Theoretical energies of low-lying states of light helium-like ions

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A rigorous quantum electrodynamical calculation is presented for energy levels of the $1\,^1S$, $2\,^1S$, $2\,^3S$, $2\,^1P_1$, and $2\,^3P_{0,1,2}$ states of helium-like ions with the nuclear charge $Z = 3, \ldots, 12$. The calculational approach accounts for all relativistic, quantum electrodynamical, and recoil effects up to orders $m\alpha^6$ and $m^2/M\alpha^5$, thus advancing the previously reported theory of light helium-like ions by one order in α.

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I. INTRODUCTION

Atomic helium and light helium-like ions have long been attractive subjects of theoretical and experimental investigations. From the theoretical point of view, helium-like atoms are the simplest few-body systems. As such, they are traditionally used as a testing ground for different methods of the description of atomic structure. On the experimental side, small natural line widths of transitions between the metastable ^3P and ^3S states of helium-like ions permit spectroscopic measurements of high precision. For atomic helium, experimental investigations are nowadays carried out with the relative accuracy up to 7×10^{-12} [1]. An advantage of the helium-like ions as compared to, for example, hydrogen-like ones, is that the transition frequency increases slowly with the nuclear charge number Z ($\sim Z$). This feature ensures that wavelengths of a significant part of the helium isoelectronic sequence fall in the region suitable for accurate experimental determination.

There are presently two main theoretical approaches that allow one to systematically account for the electron-correlation, relativistic, and quantum electrodynamical (QED) effects in few-electron systems. The first one, traditionally used for light systems, relies on an expansion of the relativistic and QED effects in terms of α and $Z\alpha$ (where α is the fine-structure constant) and treats the nonrelativistic electron-electron interaction nonperturbatively. This approach started with the pioneering works of Araki [2] and Sucher [3], who derived the expression for the Lamb shift in many-electron systems complete through the order $m\alpha^5$. The other approach aims primarily at high-Z ions. It does not use any expansion in the binding-strength parameter $Z\alpha$ (and thus is often referred to as the *all-order* approach) but treats the electron-electron interaction within the perturbative expansion with the parameter $1/Z$. A systematic formulation of this method is presented in Ref. [4].

These two approaches can be considered as complementary, the first being clearly preferable for light atoms and the second for heavy ions. The intermediate region of nuclear charges around $Z = 12$ is the most difficult one for theory, as contributions not (yet) accounted by either of these methods have their maximal value there. In order to provide accurate predictions for the whole isoelectronic sequence, it is necessary to combine these two approaches.

For the first time a combination of the complementary approaches was made by Drake [5]. His results for energies of helium-like ions comprise all effects up to order $m\alpha^5$ in the low-Z region, whereas in the high-Z region, they are complete up to the next-to-the-leading order in $1/Z$ for nonradiative effects and to the leading order for radiative effects. Since then, significant progress was achieved in theoretical understanding of energy levels of atomic helium, whose description is now complete through order $m\alpha^6$ [6,7]. Also in the high-Z region, theoretical energies have recently been significantly improved by a rigorous treatment of the two-electron QED corrections [8], which completed the $O(1/Z)$ part of the radiative effects.

In the present investigation we aim to improve theoretical predictions of the $n = 1$ and $n = 2$ energy levels of light helium-like ions. To this end, we perform a calculation that includes all QED and recoil effects up to orders $m\alpha^6$ and $m^2/M\alpha^5$ (where M is the nuclear mass). In order to establish a basis for merging the current approach with the all-order calculations, we perform an extensive analysis of the $1/Z$ expansion of individual corrections. This analysis also provides an effective test of consistency of our calculational results and of the $1/Z$-expansion data available in the literature.

II. THEORY OF THE ENERGY LEVELS

In this section, we present a summary of contributions to the energy levels of two-electron atoms complete up to orders $m\alpha^6$ and $m^2/M\alpha^5$.

According to QED theory, energy levels of atoms are represented by an expansion in powers of α of the form

$$E(\alpha) = E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + \cdots, \quad (1)$$

where $E^{(n)} \equiv m\alpha^n \mathcal{E}^{(n)}$ is a contribution of order α^n and may include powers of $\ln\alpha$. Each of $\mathcal{E}^{(n)}$ is in turn expanded in powers of the electron-to-nucleus mass ratio m/M:

$$\mathcal{E}^{(n)} = \mathcal{E}^{(n)}_\infty + \mathcal{E}^{(n)}_M + \mathcal{E}^{(n)}_{M^2} + \cdots, \quad (2)$$

where $\mathcal{E}^{(n)}_M$ denotes the correction of first order in m/M and $\mathcal{E}^{(n)}_{M^2}$ is the second-order correction. Note that, for the nonrelativistic energy, it is more natural to expand in m_r/M (where m_r is the reduced mass) rather than in m/M, since such expansion has smaller coefficients. For the relativistic corrections, however, the natural recoil expansion parameter is m/M, so for consistency we use it for the nonrelativistic energy as well.

The terms of the double perturbation expansion (1) and (2) are expressed as expectation values of some effective Hamiltonians (in some cases, of nonlocal operators) and as second- and higher order perturbation corrections induced by these Hamiltonians (operators). It is noteworthy that the expansion (1) is employed also for the states that are mixed by the relativistic effects, namely $2\,^1P_1$ and $2\,^3P_1$. The mixing effects are treated perturbatively. (So, the leading effect due to the $2\,^1P_1$–$2\,^3P_1$ mixing appears naturally as the second-order $m\alpha^6$ correction, together with contributions from other intermediate states.) This differs from the approach used, for example, in Ref. [5], where a two-by-two matrix was constructed for this pair of states and the energies were obtained by a diagonalization.

The leading contribution to the energy $\mathcal{E}^{(2)}_\infty \equiv \mathcal{E}_0$ is the eigenvalue of the nonrelativistic Hamiltonian,

$$H^{(2)} \equiv H_0 = \sum_a \left(\frac{\vec{p}_a^{\,2}}{2} - \frac{Z}{r_a}\right) + \sum_{a<b} \frac{1}{r_{ab}}. \tag{3}$$

The first- and second-order recoil corrections to the nonrelativistic energy are given by

$$\mathcal{E}^{(2)}_M = -\frac{m}{M}\mathcal{E}^{(2)}_\infty + \langle H^{(2)}_{\rm rec}\rangle, \tag{4}$$

$$\mathcal{E}^{(2)}_{M^2} = \left(\frac{m}{M}\right)^2 \mathcal{E}^{(2)}_\infty - 2\frac{m}{M}\langle H^{(2)}_{\rm rec}\rangle + \left\langle H^{(2)}_{\rm rec}\frac{1}{(\mathcal{E}_0 - H_0)'}H^{(2)}_{\rm rec}\right\rangle, \tag{5}$$

where

$$H^{(2)}_{\rm rec} = \frac{m}{M}\sum_{a<b} \vec{p}_a \cdot \vec{p}_b \tag{6}$$

is the mass polarization operator.

The leading relativistic correction $\mathcal{E}^{(4)}_\infty$ is given by the expectation value of the Breit-Pauli Hamiltonian $H^{(4)}$ [9],

$$\begin{aligned} H^{(4)} = {} & \sum_a \left[-\frac{\vec{p}_a^{\,4}}{8} + \frac{\pi Z}{2}\delta^3(r_a) + \frac{Z}{4}\vec{\sigma}_a \cdot \frac{\vec{r}_a}{r_a^3} \times \vec{p}_a\right] \\ & + \sum_{a<b} \Bigg\{ -\pi\delta^3(r_{ab}) - \frac{1}{2} p_a^i \left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i r_{ab}^j}{r_{ab}^3}\right) p_b^j \\ & - \frac{2\pi}{3}\vec{\sigma}_a \cdot \vec{\sigma}_b \delta^3(r_{ab}) + \frac{\sigma_a^i \sigma_b^j}{4 r_{ab}^3}\left(\delta^{ij} - 3\frac{r_{ab}^i r_{ab}^j}{r_{ab}^2}\right) \\ & + \frac{1}{4 r_{ab}^3}[2(\vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_a) \\ & + (\vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_a)] \Bigg\}. \end{aligned} \tag{7}$$

