_i}{2} \ln^2 K - D_i \ln K \right\}
\]

where \( K \geq E_h \) is a free parameter. One can easily show that the result does not depend on the choice of \( K \).

### 3 Regularization

From now on, we will present formulas explicitly for the two-electron atom. We will also use the short-hand notation \( r \equiv r_{12} \).

For the numerical evaluation of the perturbations induced by the Breit Hamiltonian, it is advantageous to transform formulas to a more regular form, which leads to a much better numerical convergence. For the perturbed wave-function part of \( P_{L1} \), we introduce the following (non-Hermitian) regularized Breit operator \( H_{\text{Breit}}' \)

\[
H_{\text{Breit}}' = -\frac{1}{2} (E - V)^2 + \frac{1}{4} \nabla_1^2 \nabla_2^2 - \frac{Z}{4} \frac{\hat{r}_1}{r_1^3} \cdot \nabla_1 - \frac{Z}{4} \frac{\hat{r}_2}{r_2^3} \cdot \nabla_2 - \frac{1}{2} p^1_i \left( \frac{\delta g^i}{r} + \frac{r^i r^j}{r^3} \right) p^j_2.
\]

It can be shown that for any trial function \(|\phi\rangle\), the following identity holds

\[
H_{\text{Breit}}(\phi) = H_{\text{Breit}}'(\phi) + \{ H - E, Q \} |\phi\rangle.
\]

Using the identity (18), we transform the perturbed wave-function part of \( P_{L1} \) to a more regular form as follows

\[
P_{L1,\text{pert}}(k) = 2 \left| H_{\text{Breit}}' \right| \frac{1}{E - H - k} \frac{1}{\tilde{P}} - 2 \left( \langle Q | \langle Q \rangle \right| \frac{1}{E - H - k} \frac{1}{\tilde{P}} \right).
\]

For the vertex part of \( P_{L1} \), we use a more complicated, Hermitian version of the regularized Breit operator,

\[
H_{\text{Breit}}'' = -\frac{1}{2} (E - V)^2 + \frac{1}{4} \nabla_1^2 \nabla_2^2
- \frac{Z}{4} \frac{\hat{r}_1}{r_1^3} \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \tilde{P}_1
- \frac{Z}{4} \frac{\hat{r}_2}{r_2^3} \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \tilde{P}_2
- \frac{1}{2} p^1_i \left( \frac{\delta g^i}{r} + \frac{r^i r^j}{r^3} \right) p^j_2.
\]

For this operator, the following identity holds

\[
H_{\text{Breit}} = H_{\text{Breit}}'' + \{ H - E, Q' \} - \frac{1}{2} (H - E)^2,
\]

where \( Q' = Q - \frac{E}{2} \). Using this identity, we derive the following regularized expression for the vertex part of \( P_{L1} \),
\[ P_{\text{ver}}(k) = \left\langle \vec{P} \right| \frac{1}{E - H - k} \left[ H'_{\text{Breit}} - 2kQ \right. \]
\[ + k\vec{E} - \frac{k^2}{2} - \langle H_{\text{Breit}} \rangle \left. \right| \frac{1}{E - H - k} \vec{P} \right. \]
\[ - \left\langle (2\vec{P} Q + (k - E)\vec{P}) \right| \frac{1}{E - H - k} \vec{P} \right. \]
\[ - \frac{1}{2} \langle \vec{P}^2 \rangle. \] (23)

### 4 Angular reduction

We now turn to performing the angular reduction of the above formulas for the $3S$ and $3P$ states of a two-electron atom. The angular reduction is carried out in Cartesian coordinates. The representation of wave functions in Cartesian coordinates is discussed in detail in Ref. [21].

