Relativistic Bethe logarithm for triplet states of helium-like ions

Vladimir A. Yerokhin
Peter the Great St. Petersburg Polytechnic University, Polytekhnicheskaya 29, 195251 St. Petersburg, Russia

Vojtěch Patkóš
Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Prague 2, Czech Republic

Krzysztof Pachucki
Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

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We report a calculation of relativistic corrections of order $m\alpha^7$ to the Bethe logarithm for the $2\,^3S$ and $2\,^3P$ 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 [V. Patkóš, V. A. Yerokhin, K. Pachucki, 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.

I. 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 α is the fine-structure constant). At the present level of experimental and theoretical interest, QED effects of higher orders in α 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 [10–12] and recently for the $2\,^3S$ and $2\,^3P$ states [13]. 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 [14, 15]. In view of this discrepancy, it is important to cross-check the calculations of the $m\alpha^7$ effects reported in Refs. [13, 14, 16]. 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 $2\,^3S$ and $2\,^3P$ 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.

II. BASIC FORMULAS

A. Nonrelativistic Bethe logarithm

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

$$\mathcal{H} = \sum_a \frac{\vec{\pi}_a^{\,2}}{2\,m} + V + e\sum_a \phi(\vec{r}_a) \tag{1}$$

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

$$V = -\sum_a \frac{Z\alpha}{r_a} + \sum_{a<b} \frac{\alpha}{r_{ab}}\,, \tag{2}$$

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 Hamiltonan (1) and has the

form

$$E_L(\Lambda) = \frac{e^2}{m^2}\int_{|\boldsymbol{k}|<\Lambda}\frac{d^3k}{(2\pi)^3 2k}\left(\delta^{ij}-\hat{\boldsymbol{k}}^i\hat{\boldsymbol{k}}^j\right) \times\sum_{ab}\langle\psi|p_a^i\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}_a}\,\frac{1}{E-H-k}\,p_b^j\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_b}|\psi\rangle\,, \quad (3)$$

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

$$E_L^{(5)}(\Lambda) = \frac{2\alpha}{3\pi m^2}\int_0^\Lambda dk\, k\, P_{nd}(k)\,, \quad (4)$$

$$P_{nd}(k) = \left\langle\vec{P}\,\frac{1}{E-H-k}\,\vec{P}\right\rangle, \quad (5)$$

where $\vec{P}\equiv\sum_a\vec{p}_a$.

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

$$k\,P_{nd}(k) = \left\langle\nabla^2\right\rangle + \frac{1}{k}\,D + \dots\,, \quad (6)$$

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

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

$$\ln k_0 = \frac{\langle\vec{P}\,(H-E)\,\ln[2\,(H-E)/E_h]\,\vec{P}\rangle}{\langle\vec{P}\,(H-E)\,\vec{P}\rangle} = -\frac{1}{D}\int_0^\infty dk\left[k\,P_{nd}(k) - \left\langle\nabla^2\right\rangle - \frac{D}{k}\,\theta(k-E_h/2)\right], \quad (7)$$

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

B. 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

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

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

$$E_L^{(7)}(\Lambda) = E_{L1}(\Lambda)+E_{L2}(\Lambda)+E_{L3}(\Lambda) = \frac{2\alpha}{3\pi m^2}\int_0^\Lambda dk\,k\Big[P_{L1}(k)+P_{L2}(k)+P_{L3}(k)\Big]. \quad (9)$$

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

$$P_{L1}(k) = 2\left\langle H_{\rm Breit}\frac{1}{(E-H)'}\,\vec{P}\,\frac{1}{E-H-k}\,\vec{P}\right\rangle, + \left\langle\vec{P}\,\frac{1}{E-H-k}\left[H_{\rm Breit}-\langle H_{\rm Breit}\rangle\right]\frac{1}{E-H-k}\,\vec{P}\right\rangle. \quad (10)$$

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

$$P_{L2}(k) = 2\left\langle\vec{\delta j}\,\frac{1}{E-H-k}\,\vec{P}\right\rangle. \quad (11)$$