The finite-nuclear-mass correction to the Breit contribution $\mathcal{E}^{(4)}_M$ is conveniently separated into the mass scaling, the mass polarization, and the operator parts. The mass scaling prefactor is $(m_r/m)^4$ for the first term in Eq. (7) and $(m_r/m)^3$, for all the others. The mass polarization part represents the first-order perturbation of $\mathcal{E}^{(4)}_\infty$ by the mass-polarization operator (6). The operator part is given by the expectation value of the recoil addition to the Breit-Pauli Hamiltonian,

$$H^{(4)}_{\rm rec} = \frac{Zm}{2M}\sum_{ab}\left[\frac{\vec{r}_a}{r_a^3} \times \vec{p}_b \cdot \vec{\sigma}_a - p_a^i\left(\frac{\delta^{ij}}{r_a} + \frac{r_a^i r_a^j}{r_a^3}\right)p_b^j\right]. \tag{8}$$

$\mathcal{E}^{(5)}_\infty$ is the leading QED correction [2,3]. We divide it into logarithmic and nonlogarithmic parts, $\mathcal{E}^{(5)}_\infty = \mathcal{E}^{(5)}_\infty(\log) + \mathcal{E}^{(5)}_\infty(\text{nlog})$, which are given by

$$\mathcal{E}^{(5)}_\infty(\log) = \frac{14}{3}\ln(Z\alpha)\sum_{a<b}\langle\delta^3(r_{ab})\rangle + \frac{4Z}{3}\ln[(Z\alpha)^{-2}]\sum_a\langle\delta^3(r_a)\rangle \tag{9}$$

and

$$\begin{aligned} \mathcal{E}^{(5)}_\infty(\text{nlog}) = {} & \frac{164}{15}\sum_{a<b}\langle\delta^3(r_{ab})\rangle - \frac{14}{3}\sum_{a<b}\widetilde{Q}_{ab} \\ & + \left[\frac{19}{30} - \ln\left(\frac{k_0}{Z^2}\right)\right]\frac{4Z}{3}\sum_a\langle\delta^3(r_a)\rangle + \langle H^{(5)}_{\rm fs}\rangle, \end{aligned} \tag{10}$$

where

$$\widetilde{Q}_{ab} = \left\langle \frac{1}{4\pi r_{ab}^3} + \delta^3(r_{ab})\ln Z \right\rangle \tag{11}$$

and the singular operator r^{-3} is defined by

$$\left\langle\frac{1}{r^3}\right\rangle \equiv \lim_{a\to 0}\int d^3r\,\phi^*(\vec{r})\phi(\vec{r}) \times \left[\frac{1}{r^3}\Theta(r-a) + 4\pi\delta^3(r)(\gamma + \ln a)\right], \tag{12}$$

where γ is the Euler constant. The Bethe logarithm is defined as

$$\ln(k_0) = \frac{\left\langle\sum_a \vec{p}_a(H_0 - \mathcal{E}_0)\ln[2(H_0 - \mathcal{E}_0)]\sum_b \vec{p}_b\right\rangle}{2\pi Z\left\langle\sum_c \delta^3(r_c)\right\rangle}. \tag{13}$$

The operator $H^{(5)}_{\rm fs}$ is the anomalous magnetic moment correction to the spin-dependent part of the Breit-Pauli Hamiltonian. $H^{(5)}_{\rm fs}$ does not contribute to the energies of the singlet states nor to the spin-orbit averaged levels but it yields the $m\alpha^5$ contribution to the fine-structure splitting. It is given by

$$\begin{aligned} H^{(5)}_{\rm fs} = {} & \frac{Z}{4\pi}\sum_a \vec{\sigma}_a \cdot \frac{\vec{r}_a}{r_a^3} \times \vec{p}_a \\ & + \sum_{a<b}\Bigg\{\frac{1}{4\pi}\frac{\sigma_a^i\sigma_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\frac{r_{ab}^i r_{ab}^j}{r_{ab}^2}\right) \\ & + \frac{1}{4\pi r_{ab}^3}[2(\vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_a) \\ & + (\vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_a)]\Bigg\}. \end{aligned} \tag{14}$$

We note that despite the presence of terms with $\ln Z$ in Eq. (10), the correction $\mathcal{E}^{(5)}_\infty(\text{nlog})$ does not have logarithmic terms in its $1/Z$ expansion.

The recoil correction $\mathcal{E}_M^{(5)}$ consists of four parts [10]:

$$\mathcal{E}_M^{(5)} = \frac{m}{M}(\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3) + \langle H^{(5)}_{\text{fs,rec}}\rangle, \tag{15}$$

where

$$\mathcal{E}_1 = -3\mathcal{E}_\infty^{(5)} + \frac{4Z}{3}\sum_a \langle\delta^3(r_a)\rangle - \frac{14}{3}\sum_{a<b}\langle\delta^3(r_{ab})\rangle, \tag{16}$$

$$\mathcal{E}_2 = Z^2\left[-\frac{2}{3}\ln(Z\alpha) + \frac{62}{9} - \frac{8}{3}\ln\left(\frac{k_0}{Z^2}\right)\right]\sum_a\langle\delta^3(r_a)\rangle - \frac{14Z^2}{3}\sum_a \widetilde{Q}_a, \tag{17}$$

with $\widetilde{Q}_a$ defined analogously to Eq. (11), and $(m/M)\mathcal{E}_3$ is the first-order perturbation of $\mathcal{E}_\infty^{(5)}$ due to the mass-polarization operator (6). The operator $H^{(5)}_{\text{fs,rec}}$ yields a nonvanishing contribution to the fine-structure splitting only. It is given by

$$H^{(5)}_{\text{fs,rec}} = \frac{m}{M}\frac{Z}{4\pi}\sum_{ab}\frac{\vec{r}_a}{r_a^3}\times\vec{p}_b\cdot\vec{\sigma}_a. \tag{18}$$

We note that the last term in Eq. (16) was omitted in the original derivation of Ref. [10].

The complete result for the $m\alpha^6$ correction $\mathcal{E}_\infty^{(6)}$ to the energy levels was derived by one of the authors (K.P.) in a series of papers [6,7,11,12] as

$$\mathcal{E}_\infty^{(6)} = -\ln(Z\alpha)\pi\sum_{a<b}\langle\delta^3(r_{ab})\rangle + E_{\text{sec}} + \langle H^{(6)}_{\text{nrad}} + H^{(6)}_{R1} + H^{(6)}_{R2} + H^{(6)}_{\text{fs}} + H^{(6)}_{\text{fs,amm}}\rangle. \tag{19}$$

The first term in this expression contains the complete logarithmic dependence of the $m\alpha^6$ correction. The part of it proportional to $\ln\alpha$ was first obtained in Ref. [13]. The remaining logarithmic part proportional to $\ln Z$ was implicitly present in formulas reported in Ref. [6,7]. (It originates from the expectation value of the operator $1/r_{ab}^3$.) In Eq. (19), we group all logarithmic terms together so that the remaining part does not have any logarithms in its $1/Z$ expansion.