We start with the nonrelativistic Bethe logarithm. The angular reduction of $P_{\text{nd}}$ for the $3S$ reference state is trivial, since only one angular symmetry ($3P^r$) of intermediate states is allowed. For the $3P$ reference state, we decompose the Cartesian product of the current $j^i \equiv P^i$ and the wave function $\phi^k$ into a sum of irreducible tensors of the rank $L = 0, 1, 2$ as follows

\[ j^i \phi^k = \frac{1}{3} \delta^{ik} \vec{j} \cdot \vec{\phi} + \frac{1}{2} \epsilon_{kl} (\vec{j} \times \vec{\phi})_l \]
\[ + \frac{1}{2} \left[ j^i \phi^k + j^k \phi^i - \frac{2}{3} \delta^{ik} \vec{j} \cdot \vec{\phi} \right]. \] (24)

This decomposition leads to the separation of $P_{\text{nd}}$ into the contributions with $3S$, $3P^r$, and $3D^c$ intermediate states,

\[ P_{\text{nd}}(k) = \frac{1}{3} \left\langle \Psi_0 \right| \frac{1}{E - H - k} \left| \phi \right. \right|_{3S} \Psi_0 \right. \]
\[ + \frac{1}{2} \left\langle \Psi_1 \right| \frac{1}{E - H - k} \left| \phi \right. \right|_{3P^r} \Psi_1 \right. \]
\[ + \frac{1}{4} \left\langle \Psi_2 \right| \frac{1}{E - H - k} \left| \phi \right. \right|_{3D^c} \Psi_2 \right. \] (25)

where $\Psi_0 = \vec{j} \cdot \vec{\phi}$, $\Psi_1 = \vec{j} \times \vec{\phi}$ and $\Psi_2 \equiv j^i \phi^k + j^k \phi^i - \frac{2}{3} \delta^{ik} (\vec{j} \cdot \vec{\phi})$ and the summation over the repeated indices is implicit.

The angular reduction of $P_{L1}$ and $P_{L2}$ follows the same pattern as for the leading contribution $P_{\text{nd}}$. For $P_{L3}$, we need first to perform the angular integration over $k$. It is carried out with help of the following formulas

\[ \int \frac{d^4 k}{4\pi} \left( \delta^{ij} - k^i k^j \right) = \frac{1}{3} \delta^{ij}, \]
\[ \int \frac{d^4 k}{4\pi} \left( k^i k^j k^k k^l \right) = \frac{1}{15} \left( \delta^{ij} \delta^{kl} + \delta^{il} \delta^{jk} + \delta^{ik} \delta^{jl} \right), \] (26)

\[ \int \frac{d^4 k}{4\pi} \left( k^i \delta^{jk} \right) = \frac{1}{3} \delta^{ij}, \]
\[ \int \frac{d^4 k}{4\pi} \left( k^i k^j k^k k^l \right) = \frac{1}{15} \left( \delta^{ij} \delta^{kl} + \delta^{il} \delta^{jk} + \delta^{ik} \delta^{jl} \right). \] (27)

Performing the angular integration and using the fact that $\vec{L} = \vec{r}_1 \times \vec{p}_1 + \vec{r}_2 \times \vec{p}_2$ is the angular momentum operator commuting with $\vec{H}$, we obtain

\[ P_{L3}(k) = \frac{k^2}{10} \left[ 3 \left( \left\langle p_1^i r_1^j + p_2^i r_2^j \right\rangle^{(2)} \left( \frac{1}{E - H - k} \left( r_1^i p_1^j + r_2^i p_2^j \right) \right)^{(2)} \right) \right. \]
\[ - \frac{5}{2k} \left( \vec{L}^2 \right) - 2 \left( \left\langle p_1^i \left( 2 \delta^{ij} r_1^k - r_1^i r_2^k \right) \right\rangle \left( \frac{1}{E - H - k} \left( p_1^i + p_2^i \right) \right) \right), \] (28)

where $(a^i b^j)^{(2)} = (a^i b^j + a^j b^i)/2 - (\vec{a} \cdot \vec{b}) \delta^{ij}/3$.