The correction to the current δj^i is obtained from the Breit-Pauli Hamiltonian, specifically from the first and fourth terms of Eq. (8), with the result

$$\delta j^i = -\frac{1}{2m^2}\sum_a p_a^i\,p_a^2 - \frac{\alpha}{2m}\sum_{a,b}\left(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i r_{ab}^j}{r_{ab}^3}\right)p_b^j\,. \quad (12)$$

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

$$P_{L3}(k) = \frac{3k^2}{8\pi}\int d\hat{\boldsymbol{k}}\left(\delta^{ij}-\hat{\boldsymbol{k}}^i\hat{\boldsymbol{k}}^j\right)\left[\left\langle\sum_a p_a^i\,(\hat{\boldsymbol{k}}\cdot\boldsymbol{r_a})\,\frac{1}{E-H-k}\sum_b(\hat{\boldsymbol{k}}\cdot\boldsymbol{r}_b)p_b^j\right\rangle - \left\langle\sum_a p_a^i\,(\hat{\boldsymbol{k}}\cdot\boldsymbol{r}_a)^2\,\frac{1}{E-H-k}\sum_b p_b^j\right\rangle\right]. \quad (13)$$

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

$$k\,P_{Li}(k) = G_i k^2 + F_i k + A_i + \frac{B_i}{\sqrt{k}} + \frac{C_i\,\ln k}{k} + \frac{D_i}{k} + \dots\,, \quad (14)$$

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 $\Delta E_{Li}(\Lambda)$ in Eq. (9) are defined as

$$E_{Li} = \frac{2\alpha}{3\pi m^2}\int_0^\infty dk\left\{k\,P_{Li}(k) - k^2 G_i - k\,F_i - A_i - \frac{B_i}{\sqrt{k}} - \left[\frac{C_i\,\ln k}{k} + \frac{D_i}{k}\right]\theta(k-E_h)\right\}. \quad (15)$$

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

$$\begin{aligned} E_{Li} \;=& \frac{2\alpha}{3\pi m^2}\left\{\int_0^K dk\,k\,P_{Li}(k) + \int_K^\infty dk\left[kP_{Li}(k) - G_i k^2 - F_i k - A_i - \frac{B_i}{k^{1/2}} - \frac{C_i\ln k}{k} - \frac{D_i}{k}\right]\right. \\ & - G_i\frac{K^3}{3} - F_i\frac{K^2}{2} - A_i K - 2B\sqrt{K_i} \\ & \left. - \frac{C_i}{2}\ln^2 K - D_i\ln K\right\}, \end{aligned} \quad (16)$$

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

III. 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 $H'_{\rm Breit}$

$$\begin{aligned} H'_{\rm Breit} =& -\frac{1}{2}(E-V)^2 + \frac{1}{4}\nabla_1^2\nabla_2^2 - \frac{Z}{4}\frac{\vec r_1}{r_1^3}\cdot\vec\nabla_1 \\ & - \frac{Z}{4}\frac{\vec r_2}{r_2^3}\cdot\vec\nabla_2 - \frac{1}{2}\,p_1^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right)p_2^j. \end{aligned} \quad (17)$$

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

$$H_{\rm Breit}|\phi\rangle = H'_{\rm Breit}|\phi\rangle + \big\{H - E, Q\big\}|\phi\rangle\,, \quad (18)$$

where

$$Q = -\frac{1}{4}\left(\frac{Z}{r_1} + \frac{Z}{r_2} - \frac{2}{r}\right). \quad (19)$$

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

$$\begin{aligned} P_{L1,\rm pwf}(k) =& 2\Big\langle H'_{\rm Breit}\frac{1}{(E-H)'}\,\vec P\,\frac{1}{E-H-k}\,\vec P\Big\rangle \\ & - 2\Big\langle\big[Q - \langle Q\rangle\big]\,\vec P\,\frac{1}{E-H-k}\,\vec P\Big\rangle. \end{aligned} \quad (20)$$