The term E_{sec} in Eq. (19) is the second-order perturbation correction induced by the Breit-Pauli Hamiltonian. (More specifically, it is the finite residual after separating divergent contributions that cancel out in the sum with the expectation value of the effective $m\alpha^6$ Hamiltonian.) The first part of the effective Hamiltonian, $H^{(6)}_{\text{nrad}}$, originates from the nonradiative part of the electron-nucleus and the electron-electron interaction. The next two terms, $H^{(6)}_{R1}$ and $H^{(6)}_{R2}$, are due to the one-loop and two-loop radiative effects, respectively. The last two parts, $H^{(6)}_{\text{fs}}$ and $H^{(6)}_{\text{fs,amm}}$, are the spin-dependent operators first derived by Douglas and Kroll [14]. They do not contribute to the energies of the singlet states nor to the spin-orbit averaged levels. Expressions for these operators are well known and are given, for example, by Eqs. (3) and (7) of Ref. [15]. The nonradiative part of the $m\alpha^6$ effective Hamiltonian is rather complicated. For simplicity, we present it specifically for a two-electron atom. The corresponding expression reads [6,7]

$$\begin{aligned}
H^{(6)}_{\text{nrad}} &= -\frac{\mathcal{E}_0^3}{2} + \left[\left(-\mathcal{E}_0 + \frac{3}{2}\vec{p}_2^{\,2} + \frac{1-2Z}{r_2}\right)\frac{Z\pi}{4}\delta^3(r_1) + (1\leftrightarrow 2)\right] + \frac{\vec{P}^2}{6}\pi\delta^3(r) - \frac{(3+\vec{\sigma}_1\cdot\vec{\sigma}_2)}{24}\pi\,\vec{p}\,\delta^3(r)\,\vec{p} \\
&\quad - \left(\frac{Z}{r_1}+\frac{Z}{r_2}\right)\frac{\pi}{2}\delta^3(r) + \left(\frac{13}{12} + \frac{8}{\pi^2} - \frac{3}{2}\ln(2) - \frac{39\zeta(3)}{4\pi^2}\right)\pi\delta^3(r) + \frac{\mathcal{E}_0^2 + 2\mathcal{E}^{(4)}}{4r} - \frac{\mathcal{E}_0}{r^2}\frac{(31+5\vec{\sigma}_1\cdot\vec{\sigma}_2)}{32} \\
&\quad - \frac{\mathcal{E}_0}{2r}\left(\frac{Z}{r_1}+\frac{Z}{r_2}\right) + \frac{\mathcal{E}_0}{4}\left(\frac{Z}{r_1}+\frac{Z}{r_2}\right)^2 \\
&\quad - \frac{1}{r^2}\left(\frac{Z}{r_1}+\frac{Z}{r_2}-\frac{1}{r}\right)\frac{(23+5\vec{\sigma}_1\cdot\vec{\sigma}_2)}{32} \\
&\quad - \frac{1}{4r}\left(\frac{Z}{r_1}+\frac{Z}{r_2}\right)^2 + \frac{Z^2}{2r_1r_2}\left(\mathcal{E}_0 + \frac{Z}{r_1} + \frac{Z}{r_2} - \frac{1}{r}\right) \\
&\quad - Z\left(\frac{\vec{r}_1}{r_1^3} - \frac{\vec{r}_2}{r_2^3}\right)\cdot\frac{\vec{r}}{r^3}\frac{(13+5\vec{\sigma}_1\cdot\vec{\sigma}_2)}{64} \\
&\quad + \frac{Z}{4}\left(\frac{\vec{r}_1}{r_1^3} - \frac{\vec{r}_2}{r_2^3}\right)\cdot\frac{\vec{r}}{r^2} - \frac{Z^2}{8}\frac{r_1^i}{r_1^3}\frac{(r^ir^j - 3\delta^{ij}r^2)}{r}\frac{r_2^j}{r_2^3} \\
&\quad + \left[\frac{Z^2}{8}\frac{1}{r_1^2}\vec{p}_2^{\,2} + \frac{Z^2}{8}\vec{p}_1\frac{1}{r_1^2}\vec{p}_1 + \vec{p}_1\frac{1}{r^2}\vec{p}_1\frac{(47+5\vec{\sigma}_1\cdot\vec{\sigma}_2)}{64} + (1\leftrightarrow 2)\right] + \frac{1}{4}p_1^i\left(\frac{Z}{r_1}+\frac{Z}{r_2}\right)\frac{(r^ir^j + \delta^{ij}r^2)}{r^3}p_2^j \\
&\quad + P^i\frac{(3r^ir^j - \delta^{ij}r^2)}{r^5}P^j\frac{(-3+\vec{\sigma}_1\cdot\vec{\sigma}_2)}{192} \\
&\quad - \left[\frac{Z}{8}p_2^k\frac{r_1^i}{r_1^3}\left(\delta^{jk}\frac{r^i}{r} - \delta^{ik}\frac{r^j}{r} - \delta^{ij}\frac{r^k}{r} - \frac{r^ir^jr^k}{r^3}\right)p_2^j + (1\leftrightarrow 2)\right] - \frac{\mathcal{E}_0}{8}p_1^2p_2^2 - \frac{1}{4}p_1^2\left(\frac{Z}{r_1}+\frac{Z}{r_2}\right)p_2^2 \\
&\quad + \frac{1}{4}\vec{p}_1\times\vec{p}_2\frac{1}{r}\vec{p}_1\times\vec{p}_2 + \frac{1}{8}p_1^kp_2^l \times\left(-\delta^{jl}\frac{r^ir^k}{r^3} - \delta^{ik}\frac{r^jr^l}{r^3} + 3\frac{r^ir^jr^kr^l}{r^5}\right)p_1^ip_2^j \\
&\quad + \ln(Z)\pi\delta^3(r),
\end{aligned} \tag{20}$$

where $\vec{P} = \vec{p}_1 + \vec{p}_2$, $\vec{p} = (\vec{p}_1 - \vec{p}_2)/2$, and $\vec{r} = \vec{r}_1 - \vec{r}_2$. We note that the operator $H^{(6)}_{\text{nrad}}$ is defined in such a way that its expectation values does not contain any logarithmic terms in the $1/Z$ expansion, as the last term of Eq. (20) is compensated by the corresponding contribution from the $1/r^3$ operator.

The effective Hamiltonians induced by the radiative effects are [6,16,17]

$$H^{(6)}_{R1} = Z^2\left[\frac{427}{96} - 2\ln(2)\right]\pi[\delta^3(r_1)+\delta^3(r_2)] + \left[\frac{6\zeta(3)}{\pi^2} - \frac{697}{27\pi^2} - 8\ln(2) + \frac{1099}{72}\right]\pi\delta^3(r) \tag{21}$$

and

$$H^{(6)}_{R2} = Z\left[-\frac{9\zeta(3)}{4\pi^2} - \frac{2179}{648\pi^2} + \frac{3\ln(2)}{2} - \frac{10}{27}\right]\pi \times[\delta^3(r_1)+\delta^3(r_2)] + \left[\frac{15\zeta(3)}{2\pi^2} + \frac{631}{54\pi^2} - 5\ln(2) + \frac{29}{27}\right]\pi\delta^3(r). \tag{22}$$

The second-order correction can be represented as

$$E_{\rm sec} = \left\langle H^{(4)'}_{\rm nfs}\frac{1}{(E_0-H_0)'}H^{(4)'}_{\rm nfs}\right\rangle + 2\left\langle H^{(4)}_{\rm nfs}\frac{1}{(E_0-H_0)'}H^{(4)}_{\rm fs}\right\rangle + \left\langle H^{(4)}_{\rm fs}\frac{1}{(E_0-H_0)'}H^{(4)}_{\rm fs}\right\rangle, \tag{23}$$

where $H^{(4)}_{\rm nfs}$ and $H^{(4)}_{\rm fs}$ are the spin-independent and spin-dependent parts of the Breit-Pauli Hamiltonian (7), respectively. The operator $H^{(4)'}_{\rm nfs}$ is obtained from $H^{(4)}_{\rm nfs}$ by a transformation that eliminates divergences in the second-order matrix elements [6]. The transformed operator is given by

$$H^{(4)'}_{\rm nfs} = -\frac{1}{2}(\mathcal{E}_0 - V)^2 - p_1^i\frac{1}{2r}\left(\delta^{ij}+\frac{r^ir^j}{r^2}\right)p_2^j + \frac{1}{4}\vec{\nabla}_1^2\vec{\nabla}_2^2 - \frac{Z}{4}\frac{\vec{r}_1}{r_1^3}\cdot\vec{\nabla}_1 - \frac{Z}{4}\frac{\vec{r}_2}{r_2^3}\cdot\vec{\nabla}_2, \tag{24}$$

where $\vec{\nabla}_1^2\vec{\nabla}_2^2$ is understood as a differentiation of the wave function on the right-hand side as a function [omitting $\delta^3(r)$] and $V = -Z/r_1 - Z/r_2 + 1/r$.

An intriguing feature of the formulas presented in this section is that their logarithmic dependence enters only in the form of $\ln(Z\alpha)$. This is not at all obvious *a priori* since $\ln(Z\alpha)$ appears naturally only in contributions induced by the electron-nucleus interaction. The effects of the electron-electron interaction usually yield logarithms of α, whereas logarithms of Z are implicitly present in matrix elements of singular operators. The fact that logarithms of α and logarithms of Z have coefficients that match each other comes "accidentally" from the derivation.