The angular reduction of the last term in Eq. (28) is exactly the same as for $P_{\text{nd}}$, $P_{L1}$ and $P_{L2}$. Let us now consider the angular reduction of the first term in Eq. (28), which will be referred to as the symmetric part $P_{L3}^{\text{sym}}$. In the case of the $3S$ reference state, there is a single angular-symmetry contribution of the $3D^c$ type in the resolvent. The result reads

\[ P_{L3}^{\text{sym}}(k) = \frac{3k^2}{40} \left\langle \Psi_2 \right| \frac{1}{E - H - k} \left| \phi \right. \right|_{3D^c} \Psi_2 \right. \] (29)

where

\[ \left| \Psi_2 \right\rangle = \left( r_1^i p_1^k + r_1^k p_1^i - \frac{2}{3} \delta^{ik} r_1^j p_1^j \right) \left( r_2^i p_2^k + r_2^k p_2^i - \frac{2}{3} \delta^{ik} r_2^j p_2^j \right) \right| \phi \rangle. \] (30)

In order to perform the angular reduction of the symmetric part for the $3P$ state, we use the following identity:

\[ \frac{1}{2} \sum_a \left( r_a^i p_a^k + r_a^k p_a^i \right) \phi^k = T^{ijk} + \epsilon^{ikl} T^{lj} + \epsilon^{jkl} T^{li} \]
\[ + \delta^{ik} T^j + \delta^{jk} T^i + \delta^{ij} T^{lk}, \] (31)

where $T^i$, $T^{ij}$, and $T^{ijk}$ are the irreducible Cartesian tensors of the first, second, and third rank, respectively.

\[ T^{ijk} = \sum_a \left( r_a^i p_a^k \phi^k \right)^{(3)}, \] (32)

\[ T^{ij} = \frac{1}{12} \sum_a \left[ \epsilon^{ilm} \left( r_a^i p_a^l + r_a^l p_a^i \right) \phi^m + \epsilon^{ilm} \left( r_a^i p_a^l + r_a^l p_a^i \right) \phi^m \right], \] (33)

\[ T^i = \frac{1}{20} \sum_a \left[ 3 \left( r_a^i p_a^l + r_a^l p_a^i \right) \phi^l - 2 r_a^l p_a^l \phi^l \right], \] (34)
\[ T'^i = \frac{1}{10} \sum_a \left[ 4r_a^l p_a^l \phi^l - r_a^l p_a^l \phi^l - r_a^l p_a^l \phi^l \right]. \] (35)

Every \( T \) is a symmetric and traceless tensor. One does not need the explicit form of \( T^{ijk} \) because when projected onto the state with \( L = 3 \), it automatically becomes irreducible, so one can use the left side of Eq. (31) instead. As a check, all the terms except for the first one in the right-hand side of Eq. (31) should vanish when projected on the \( L = 3 \) state.

The symmetric part is the sum of the \( L = 1, 2, \) and 3 parts, given by

\[ P^{\text{sym}}_{L3}(k) = \frac{3k^2}{2} \left[ \frac{4}{3} \left\langle T^{i i} \right| \frac{1}{E - H - k} \left| 3_{P_o}^o \right| T^i \right] + \frac{6}{5} \left\langle T^{i j} \right| \frac{1}{E - H - k} \left| 3_{P_o}^o \right| T^{ij} \right] + \frac{1}{5} \left\langle T^{i j k} \right| \frac{1}{E - H - k} \left| 3_{P_o}^o \right| T^{i j k} \right]. \] (36)

5 Numerical evaluation

For the numerical evaluation of the relativistic corrections to the Bethe logarithm, we need to be able to compute the integrands \( P_{Li}(k) \) for different values of \( k \) with a high precision. The crucial part is to obtain highly accurate basis-set representations of the electron propagator \((E - H - k)^{-1}\) for various angular-momentum symmetries. The general idea is to use the variational optimization of the basis for the cases when the integrand has a form of a symmetric second-order perturbation correction, since then it obey the variational principle [22]. Specifically, variational optimization can be used for the nonrelativistic contribution \( P_{nd}(k) \) and for the symmetric part of the retardation contribution, \( P_{L3}^{\text{sym}}(k) \). These two cases cover all angular-momentum symmetries in the electron propagator required in this work. Specifically, for the \( ^3S \) reference state there are only two symmetries required (\( ^3P \) and \( ^3D \)), whereas for the \( ^3P \) reference state there are six different symmetries contributing to the final result. For each angular-momentum symmetry, we perform a variational optimization of \( P_{nd}(k) \) and \( P_{L3}^{\text{sym}}(k) \) for four values of the photon momentum \( k_i = (10^4, 10^2, 10^3, 10^4) \). The optimization was carried out gradually increasing the size of the basis until the convergence condition for the relative accuracy \( \epsilon = 10^{-12} \) or the maximum size of the basis \( N = 1400 \) was reached. The optimized values of nonlinear parameters were stored and then used for computation of \( P_{Li}(k) \).