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

$$H''_{\rm Breit} = -\frac{1}{2}(E-V)\left(E - \frac{1}{r}\right) + \frac{1}{4}\nabla_1^2\nabla_2^2 - \frac{Z}{4}\vec p_1\left(\frac{1}{r_1} + \frac{1}{r_2}\right)\vec p_1 - \frac{Z}{4}\vec p_2\left(\frac{1}{r_1} + \frac{1}{r_2}\right)\vec p_2 - \frac{1}{2}\,p_1^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right)p_2^j. \quad (21)$$

For this operator, the following identity holds

$$H_{\rm Breit} = H''_{\rm Breit} + \big\{H - E, Q'\big\} - \frac{1}{2}\,(H-E)^2\,, \quad (22)$$

where $Q' = Q - \frac{E}{2}$. Using this identity, we derive the following regularized expression for the vertex part of P_{L1},

$$\begin{aligned} P_{\rm ver}(k) =& \Big\langle\vec P\,\frac{1}{E-H-k}\Big[H''_{\rm Breit} - 2kQ + kE - \frac{k^2}{2} - \langle H_{\rm Breit}\rangle\Big]\frac{1}{E-H-k}\,\vec P\Big\rangle \\ & - \Big\langle\big[2\vec P\,Q + (k-E)\vec P\big]\frac{1}{E-H-k}\,\vec P\Big\rangle - \frac{1}{2}\Big\langle\vec P^2\Big\rangle. \end{aligned} \quad (23)$$

IV. 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. [17].

We start with the nonrelativistic Bethe logarithm. The angular reduction of P_{nd} for the ${}^3S$ reference state is trivial, since only one angular symmetry (${}^3P^o$) 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 ϕ^k into a sum of irreducible tensors of the rank $L = 0$, 1, and 2 as follows

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

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

$$P_{nd}(k) \;= \frac{1}{3}\left\langle\phi^i\middle|j^i\,\frac{1}{E-H-k}\middle|_{{}^3S}\,j^k\middle|\phi^k\right\rangle + \frac{1}{2}\left\langle\Psi_1^i\,\frac{1}{E-H-k}\middle|_{{}^3P^e}\,\Psi_1^i\right\rangle + \frac{1}{4}\left\langle\Psi_2^{ik}\,\frac{1}{E-H-k}\middle|_{{}^3D^e}\,\Psi_2^{ik}\right\rangle, \tag{25}$$

where $\vec{\Psi}_1 = \vec{j}\times\vec{\phi}$ and $\Psi_2^{ik} = j^i\phi^k + j^k\phi^i - \frac{2}{3}\,\delta^{ik}\big(\vec{j}\cdot\vec{\phi}\big)$ 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_{nd}. For P_{L3}, we need first to perform the angular integration over $\hat{\boldsymbol{k}}$. It is carried out with help of the following formulas

$$\int\frac{d\hat{\boldsymbol{k}}}{4\pi}\,\hat{\boldsymbol{k}}^i\hat{\boldsymbol{k}}^j \;= \frac{1}{3}\delta^{ij}\,,\quad \int\frac{d\hat{\boldsymbol{k}}}{4\pi}\,\hat{\boldsymbol{k}}^i\hat{\boldsymbol{k}}^j\hat{\boldsymbol{k}}^k\hat{\boldsymbol{k}}^l = \frac{1}{15}\left(\delta^{ij}\delta^{kl} + \delta^{il}\delta^{kj} + \delta^{ik}\delta^{jl}\right), \tag{26}$$

$$\int\frac{d\hat{\boldsymbol{k}}}{4\pi}\left(\delta^{ij} - \hat{\boldsymbol{k}}^i\hat{\boldsymbol{k}}^j\right)\hat{\boldsymbol{k}}^n\hat{\boldsymbol{k}}^m r_1^n r_2^m = \frac{1}{15}\left(4\,\delta^{ij}(\boldsymbol{r}_1\cdot\boldsymbol{r}_2) - r_1^i r_2^j - r_1^j r_2^i\right). \tag{27}$$