The complete result for the corrections of order $m\alpha^7$ for the helium Lamb shift is not presently available (but it is known for the fine-structure splitting [15,18]). One can, however, easily generalize some of the hydrogenic results, namely those that are proportional to the electron density at the nucleus. These are (i) the one-loop radiative correction of order $m\alpha(Z\alpha)^6\ln^2(Z\alpha)^{-2}$, (ii) the two-loop radiative correction of order $m\alpha^2(Z\alpha)^5$, and (iii) the nonrelativistic correction due to the finite nuclear size. The first two effects yield the main contribution to the higher order remainder function of S states in light hydrogen-like ions. We expect that they dominate for light helium-like ions as well.

Following Ref. [5], we approximate the higher order radiative ("rad") and the finite-nuclear-size ("fs") correction to the energies of helium-like ions by

$$\mathcal{E}^{(7+)}_{\rm rad} = \mathcal{E}^{(7+)}_{\rm rad,H}\frac{\left\langle\sum_i\delta^3(r_i)\right\rangle}{\left\langle\sum_i\delta^3(r_i)\right\rangle_{\rm H}}, \tag{25}$$

$$E_{\rm fs} = E_{\rm fs,H}\frac{\left\langle\sum_i\delta^3(r_i)\right\rangle}{\left\langle\sum_i\delta^3(r_i)\right\rangle_{\rm H}}, \tag{26}$$

where the subscript H corresponds to the "hydrogenic" limit, that is, the limit of the noninteracting electrons and

$$\left\langle\sum_i\delta^3(r_i)\right\rangle_{\rm H} = \frac{Z^3}{\pi}\left(1+\frac{\delta_{l,0}}{n^3}\right). \tag{27}$$

The approximation of Eqs. (25) and (26) is exact for the aforementioned corrections proportional to the electron density at the nucleus. It is expected also to provide a meaningful estimate for contributions that weakly depend on n [such as the nonlogarithmic radiative correction of order $m\alpha(Z\alpha)^6$]. Moreover, this approximation is exact to the leading order in the $1/Z$ expansion, thus providing a meaningful estimate for high-Z helium-like ions as well.

For all the states under consideration except $2\,^1P_1$ and $2\,^3P_1$, the "hydrogenic" remainder function is just the sum of the corresponding remainders for the two electrons in the configuration:

$$\mathcal{E}^{(7+)}_{\rm rad,H} = \mathcal{E}^{(7+)}_{\rm rad}(1s) + \mathcal{E}^{(7+)}_{\rm rad}(nlj). \tag{28}$$

For the $2\,^1P_1$ and $2\,^3P_1$ states, the Dirac levels need to be first transformed from the jj to the LS coupling and thus [5]

$$\begin{aligned}\mathcal{E}^{(7+)}_{\rm rad,H}(2\,^1P_1) &= \mathcal{E}^{(7+)}_{\rm rad}(1s) + \tfrac{2}{3}\mathcal{E}^{(7+)}_{\rm rad}(2p_{3/2}) + \tfrac{1}{3}\mathcal{E}^{(7+)}_{\rm rad}(2p_{1/2}),\\ \mathcal{E}^{(7+)}_{\rm rad,H}(2\,^3P_1) &= \mathcal{E}^{(7+)}_{\rm rad}(1s) + \tfrac{1}{3}\mathcal{E}^{(7+)}_{\rm rad}(2p_{3/2}) + \tfrac{2}{3}\mathcal{E}^{(7+)}_{\rm rad}(2p_{1/2}).\end{aligned} \tag{29}$$

In our calculation, the one-electron remainder function $\mathcal{E}^{(7+)}_{\rm rad}(nlj)$ includes all known contributions of order $m\alpha^7$ and higher coming from (i) the one-loop radiative correction, (ii) the two-loop radiative correction, (iii) the three-loop radiative correction. (See the reviews in Refs. [19,20] for an update on the two-loop remainder function.)

Besides the finite-nuclear-size and radiative corrections, there are also nonradiative effects, denoted as $\mathcal{E}^{(7+)}_{\rm nrad}$ and estimated within the $1/Z$ expansion. More specifically, we include the higher order remainder due to the one-electron Dirac energy and due to the one-photon exchange correction. They enter at the order $m\alpha^8$ only but are enhanced by factors of Z^8 and Z^7, respectively. Despite this enhancement, numerical contributions of these effects are rather small for the ions considered in the present work.

III. RESULTS AND DISCUSSION

A. Numerical results

The nonrelativistic energies and wave functions are obtained by minimizing the energy functional with the basis set constructed with the fully correlated exponential functions. The choice of the basis set and the general strategy of optimization of the nonlinear parameters follow the main lines of the approach developed by Korobov [21,22]. The calculational scheme is described in previous publications [6,7,15] and will not be repeated here. Numerical values of the nonrelativistic energies of helium-like ions with the nuclear charge $Z = 3,\ldots,12$ are presented in Table I. The results were obtained with $N = 2000$ basis functions and are accurate to about 18 decimals (more than shown in the table). The energy levels of the helium atom traditionally attract special attention, so we present the corresponding results in full length. Our numerical values of the upper variational limit of the nonrelativistic energies of helium are

$$\mathcal{E}^{(2)}_\infty(1\,^1S) = -2.903\,724\,377\,034\,119\,598\,310^{+0}_{-2}, \tag{30}$$

$$\mathcal{E}^{(2)}_\infty(2\,^1S) = -2.145\,974\,046\,054\,417\,415\,799^{+0}_{-8}, \tag{31}$$

TABLE I. Nonrelativistic energies of helium-like ions $\mathcal{E}^{(2)}_{\infty}$, $\mathcal{E}^{(2)}_{M}$, and $\mathcal{E}^{(2)}_{M^2}$. For the helium atom, the nonrelativistic energy $\mathcal{E}^{(2)}_{\infty}$ is given in the text [see Eqs. (30)–(34)]. For $\mathcal{E}^{(2)}_{\infty}$ and $\mathcal{E}^{(2)}_{M}$, the results of fitting the numerical data to the form $\mathcal{E} = \sum_i c_i/Z^i$ are also presented. The $1/Z$ expansion of the second-order recoil correction $\mathcal{E}^{(2)}_{M^2}$ was not studied since this correction is relevant for the light atoms only. Atomic units are used.