For a given value of \( k \), the functions \( P_{Li}(k) \) were computed with a basis obtained by merging together the optimized sets for the two closest \( k_i \) points, thus essentially doubling the number of the basis functions. In this way, we were able to compute the functions \( P_{L2}(k) \) for \( k \leq 10^4 \) and \( P_{L3}(k) \) for \( k \leq 10^3 \) with 10-12 digits of accuracy. The calculation of \( P_{L1}(k) \) is more complicated since it involves the Breit Hamiltonian, which remains quite singular even after the regularization, so that additional steps are needed. First, we compute and store the reference-state wave function perturbed by the regularized Breit Hamiltonian \( H_{\text{Breit}} \), \( |\delta \psi \rangle = 1/(E - H)^{1/2} \). In order to get accurate results for the perturbed wave function, we optimize basis for the symmetric second-order correction induced by \( H_{\text{Breit}} \) and use this basis for calculating the perturbed wave function. The convergence of results is rather slow, which is due to the fact that the perturbed wave function \( |\delta \psi \rangle \) has an integrable singularity at \( r_a \to 0 \). In order to represent such wave functions with the exponential basis, very large (both positive and negative) values of nonlinear parameters were required. In order to effectively span large regions of parameters, we used non-uniform distributions, see Ref. [21] for details. In actual calculations, we performed the variational optimization gradually increasing the basis size up to \( N = 1200 \) and then doubled the basis when computing the perturbed wave function. For other electron propagators in \( P_{L1}(k) \), we used the same numerical procedure as for \( P_{L2}(k) \) and \( P_{L3}(k) \). In this way, we were able to compute the function \( P_{L1}(k) \) for \( k \leq 10^4 \) with accuracy of about 9 digits.

The final step is the computation of the relativistic corrections \( E_{Li} \) according to Eq. (16). The interval of the photon momenta \( k \in (0, \infty) \) is split in two by the parameter \( K \). In this work, we use \( K = 100 \). The integral over the interval \( (0, K) \) is carried out analytically, by diagonalizing the Hamiltonian matrix and using the spectral representation of the electron propagator. We note that the principal value of the integral should be taken when the intermediate-state energies smaller than the reference-state energy occur. In this way, the integral over \((0, K)\) is evaluated without any loss of numerical precision. The second part of the integral over \((K, \infty)\) is evaluated by integrating the large-\( k \) expansion of the integrand, with the coefficients of the expansion obtained by fitting the numerical values of the integrand to the known form of the asymptotic expansion.

For \( P_{L2} \) and \( P_{L3} \), we use the large-\( k \) expansion of the form [9]

\[ kP_{Li}(k) - k^2G_i - kF_i - A_i - \frac{B_i}{\sqrt{k}} - \frac{C_i}{k} \ln k - \frac{D_i}{k}, \] (37)

where the coefficients \( c_{m,n} \) are obtained from the fitting procedure. The large-\( k \) expansion of \( P_{L1} \) is more complicated, [9]

\[ kP_{L1}(k) - A_1 - \frac{B_1}{\sqrt{k}} - \frac{C_1}{k} \ln k - \frac{D_1}{k}, \] (38)
with coefficients $c_{m,n}$ to be determined numerically. The coefficients $G_i$, $F_i$, $A_i$, $B_i$, $C_i$, and $D_i$ are known analytically; their explicit formulas are presented in Refs. [15,16]. Note that the definition of $P_{i,2}$ in this work (and, therefore, definitions of the corresponding asymptotic constants) differs from Refs. [15,16] by a factor of 2.