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 H, we obtain

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

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

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

$$P_{L3}^{\rm sym}(k) = \frac{3k^2}{40}\left\langle\Psi_2^{ik}\,\frac{1}{E-H-k}\middle|_{{}^3D^e}\,\Psi_2^{ik}\right\rangle, \tag{29}$$

where

$$\begin{aligned} \big|\Psi_2^{ik}\big\rangle = \Big(& r_1^i p_1^k + r_1^k p_1^i - \frac{2}{3}\,\delta^{ik}\boldsymbol{r}_1\cdot\boldsymbol{p}_1 \\ &+ r_2^i p_2^k + r_2^k p_2^i - \frac{2}{3}\,\delta^{ik}\boldsymbol{r}_2\cdot\boldsymbol{p}_2\Big)\big|\phi\big\rangle. \end{aligned} \tag{30}$$

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

$$\begin{aligned} \frac{1}{2}\sum_a\big(r_a^i p_a^j + r_a^j p_a^i\big)\,\phi^k = T^{ijk} + \epsilon^{ikl}\,T^{lj} + \epsilon^{jkl}\,T^{li} \\ + \delta^{ik}\,T^j + \delta^{jk}\,T^i + \delta^{ij}\,T'^k, \end{aligned} \tag{31}$$

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

$$T^{ijk} \equiv \sum_a (r_a^i\,p_a^j\,\phi^k)^{(3)}\,, \tag{32}$$

$$\begin{aligned} T^{ij} =& \frac{1}{12}\sum_a\Big[\epsilon^{jlm}\left(r_a^i\,p_a^l + r_a^l\,p_a^i\right)\phi^m \\ &+ \epsilon^{ilm}\left(r_a^j\,p_a^l + r_a^l\,p_a^j\right)\phi^m\Big], \end{aligned} \tag{33}$$

$$T^i = \frac{1}{20}\sum_a\Big[3\left(r_a^i\,p_a^l + r_a^l\,p_a^i\right)\phi^l - 2\,r_a^l\,p_a^l\,\phi^i\Big], \tag{34}$$

$$T'^i = \frac{1}{10}\sum_a\Big[4r_a^l\,p_a^l\,\phi^i - r_a^i\,p_a^l\,\phi^l - r_a^l\,p_a^i\,\phi^l\Big]. \tag{35}$$

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 is 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

$$P_{L3}^{\rm sym}(k) = \frac{3\,k^2}{2}\left[\frac{4}{3}\left\langle T^{\dagger i}\;\frac{1}{E-H-k}\right|_{{}^3P^o} T^i\right\rangle + \frac{6}{5}\left\langle T^{\dagger ij}\;\frac{1}{E-H-k}\right|_{{}^3D^o} T^{ij}\right\rangle + \frac{1}{5}\left\langle T^{\dagger ijk}\;\frac{1}{E-H-k}\right|_{{}^3F^o} T^{ijk}\right\rangle\Bigg]. \quad (36)$$

V. 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 obeys the variational principle [18]. Specifically, variational optimization can be used for the nonrelativistic contribution $P_{nd}(k)$ and for the symmetric part of the retardation contribution, $P_{L3}^{\rm sym}(k)$. 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 $P_{L3}^{\rm sym}(k)$ for four values of the photon momentum $k_i = (10^1, 10^2, 10^3, 10^4)$. The optimization was carried out with 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 $k \le 10^4$ and $P_{L3}(k)$ for $k \le 10^3$ 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 $H'_{\rm Breit}$, $|\delta\psi\rangle = 1/(E-H)'|H'_{\rm Breit}\rangle$. In order to get accurate results for the perturbed wave function, we optimize basis for the symmetric second-order correction induced by $H'_{\rm Breit}$ 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. [17] 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 were able to compute the function $P_{L1}(k)$ for $k \le 10^4$ 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,∞) 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]

$$kP_{Li}(k) - k^2 G_i\; - kF_i - A_i - \frac{B_i}{\sqrt{k}} - \frac{C_i\ln k}{k} - \frac{D_i}{k} = \frac{1}{k}\sum_{m=1}^{M}\frac{c_{m,2}\sqrt{k} + c_{m,1}\ln k + c_{m,0}}{k^m}\,, \quad (37)$$

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

$$kP_{L1}(k) - A_1 - \frac{B_1}{\sqrt{k}}\; - \frac{C_1\ln k}{k} - \frac{D_1}{k} = \frac{1}{k}\sum_{m=1}^{M}\sum_{n=0}^{m}\frac{c_{m,n}\ln^n k}{k^{m/2}}\,, \quad (38)$$

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; explicit formulas them are presented in Ref. [13]. Note that the definition of P_{L2} in this work (and, therefore, definitions of the corresponding asymptotic constants) differ from Ref. [13] by a factor of 2.