Z	$1\,^1S$	$2\,^1S$	$2\,^3S$	$2\,^1P$	$2\,^3P$
$\mathcal{E}^{(2)}_{\infty} + Z^2(1+1/n^2)/2$					
3	1.720 086 587 330 694	0.584 123 254 404 560	0.514 272 627 429 260	0.631 648 922 219 983	0.597 284 318 602 632
4	2.344 433 761 576 413	0.815 126 104 651 679	0.702 833 410 222 385	0.889 228 377 083 556	0.825 026 856 929 027
5	2.969 028 419 757 218	1.046 471 967 118 562	0.891 102 651 185 767	1.147 716 734 692 201	1.051 862 307 786 520
6	3.593 753 398 101 470	1.277 982 298 711 029	1.079 244 097 692 043	1.406 667 686 611 591	1.278 289 303 511 949
7	4.218 554 851 227 295	1.509 584 284 500 004	1.267 318 262 508 963	1.665 883 599 383 315	1.504 498 255 070 109
8	4.843 404 877 242 074	1.741 242 692 371 423	1.455 352 679 914 990	1.925 264 764 124 369	1.730 577 283 616 668
9	5.468 287 636 040 509	1.972 938 360 878 370	1.643 361 670 481 692	2.184 755 723 292 205	1.956 572 706 521 290
10	6.093 193 484 962 451	2.204 659 953 768 328	1.831 353 415 926 627	2.444 323 260 421 919	2.182 511 179 215 097
11	6.718 116 223 927 278	2.436 400 325 538 931	2.019 332 929 131 276	2.703 946 297 095 311	2.408 409 121 058 957
12	7.343 051 687 353 070	2.668 154 743 908 730	2.207 303 452 397 112	2.963 610 824 902 483	2.634 277 196 002 167
$1/Z$-expansion coefficients					
c_{-1}	5/8	169/729	137/729	1705/6561	1481/6561
c_0	−0.157 666 43	−0.114 510 14	−0.047 409 30	−0.157 028 66	−0.072 998 98
c_1	0.008 699 03	0.009 327 61	−0.004 872 28	0.026 106 26	−0.016 585 30
c_2	−0.000 888 69	−0.001 284 99	−0.003 457 75	0.005 782 46	−0.010 353 67
c_3	−0.001 036 59	0.006 194 73	−0.002 030 70	−0.005 033 12	−0.005 427 43
c_4	−0.000 610 67	−0.001 471 94	−0.001 278 08	−0.007 099 02	−0.002 001 75
c_5	−0.000 388 13	−0.003 775 51	−0.000 934 77	−0.001 103 32	0.000 100 74
$\mathcal{E}^{(2)}_{M}/(Z^2 m/M)$					
2	0.765 698 46	0.538 869 48	0.545 667 88	0.542 471 90	0.517 147 94
3	0.840 987 69	0.562 509 01	0.569 810 61	0.582 725 90	0.524 732 09
4	0.879 755 41	0.576 178 76	0.582 830 44	0.608 268 18	0.529 299 61
5	0.903 348 97	0.584 990 29	0.590 909 14	0.625 203 60	0.532 349 14
6	0.919 210 60	0.591 123 83	0.596 399 30	0.637 117 06	0.534 516 27
7	0.930 603 34	0.595 633 60	0.600 370 03	0.645 913 88	0.536 130 48
8	0.939 181 63	0.599 086 96	0.603 374 29	0.652 661 02	0.537 377 39
9	0.945 873 29	0.601 815 29	0.605 726 19	0.657 993 92	0.538 368 63
10	0.951 238 85	0.604 024 79	0.607 617 17	0.662 312 12	0.539 175 09
11	0.955 636 86	0.605 850 39	0.609 170 53	0.665 878 55	0.539 843 79
12	0.959 307 33	0.607 384 02	0.610 469 21	0.668 872 98	0.540 407 11
$1/Z$-expansion coefficients					
c_0	1	5/8	5/8	$5/8 + 2^9/3^8$	$5/8 - 2^9/3^8$
c_1	−0.491 706 5	−0.219 681 2	−0.176 992 4	−0.422 232 8	−0.082 563 1
c_2	0.039 651 7	0.100 337 6	0.030 684 4	0.133 727 0	0.045 923 6
c_3	0.012 972 5	−0.009 874 4	0.009 154 5	0.162 310 7	0.009 983 7
c_4	−0.000 022 6	−0.006 744 6	0.003 896 3	−0.000 445 3	−0.007 945 4
c_5	0.003 037 4	0.008 949 1	0.001 835 8	−0.099 048 5	−0.011 326 2
$\mathcal{E}^{(2)}_{M^2}/(Z^2 m^2/M^2)$					
2	−0.923 067 75	−0.575 065 28	−0.561 902 54	−0.596 056 62	−0.552 238 02
3	−1.015 027 87	−0.623 263 22	−0.591 803 40	−0.687 746 68	−0.574 156 42
4	−1.061 762 41	−0.651 489 97	−0.607 626 64	−0.742 385 92	−0.583 335 75
5	−1.090 051 34	−0.669 682 17	−0.617 364 45	−0.776 892 85	−0.588 425 34
6	−1.109 014 61	−0.682 312 57	−0.623 951 64	−0.800 354 77	−0.591 687 77
7	−1.122 610 79	−0.691 572 88	−0.628 701 72	−0.817 261 02	−0.593 967 08
8	−1.132 835 81	−0.698 645 59	−0.632 288 26	−0.829 994 71	−0.595 653 31
9	−1.140 805 12	−0.704 220 80	−0.635 091 75	−0.839 919 81	−0.596 952 97
10	−1.147 190 96	−0.708 727 06	−0.637 343 21	−0.847 868 27	−0.597 986 12
11	−1.152 422 61	−0.712 444 12	−0.639 190 98	−0.854 374 66	−0.598 827 53
12	−1.156 787 03	−0.715 562 17	−0.640 734 67	−0.859 797 49	−0.599 526 27

TABLE II. The leading relativistic corrections $\mathcal{E}^{(4)}_\infty$ and $\mathcal{E}^{(4)}_M$ for helium-like atoms and their $1/Z$-expansion coefficients. The analytical results for the coefficient c_1 for $\mathcal{E}^{(4)}_\infty$ were taken from Ref. [29] for the $1\,^1S$, $2\,^3S$, $2\,^3P_0$, and $2\,^3P_2$ states. For the other states, this coefficient was evaluated numerically to high accuracy in this work by the same method as in Ref. [29]. The c_0 coefficient of $\mathcal{E}^{(4)}_M$ for the S states originates from the one-electron recoil effect and is well known from the hydrogen theory. For the P states, it contains also the two-electron contribution, which was derived in Ref. [36]. The remaining $1/Z$-expansion coefficients were obtained by fitting the numerical data for $\mathcal{E}^{(4)}_\infty$ and $\mathcal{E}^{(4)}_M$. Atomic units are used.

Z	$1\,^1S$	$2\,^1S$	$2\,^3S$	$2\,^1P_1$	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$
$\mathcal{E}^{(4)}_\infty/Z^4$							
2	−0.121 984 67	−0.127 135 46	−0.135 279 87	−0.127 501 60	−0.118 042 52	−0.123 316 23	−0.123 729 58
3	−0.145 794 73	−0.131 881 23	−0.142 840 30	−0.130 953 91	−0.121 128 29	−0.126 601 86	−0.124 410 72
4	−0.163 263 53	−0.136 297 75	−0.147 356 68	−0.133 229 53	−0.126 667 74	−0.130 512 05	−0.125 569 23
5	−0.176 048 64	−0.139 882 98	−0.150 310 08	−0.134 786 60	−0.131 522 71	−0.133 708 51	−0.126 557 82
6	−0.185 674 19	−0.142 737 56	−0.152 383 24	−0.135 917 90	−0.135 444 97	−0.136 216 54	−0.127 342 75
7	−0.193 138 21	−0.145 028 97	−0.153 916 10	−0.136 778 46	−0.138 596 36	−0.138 199 25	−0.127 965 82
8	−0.199 077 87	−0.146 895 44	−0.155 094 63	−0.137 455 97	−0.141 156 38	−0.139 793 29	−0.128 467 48
9	−0.203 909 05	−0.148 439 23	−0.156 028 56	−0.138 003 71	−0.143 266 17	−0.141 097 57	−0.128 878 10
10	−0.207 911 70	−0.149 734 47	−0.156 786 71	−0.138 455 96	−0.145 029 86	−0.142 182 11	−0.129 219 51
11	−0.211 280 06	−0.150 835 16	−0.157 414 35	−0.138 835 82	−0.146 523 58	−0.143 096 91	−0.129 507 41
12	−0.214 152 65	−0.151 781 23	−0.157 942 44	−0.139 159 46	−0.147 803 54	−0.143 878 26	−0.129 753 21
$1/Z$-expansion coefficients							
c_0	−1/4	−21/128	−21/128	−55/384	−21/128	−59/384	−17/128
c_1	0.480 139 61	0.169 478 18	0.076 935 23	0.055 403 03	0.219 768 22	0.130 428 76	0.040 638 72
c_2	−0.636 506 86	−0.281 858 62	−0.042 775 47	−0.090 632 15	−0.303 523 35	−0.162 129 41	−0.047 315 68
c_3	0.456 314 23	0.202 919 21	0.010 473 95	0.156 412 39	0.091 746 25	0.042 468 90	0.002 244 38
c_4	−0.171 179 61	−0.042 542 10	−0.004 460 83	−0.178 042 53	−0.008 844 33	−0.004 319 44	−0.000 236 51
c_5	0.018 587 49	0.018 861 71	−0.001 566 73	0.059 068 31	0.015 552 82	0.007 698 46	0.003 691 05
$\mathcal{E}^{(4)}_M/(Z^4 m/M)$							
2	−0.134 960 7	−0.004 351 6	0.005 574 1	−0.003 655 3	0.015 596 8	0.016 677 1	0.012 760 7
3	−0.123 759 2	−0.001 616 1	0.011 426 9	−0.008 574 4	0.026 148 2	0.026 855 2	0.019 248 5
4	−0.107 627 1	0.002 303 9	0.015 288 3	−0.012 139 6	0.032 666 5	0.032 185 5	0.021 650 8
5	−0.093 784 1	0.005 792 4	0.017 933 4	−0.014 451 6	0.037 580 2	0.035 768 1	0.022 926 5
6	−0.082 625 7	0.008 672 2	0.019 840 8	−0.015 970 4	0.041 407 7	0.038 388 7	0.023 736 9
7	−0.073 647 0	0.011 026 9	0.021 276 3	−0.017 005 1	0.044 450 5	0.040 395 3	0.024 304 7
8	−0.066 337 0	0.012 965 9	0.022 393 8	−0.017 736 6	0.046 915 2	0.041 981 4	0.024 727 6
9	−0.060 299 1	0.014 581 1	0.023 287 6	−0.018 271 0	0.048 946 2	0.043 266 3	0.025 056 1
10	−0.055 241 6	0.015 943 0	0.024 018 4	−0.018 672 8	0.050 645 5	0.044 328 0	0.025 319 3
11	−0.050 950 5	0.017 104 5	0.024 626 8	−0.018 982 2	0.052 086 4	0.045 219 7	0.025 535 1
12	−0.047 267 8	0.018 105 5	0.025 141 1	−0.019 225 6	0.053 322 8	0.045 979 1	0.025 715 5
$1/Z$-expansion coefficients							
c_0	0	1/32	1/32	−0.020 744 7	0.069 205 9	0.055 392 0	0.027 764 2
c_1	−0.645 040 2	−0.182 643 4	−0.078 412 4	0.002 583 0	−0.217 113 6	−0.125 397 2	−0.025 605 0
c_2	0.972 372 8	0.314 800 3	0.062 834 3	0.220 104 6	0.332 302 1	0.157 607 0	0.015 453 2
c_3	−0.460 091 9	−0.188 443 6	−0.018 866 9	−0.387 495 1	−0.152 038 8	−0.096 226 5	−0.036 663 9
c_4	−0.040 368 0	−0.048 228 2	0.000 413 8	−0.046 282 4	−0.252 878 4	−0.030 160 4	−0.017 642 5