The fitting was performed as follows. At the first step, we store numerical values of the functions $P_{i,2}(k)$ for different values of $k$ in the interval $k \in (5, 10^3)$ (typically, about 300 points). For $P_{i,3}(k)$, numerical cancellations in subtracting the large-$k$ asymptotics are larger, so we used a smaller interval $k \in (5, 10^2)$. At the second step, we subtract contributions of all asymptotic constants known analytically except $D_i$ from the stored values and select several variants of fitting functions and fitting intervals $k \in (k_{\text{min}}, k_{\text{max}})$ that yield the best results for the asymptotic constant $D_i$. Typically, 10-16 free parameters in the fitting ansatz were used. Finally, we use the analytical results for $D_i$ and apply the optimal fitting prescriptions to obtain results for the high-$k$ part of the integral. The scattering of results obtained with different fitting functions was used for estimating the uncertainty.

### 6 Results

The relativistic corrections to the Bethe logarithm were calculated for the helium atom in Refs. [15,16], defined as given by Eq. (15). For helium-like ions, however, this definition is not very convenient. The reason is that the $Z$ dependence of the corrections $E_{L,i}$ is quite complicated; they scale as $Z^0$ and in addition contain terms proportional to $\ln Z$ and $\ln^2 Z$. It is thus advantageous to separate out the leading $Z$ dependence and logarithmic terms from the definition, similarly to that for the nonrelativistic Bethe logarithm (7). The separation of logarithms can be achieved by changing the cutoff parameter in Eq. (15), $E_h = m\alpha^2 \to m(Z\alpha)^2$.

So, instead of corrections $E_{L,i}$ we introduce the functions $\beta_{L,i}$ that do not have logarithmic terms in their $1/Z$ expansion and are related to $E_{L,i}$ as follows

$$\beta_{L,i} = \frac{1}{Z^2(\sum_{n} \delta_3(r_n))} [E_{L,i} + \frac{2}{3\pi} \left( C_i + \frac{1}{2} \ln^2 Z^2 + D_i \ln Z^2 \right)],$$

(39)

where $C_i$ and $D_i$ are the large-$k$ asymptotic expansion constants in Eq. (15), explicit formulas for which can be found in Refs. [15,16].

In the high-$Z$ limit, the functions $\beta_{L,i}(Z)$ should approach the asymptotic values that can be obtained from the hydrogen theory. Specifically, for a two-electron $1snl$ state the large-$Z$ limit is obtained as

$$\beta_0(1snl) = \left( 1 + \frac{\delta_{L,0}}{n^3} \right)^{-1} \left[ \mathcal{L}(1s) + \frac{\mathcal{L}(nl)}{n^3} \right],$$

(40)

where $\mathcal{L}(nl)$ is the one-loop hydrogenic low-energy contribution from Refs. [8,23], $\mathcal{L}(np) = (1/3) \mathcal{L}(np_{1/2}) + (2/3) \mathcal{L}(np_{3/2})$.

Results of our numerical calculations of the relativistic corrections to the Bethe logarithm for the $2^3S$ and $2^3P$ states of helium-like atoms with $Z \leq 12$ are collected in Tables 1 and 2 and Fig. 1. We observe that the numerical values of $\beta_L$ exhibit a weak dependence on $Z$. Moreover, both for the $2^3S$ and $2^3P$ states the results are quite close to the hydrogenic $1s$ value $\mathcal{L}(1s) = -27.259909$ [23]. This behavior is similar to that of the nonrelativistic Bethe logarithm [2].

Tables 1 and 2 present also results of our numerical extrapolation of $\beta_L(Z)$ to the $Z \to \infty$ limit. The extrapolation was carried out by fitting the $1/Z$ expansion to a polynomial in $1/Z$. We observe that the fitting results are in excellent agreement with the analytical values of $\beta_0$ obtained from the hydrogen theory [8,23].