The fitting was performed as follows. At the first step, we store numerical values of the functions $P_{Li}(k)$ for different values of k in the interval $k \in (5, 10^4)$ (typically, about 300 points). For $P_{L3}(k)$, numerical cancellations in subtracting the large-k asymptotics are larger, so we used a smaller interval $k \in (5, 10^3)$. 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

TABLE I. Relativistic corrections to the Bethe logarithm for the $2\,^3S$ state.

Z	β_{L1}	β_{L2}	β_{L3}	β_L	Ref.
2	−3.335 97	16.963 35	−40.596 75	−26.969 37 (2)	
	−3.335 96	16.963 47	−40.596 75	−26.969 2 (2)	[13]
3	−3.396 19	16.917 55	−40.584 84	−27.063 48 (2)	
4	−3.433 87	16.884 51	−40.578 19	−27.127 56 (2)	
5	−3.458 95	16.861 90	−40.574 00	−27.171 05 (2)	
6	−3.476 71	16.845 75	−40.571 12	−27.202 08 (2)	
7	−3.489 91	16.833 71	−40.569 04	−27.225 24 (2)	
8	−3.500 09	16.824 41	−40.567 46	−27.243 14 (2)	
9	−3.508 17	16.817 02	−40.566 23	−27.257 38 (3)	
10	−3.514 76	16.811 02	−40.565 23	−27.268 98 (4)	
11	−3.520 21	16.806 04	−40.564 42	−27.278 59 (4)	
12	−3.524 88	16.801 85	−40.563 74	−27.286 77 (5)	
∞				−27.381 4 (6)	
				−27.381 138	[19]

TABLE II. Relativistic corrections to the Bethe logarithm for the $2\,^3P$ state.

Z	β_{L1}	β_{L2}	β_{L3}	β_L	Ref.
2	−3.292 74	16.939 85	−40.644 79	−26.997 68 (25)	
	−3.292 77	16.939 94	−40.644 78	−26.997 6 (5)	[13]
3	−3.276 93	16.915 94	−40.678 95	−27.039 94 (20)	
4	−3.267 96	16.884 90	−40.702 03	−27.085 08 (20)	
5	−3.264 40	16.861 08	−40.717 78	−27.121 09 (20)	
6	−3.263 22	16.843 21	−40.729 10	−27.149 11 (20)	
7	−3.263 01	16.829 52	−40.737 61	−27.171 10 (20)	
8	−3.263 27	16.818 77	−40.744 24	−27.188 74 (20)	
9	−3.263 80	16.810 12	−40.749 54	−27.203 21 (20)	
10	−3.264 36	16.803 03	−40.753 88	−27.215 20 (20)	
11	−3.264 92	16.797 12	−40.757 49	−27.225 29 (20)	
12	−3.265 44	16.792 11	−40.760 55	−27.233 88 (20)	
∞				−27.340 8 (30)	
				−27.341 771	[8, 19]

functions and fitting intervals $k \in (k_{\min}, k_{\max})$ that yield the best results for the asymptotic constant D_i. Typically, 10-16 free parameters in the fitting anzatz 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 were used for estimating the uncertainty.

VI. RESULTS

The relativistic corrections to the Bethe logarithm were calculated for the helium atom in Ref. [13], 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_{Li} is quite complicated; they scale as Z^6 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_{Li} we introduce the functions β_{Li} that do not have logarithmic terms in their $1/Z$ expansion and are related to E_{Li} as follows

$$\beta_{Li} = \frac{1}{Z^3\langle\sum_a \delta^3(r_a)\rangle}\Big[E_{Li} + \frac{2}{3\pi}\Big(\frac{C_i}{2}\,\ln^2 Z^2 + D_i \ln Z^2\Big)\Big], \tag{39}$$

where C_i and D_i are the large-k asymptotic expansion constants in Eq. (15), explicit formulas for which can be found in Ref. [13].