$$\mathcal{E}^{(2)}_\infty(2^3S) = -2.175\,229\,378\,236\,791\,305\,738\,977^{+0}_{-2}, \quad (32)$$

$$\mathcal{E}^{(2)}_\infty(2^1P) = -2.123\,843\,086\,498\,101\,359\,246^{+0}_{-2}, \quad (33)$$

$$\mathcal{E}^{(2)}_\infty(2^3P) = -2.133\,164\,190\,779\,283\,205\,146\,96^{+0}_{-10}. \quad (34)$$

The value for the ground state is given only for completeness, since much more accurate numerical results are available in the literature [22,23]. The numerical results for the leading relativistic correction $\mathcal{E}^{(4)}$ are summarized in Table II.

The leading QED correction $\mathcal{E}^{(5)}$ is given by Eqs. (9), (10), and (15). Computationally the most problematic part of it is represented by the Bethe logarithm $\ln(k_0)$ and its mass-polarization correction $\ln(k_0)_M$. Accurate calculations of $\ln(k_0)$ were performed by Drake and Goldman [24] for helium-like like atoms with $Z \leqslant 6$ and by Korobov [25] for $Z = 2$. Calculations of the recoil correction to the Bethe logarithm were reported by Pachucki and Sapirstein [10] for $Z = 2$ and by Drake and Goldman [24] for $Z \leqslant 6$. In the present investigation, we perform accurate evaluations of the Bethe logarithm $\ln(k_0)$ and its recoil correction $\ln(k_0)_M$ for helium-like ions with $Z \leqslant 12$. The calculational approach is described in Appendix A.

Table III summarizes the numerical results obtained and gives a comparison with the previous calculations. Numerical values for the Bethe logarithm are presented for the difference $\ln(k_0) - \ln(Z^2)$ since this difference has a weak Z dependence

TABLE III. Bethe logarithm for helium-like atoms with infinite nuclear mass, $\ln(k_0/Z^2)$, and its first-order perturbation by the mass polarization operator, $\ln(k_0)_M$. Coefficients of the $1/Z$ expansion of $\ln(k_0/Z^2)$ are also presented. The leading term c_0 is known with a high accuracy from the hydrogen theory. The higher order coefficients are obtained by fitting the numerical data.

Z	$1\,^1S$	$2\,^1S$	$2\,^3S$	$2\,^1P$	$2\,^3P$	Ref.
$\ln(k_0/Z^2)$						
2	2.983 865 861 8(1)	2.980 118 365 1(1)	2.977 742 459 29(2)	2.983 803 382 4(1)	2.983 691 003 3(2)	
	2.983 865 860 9(1)	2.980 118 364 8(1)	2.977 742 459 2(1)	2.983 803 377(1)	2.983 690 995(1)	[25]
	2.983 865 857(3)	2.980 118 36(7)	2.977 742 46(1)	2.983 803 46(3)	2.983 690 84(2)	[24]
3	2.982 624 563 0(2)	2.976 363 063 0(2)	2.973 851 709 92(4)	2.983 186 013 6(2)	2.982 958 798 2(2)	
4	2.982 503 099 1(3)	2.973 976 911 2(3)	2.971 735 578 90(7)	2.982 698 213 8(4)	2.982 443 598 4(3)	
5	2.982 591 376 1(4)	2.972 388 098 8(4)	2.970 424 964 90(8)	2.982 340 114 9(8)	2.982 089 604 9(4)	
6	2.982 716 948(1)	2.971 266 246 4(5)	2.969 537 071 9(3)	2.982 072 719(2)	2.981 835 938 5(6)	
	2.982 716 948(4)	2.971 266 24(4)	2.969 537 07(1)	2.982 072 76(2)	2.981 835 92(3)	[24]
7	2.982 839 085(3)	2.970 435 367(1)	2.968 896 814(1)	2.981 867 337(7)	2.981 646 451(2)	
8	2.982 948 318(4)	2.969 796 528(3)	2.968 413 645(2)	2.981 705 33(1)	2.981 499 939(4)	
9	2.983 043 667(8)	2.969 290 586(5)	2.968 036 227(5)	2.981 574 56(3)	2.981 383 443(7)	
10	2.983 126 46(2)	2.968 880 24(1)	2.967 733 341(9)	2.981 466 92(5)	2.981 288 68(1)	
11	2.983 198 50(3)	2.968 540 85(2)	2.967 484 93(2)	2.981 376 9(1)	2.981 210 12(2)	
12	2.983 261 47(5)	2.968 255 57(4)	2.967 277 54(3)	2.981 300 4(2)	2.981 143 96(3)	
Coefficients of the $1/Z$ expansion						
c_0	2.984 128 56	2.964 977 59	2.964 977 59	2.980 376 47	2.980 376 47	
c_1	−0.012 299 28	0.040 788 09	0.027 759 43	0.012 003 83	0.009 627 97	
c_2	0.022 449 74	−0.016 439 35	−0.001 423 95	−0.010 982 08	−0.004 810 60	
c_3	0.003 586 19	−0.012 355 03	−0.005 968 56	−0.000 482 19	−0.002 457 88	
c_4	−0.002 503 70	0.005 813 30	0.000 119 95	0.003 764 32	−0.000 236 70	
$\ln(k_0)_M/(m/M)$						
2	0.094 389 4(1)	0.017 734 4(1)	0.004 785 54(1)	−0.003 553 4(2)	0.008 709 5(1)	
	0.094 38(1)	0.017 734(1)	0.004 784(3)	−0.003 538(6)	0.008 701(4)	[24]
3	0.109 539 7(1)	0.034 210 3(1)	0.007 852 51(1)	−0.006 602 3(2)	0.016 328 3(1)	
4	0.116 919 7(1)	0.044 876 8(1)	0.009 616 61(1)	−0.007 951 2(2)	0.020 199 2(1)	
5	0.121 304 5(2)	0.052 012 4(2)	0.010 754 20(1)	−0.008 629 5(2)	0.022 479 0(1)	
6	0.124 212 9(3)	0.057 053 0(3)	0.011 547 92(1)	−0.009 015 3(2)	0.023 973 6(1)	
	0.124 21(1)	0.057 051(1)	0.011 541(1)	−0.008 98(1)	0.023 98(1)	[24]
7	0.126 283 1(4)	0.060 783 0(9)	0.012 133 20(1)	−0.009 255 6(2)	0.025 027 3(1)	
8	0.127 833 6(5)	0.063 647 0(7)	0.012 582 68(1)	−0.009 416 0(2)	0.025 809 5(2)	
9	0.129 037 1(2)	0.065 912(1)	0.012 938 76(1)	−0.009 528 7(2)	0.026 412 8(3)	
10	0.129 998 9(2)	0.067 746(1)	0.013 227 87(1)	−0.009 611 2(2)	0.026 892 2(4)	
11	0.130 785 1(2)	0.069 261(1)	0.013 467 30(1)	−0.009 673 6(2)	0.027 282 2(4)	
12	0.131 439 7(2)	0.070 534(2)	0.013 668 86(1)	−0.009 722 2(3)	0.027 605 7(4)	