Summarizing, we performed calculations of the relativistic corrections to the Bethe logarithm for the $2^3S$ and $2^3P$ states of helium-like ions with $Z \leq 12$. The leading $Z$ dependence and terms proportional to $\ln Z$ and $\ln^2 Z$ were separated out. The resulting scaled func-

### Table 1: Relativistic corrections to the Bethe logarithm for the $2^3S$ state

| $Z$ | $\beta_{L_1}$ | $\beta_{L_2}$ | $\beta_{L_3}$ | $\beta_L$ | Refs. |
|-----|----------------|----------------|----------------|----------|-------|
| 2   | -3.33597       | 16.96335       | -40.59675      | -26.96397 (2) | [15,16] |
| 3   | -3.39619       | 16.96347       | -40.59675      | -26.9692 (2)  |       |
| 4   | -3.43387       | 16.91755       | -40.58484      | -27.06348 (2) |       |
| 5   | -3.45895       | 16.86190       | -40.57819      | -27.12756 (2) |       |
| 6   | -3.47671       | 16.84575       | -40.57400      | -27.17105 (2) |       |
| 7   | -3.48991       | 16.83371       | -40.56904      | -27.22524 (2) |       |
| 8   | -3.50009       | 16.82441       | -40.56746      | -27.24314 (2) |       |
| 9   | -3.50817       | 16.81702       | -40.56623      | -27.25738 (3) |       |
| 10  | -3.51467       | 16.81102       | -40.56523      | -27.26898 (4) |       |
| 11  | -3.52021       | 16.80604       | -40.56442      | -27.27859 (4) |       |
| 12  | -3.52488       | 16.80185       | -40.56374      | -27.28677 (5) |       |
| $\infty$ |           |                |                | $-27.3814$ (6) |       |
|      |                |                |                | $-27.381138$ [23] |     |
Table 2  Relativistic corrections to the Bethe logarithm for the $2^3P$ state

| Z  | $\beta_{L1}$ | $\beta_{L2}$ | $\beta_{L3}$ | $\beta_{L}$ | Refs.  |
|----|--------------|--------------|--------------|-------------|--------|
| 2  | −3.29274     | 16.93985     | −40.64479    | −26.99768 (25) |        |
|    | −3.29277     | 16.93994     | −40.64478    | −26.9976 (5) | [15,16]|
| 3  | −3.27693     | 16.91594     | −40.67895    | −27.03994 (20) |        |
| 4  | −3.26796     | 16.88490     | −40.70203    | −27.08508 (20) |        |
| 5  | −3.26440     | 16.86108     | −40.71778    | −27.12109 (20) |        |
| 6  | −3.26322     | 16.84321     | −40.72910    | −27.14911 (20) |        |
| 7  | −3.26301     | 16.82952     | −40.73761    | −27.17110 (20) |        |
| 8  | −3.26327     | 16.81877     | −40.74424    | −27.18874 (20) |        |
| 9  | −3.26380     | 16.81012     | −40.74954    | −27.20321 (20) |        |
| 10 | −3.26436     | 16.80303     | −40.75388    | −27.21520 (20) |        |
| 11 | −3.26492     | 16.79712     | −40.75749    | −27.22529 (20) |        |
| 12 | −3.26544     | 16.79211     | −40.76055    | −27.23388 (20) |        |
| $\infty$ | −3.26322 | 16.81012 | −40.74954 | −27.3408 (30) |        |

Fig. 1  The relativistic correction to the Bethe logarithm $\beta_{L}$ for the $2^3S$ (left) and $2^3P$ (right) states of helium-like ions, as a function of the inverse nuclear charge $1/Z$. Round dots (orange) denote the numerical results, the hexagon dot (green) shows the analytical result at $Z = \infty$, and dotted line (orange) represents the numerical fit.

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Author contributions  VAY performed the numerical part of the calculation. VP and KP performed the derivation of formulas and the analytical part of the calculation.

Data Availability Statement  The datasets generated during the current study (numerical values of the functions $P_{Li}(k)$ and values of the asymptotic expansion constants) are available from the corresponding author on request. This manuscript has no associated data or the data will not be deposited.
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