In the high-Z limit, the functions $\beta_{Li}(Z)$ 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

$$\beta_0(1snl) = \Big(1 + \frac{\delta_{l,0}}{n^3}\Big)^{-1}\Big[\mathcal{L}(1s) + \frac{\mathcal{L}(nl)}{n^3}\Big], \tag{40}$$

where $\mathcal{L}(nl)$ is the one-loop hydrogenic low-energy contribution from Refs. [8, 19], $\mathcal{L}(np) = (1/3)\,\mathcal{L}(np_{1/2}) + (2/3)\,\mathcal{L}(np_{3/2})$.

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 $Z \le 12$ are collected in Tables I and II and Fig. 1. We observe that the numerical values of β_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 $\mathcal{L}(1s) = -27.259\,909$ [19]. This behaviour is similar to that of the nonrelativistic Bethe logarithm [2].

Tables I and II 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 β_0 obtained from the hydrogen theory [8, 19].

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 $Z \le 12$. The leading Z dependence and terms proportional to $\ln Z$ and $\ln^2 Z$ were separated out. The resulting scaled function β_L was found to depend weakly on Z and on the reference state. The extrapolated $Z \to \infty$ limit of the numerical results was found to be in excellent agreement with the analytical values obtained from the hydrogen theory. This constitutes a stringent check of correctness of the numerical procedure of the calculation.

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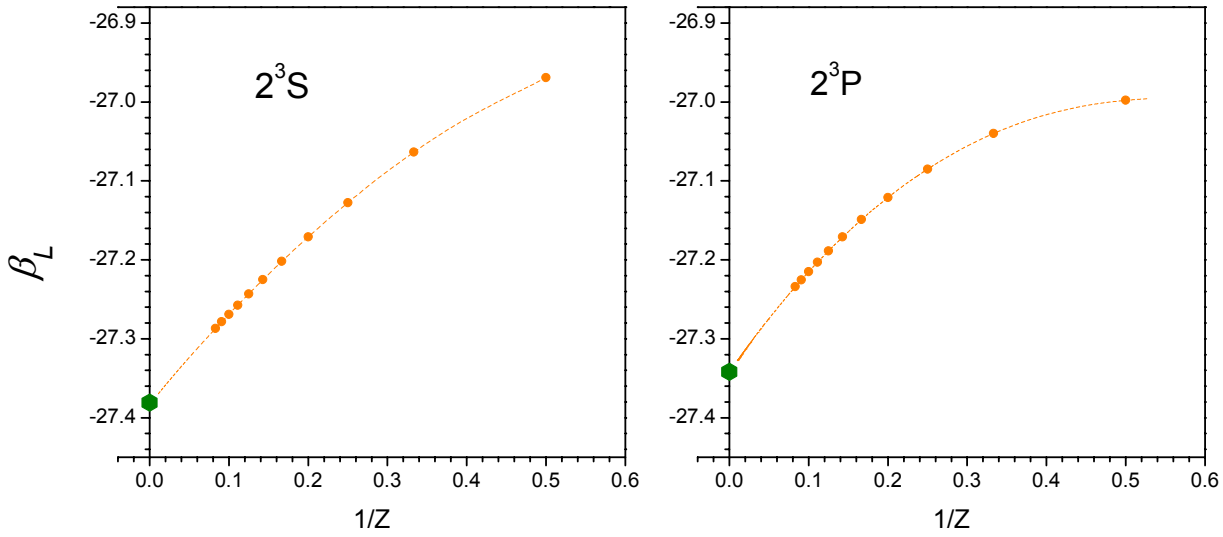

FIG. 1. The relativistic correction to the Bethe logarithm β_L for the $2\,^3S$ (left) and $2\,^3P$ (right) states of helium-like ions, as a function of the inverse nuclear charge $1/Z$. Round dots (orange) denote the numerical results, the hexagon dot (green) shows the analytical result at $Z = \infty$,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

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