and does not contain any logarithms in its $1/Z$ expansion. The table also lists the coefficients of the $1/Z$ expansion of $\ln(k_0/Z^2)$. The leading coefficient c_0 is known from the hydrogen theory; accurate numerical values can be found in Ref. [26]. The higher order coefficients were obtained by fitting our numerical data. It is interesting to compare them with the analogous results reported previously by Drake and Goldman [24]. For the next-to-the-leading coefficient c_1, the results agree up to about four to five digits for S states and to about three to four digits for P states. For the higher order coefficients, the agreement gradually deteriorates. However, the results for the sum of the two expansions agree very well with each other. More specifically, the maximal absolute deviation between the values of the Bethe logarithms for $Z > 12$ obtained with our $1/Z$-expansion coefficients and with those by Drake and Goldman is 1×10^{-8} for the $1\,^1S$ state, 3×10^{-8} for the $2\,^1S$ state, 6×10^{-9} for the $2\,^3S$ state, 1×10^{-7} for the $2\,^1P$ state, and 6×10^{-8} for the $2\,^3P$ state. So, the accuracy of these expansions is sufficient for most practical purposes.

Another part of the calculation of $\mathcal{E}^{(5)}$ that needs a separate discussion is the evaluation of the expectation value of the singular operator $1/r^3$, which is defined by Eq. (12). The calculational approach is described in Appendix B. Total results for the logarithmic and the nonlogarithmic part of the leading QED correction are summarized in Tables IV and V, respectively. The results are in good agreement with the previous calculations [5].

Table VI presents the numerical values of the $m\alpha^6$ correction, the main result of this investigation. The corresponding calculations for atomic helium were reported in Refs. [6,7]; our present numerical values agree with the ones obtained previously. Calculations performed in this work for helium-like ions were accomplished along the lines described in

TABLE IV. The leading logarithmic QED corrections $\mathcal{E}^{(5)}_\infty(\log)$ and $\mathcal{E}^{(5)}_M(\log)$. For the nonrecoil correction, we present the coefficients of the $1/Z$ expansion obtained by fitting the numerical data (except for c_0, which is known analytically). The recoil correction is very small for ions with $Z > 12$, so its $1/Z$ expansion was not studied. Atomic units are used.

Z	$1\,^1S$	$2\,^1S$	$2\,^3S$	$2\,^1P$	$2\,^3P$
$\mathcal{E}^{(5)}_\infty(\log)/[Z^4\ln(Z\alpha)^{-2}]$					
2	0.587 967 740	0.435 225 697	0.440 118 361	0.424 690 417	0.419 620 202
3	0.661 366 949	0.444 453 845	0.450 745 298	0.425 056 974	0.418 277 856
4	0.702 709 966	0.450 600 513	0.456 788 812	0.425 087 644	0.418 654 616
5	0.729 153 414	0.454 883 655	0.460 628 756	0.425 031 723	0.419 253 068
6	0.747 506 286	0.458 013 834	0.463 274 004	0.424 963 548	0.419 808 283
7	0.760 984 320	0.460 392 952	0.465 204 144	0.424 901 229	0.420 280 937
8	0.771 300 325	0.462 259 020	0.466 673 600	0.424 848 038	0.420 676 712
9	0.779 449 465	0.463 760 328	0.467 829 292	0.424 803 420	0.421 008 829
10	0.786 049 205	0.464 993 553	0.468 761 819	0.424 766 013	0.421 289 730
11	0.791 502 875	0.466 024 214	0.469 530 027	0.424 734 472	0.421 529 561
12	0.796 085 045	0.466 898 202	0.470 173 774	0.424 707 664	0.421 736 263
$1/Z$-expansion coefficients					
c_0	$8/(3\,\pi)$	$3/(2\,\pi)$	$3/(2\,\pi)$	$4/(3\,\pi)$	$4/(3\,\pi)$
c_1	−0.659 550 48	−0.137 744 61	−0.089 756 44	0.003 158 46	−0.036 478 76
c_2	0.330 586 16	0.136 452 03	0.026 693 63	0.009 117 22	0.051 362 86
c_3	−0.132 768 16	−0.061 297 50	0.005 488 16	−0.061 231 69	0.011 132 17
c_4	0.048 550 42	−0.000 485 58	0.001 979 36	0.070 367 56	−0.001 924 41
c_5	−0.005 834 76	−0.000 419 68	0.001 082 09	0.002 994 02	−0.014 225 78
$\mathcal{E}^{(5)}_M(\log)/[(m/M)Z^4\ln(Z\alpha)^{-2}]$					
2	−1.490 787 8	−1.087 827 3	−1.099 571 6	−1.048 033 4	−1.072 942 1
3	−1.503 000 7	−0.999 820 0	−1.013 525 6	−0.931 087 7	−0.972 929 1
4	−1.414 815 1	−0.900 768 2	−0.913 023 5	−0.820 369 5	−0.869 549 4
5	−1.281 038 5	−0.795 295 8	−0.805 624 3	−0.712 358 9	−0.765 222 3
6	−1.122 852 5	−0.685 953 6	−0.694 495 7	−0.605 509 9	−0.660 414 8
7	−0.950 101 1	−0.574 135 7	−0.581 137 5	−0.499 185 8	−0.555 305 8
8	−0.767 968 8	−0.460 648 8	−0.466 344 1	−0.393 108 1	−0.449 990 7
9	−0.579 443 0	−0.345 987 0	−0.350 573 6	−0.287 146 9	−0.344 527 5
10	−0.386 365 2	−0.230 468 4	−0.234 108 4	−0.181 238 4	−0.238 954 2
11	−0.189 932 1	−0.114 306 4	−0.117 131 8	−0.075 350 3	−0.133 296 7
12	0.009 045 2	0.002 350 7	0.000 232 1	0.030 534 1	−0.027 573 6

Refs. [6,7]. Here we only note that calculations for higher values of Z often exhibit a slower numerical convergence (and numerical stability) than for helium, especially so for the second-order corrections involving singular operators. The variational optimization of nonlinear parameters for the symmetric second-order corrections was performed in several steps with increasing the number of basis functions on each step up to $N = 1000$ or 1200. The final values were obtained by merging several basis sets and enlarging the number of functions up to $N = 5000$–7000. The nonsymmetric second-order corrections were evaluated as described in Ref. [15]. The calculations were performed in the quadruple, sixtuple, and octuple arithmetics implemented in FORTRAN 95 by V. Korobov [27].

Table VII presents the results for the finite-nuclear-size correction and approximate values of the higher order ($m\alpha^7$ and higher) correction to the ionization energy. The uncertainty of the total theoretical prediction originates from the higher order radiative effects; it was estimated by dividing the absolute value of this correction by Z. The values for the root-mean-square radius of nuclei were taken from Ref. [28].

B. Comparison with the all-order approach

In this section we discuss the calculational results obtained for the $m\alpha^6$ correction in more detail and make a comparison with the results obtained previously within the all-order, $1/Z$-expansion approach. The logarithmic part of the correction, $\mathcal{E}^{(6)}(\log)$, behaves as $m\alpha^3(Z\alpha)^3$ for large Z and thus corresponds to diagrams with three photon exchanges that have not yet been addressed within the all-order approach. The nonlogarithmic part $\mathcal{E}^{(6)}(\mathrm{nlog})$, however, contains some pieces that are known and identified in the following.

For all states except $2\,^1P_1$ and $2\,^3P_1$, the leading term of the $1/Z$ expansion of $\mathcal{E}^{(6)}(\mathrm{nlog})$ is of order $m(Z\alpha)^6$ and comes from the $Z\alpha$ expansion of the one-electron Dirac energy. For the $2\,^1P_1$ and $2\,^3P_1$ states, the leading term is of the previous order in $1/Z$, $m(Z\alpha)^6 Z$, and is due to the mixing of these levels. More specifically, the mixing contribution is $\delta E_{\mathrm{mix}} = |\langle 2\,^1P_1|H^{(4)}|2\,^3P_1\rangle|^2/[E_0(2\,^1P_1) - E_0(2\,^3P_1)]$ for the $2\,^1P_1$ state and that with the opposite sign for $2\,^3P_1$. The contribution of order $m(Z\alpha)^6$ for the mixing states comes from the expansion of the one-electron Dirac energy and from the expansion of δE_{mix}.

TABLE V. The leading nonlogarithmic QED corrections $\mathcal{E}^{(5)}_{\infty}(\text{nlog})$ and $\mathcal{E}^{(5)}_{M}(\text{nlog})$. For the nonrecoil part, we present the coefficients of the $1/Z$ expansion. The coefficient c_0 is known with a very good accuracy from the hydrogen theory. The remaining coefficients were obtained by numerical fitting. The radiative recoil correction is very small for ions with $Z > 12$, so its $1/Z$ expansion was not studied. Atomic units are used.

Z	$1\,^1S$	$2\,^1S$	$2\,^3S$	$2\,^1P_1$	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$
$\mathcal{E}^{(5)}_{\infty}(\text{nlog})/Z^4$							
2	−1.390 282 4	−1.021 756 7	−1.032 719 5	−0.999 104 6	−0.986 487 5	−0.987 824 8	−0.987 273 6
3	−1.552 423 4	−1.040 733 9	−1.055 874 3	−1.000 028 8	−0.984 014 5	−0.985 285 6	−0.983 645 7
4	−1.645 829 1	−1.053 494 3	−1.068 951 4	−0.999 838 9	−0.985 557 5	−0.986 317 8	−0.983 817 7
5	−1.706 668 4	−1.062 551 3	−1.077 230 3	−0.999 427 5	−0.987 480 3	−0.987 748 5	−0.984 617 0
6	−1.749 464 5	−1.069 274 8	−1.082 920 6	−0.999 028 5	−0.989 184 7	−0.989 040 9	−0.985 437 6
7	−1.781 211 9	−1.074 448 4	−1.087 066 2	−0.998 687 5	−0.990 609 4	−0.990 128 4	−0.986 162 1
8	−1.805 701 0	−1.078 546 0	−1.090 218 7	−0.998 404 7	−0.991 791 0	−0.991 033 0	−0.986 779 7
9	−1.825 165 8	−1.081 868 4	−1.092 695 9	−0.998 170 7	−0.992 776 8	−0.991 788 8	−0.987 303 6
10	−1.841 008 7	−1.084 614 8	−1.094 693 4	−0.997 975 9	−0.993 607 6	−0.992 426 0	−0.987 749 6
11	−1.854 154 5	−1.086 922 2	−1.096 338 0	−0.997 812 2	−0.994 315 0	−0.992 968 8	−0.988 132 3
12	−1.865 237 8	−1.088 887 5	−1.097 715 6	−0.997 673 3	−0.994 923 5	−0.993 435 8	−0.988 463 2
$1/Z$-expansion coefficients							
c_0	−1.995 417 0	−1.113 278 1	−1.113 278 1	−0.996 116 0	−1.002 747 5	−0.999 431 8	−0.992 800 3
c_1	1.658 816 0	0.325 517 0	0.191 147 5	−0.017 559 8	0.106 210 2	0.081 192 9	0.059 452 5
c_2	−1.226 271 4	−0.420 456 0	−0.051 603 3	−0.031 853 8	−0.146 537 2	−0.108 500 3	−0.085 893 4
c_3	0.825 843 5	0.327 325 0	−0.013 194 5	0.247 256 7	−0.016 628 5	−0.029 527 6	−0.036 773 9
c_4	−0.373 062 3	−0.114 627 2	−0.008 949 1	−0.334 953 5	0.006 846 2	0.008 201 3	0.009 431 2
c_5	0.088 160 0	0.037 575 2	0.010 984 6	0.085 299 0	0.018 205 0	0.016 141 2	0.015 502 4
$\mathcal{E}^{(5)}_{M}(\text{nlog})/[(m/M)Z^5]$							
2	3.292 520	2.455 583	2.489 805	2.385 181	2.393 644	2.393 984	2.393 698
3	2.816 621	1.914 328	1.949 969	1.811 294	1.817 918	1.818 182	1.817 751
4	2.527 383	1.642 421	1.673 220	1.526 466	1.531 293	1.531 426	1.530 930
5	2.334 128	1.478 228	1.504 411	1.356 337	1.359 930	1.359 969	1.359 460
6	2.196 193	1.368 117	1.390 605	1.243 181	1.245 918	1.245 898	1.245 400
7	2.092 908	1.289 066	1.308 659	1.162 444	1.164 573	1.164 516	1.164 039
8	2.012 719	1.229 525	1.246 828	1.101 918	1.103 606	1.103 526	1.103 074
9	1.948 679	1.183 048	1.198 512	1.054 847	1.056 206	1.056 113	1.055 685
10	1.896 366	1.145 753	1.159 714	1.017 186	1.018 295	1.018 194	1.017 790
11	1.852 835	1.115 160	1.127 873	0.986 367	0.987 283	0.987 177	0.986 794
12	1.816 049	1.089 607	1.101 272	0.960 678	0.961 441	0.961 334	0.960 971

The next term of the $1/Z$ expansion is of order $m\alpha(Z\alpha)^5$ and comes from the one-electron one-loop radiative correction and from the one-photon exchange correction. The radiative part is well known [19]. The part due to the one-photon exchange was obtained for the $1\,^1S$, $2\,^3S$, $2\,^3P_0$, and $2\,^3P_2$ states analytically in Ref. [29] and for the other states numerically in this work. For the $2\,^1P_1$ and $2\,^3P_1$ states, there is a small additional mixing contribution, which we were unable to determine unambiguously.

The exact results for the first two coefficients of the $1/Z$ expansion of $\mathcal{E}^{(6)}(\text{nlog})$ are listed in Table VI. A fit of our numerical data agrees well with these coefficients. The agreement observed shows consistency of our numerical results with independent calculations at the level of the one-photon effects. We now turn to the contribution of order $m\alpha^2(Z\alpha)^4$. This contribution is induced by nontrivial two-photon effects, so that a comparison drawn for this part will yield a much more stringent test of consistency of different approaches.

The part of $\mathcal{E}^{(6)}(\text{nlog})$ that is of order $m\alpha^2(Z\alpha)^4$ is implicitly present in the two-electron QED contribution calculated numerically in Ref. [8] to all orders in $Z\alpha$. This contribution can be represented as (see Eq. (72) of Ref. [8])

$$\Delta E^{\text{QED}}_{2\text{el}} = m\alpha^2(Z\alpha)^3[a_{31}\ln(Z\alpha)^{-2} + a_{30} + (Z\alpha)G(Z)], \tag{35}$$

where the remainder function $G(Z)$ incorporates all higher orders in $Z\alpha$. The two-electron QED correction comprises the so-called screened self-energy and vacuum-polarization contributions and the part of the two-photon exchange correction that is beyond the Breit approximation.

The coefficients a_{31} and a_{30} in Eq. (35) correspond to the second term of the $1/Z$ expansion of the leading QED correction $\mathcal{E}^{(5)}_{\infty}$. More specifically, a_{31} corresponds to the coefficient c_1 from Table IV and a_{30}, to that from Table V. The $Z = 0$ limit of the higher order remainder function $G(Z)$ corresponds to the third coefficient of the $1/Z$ expansion of the correction $\mathcal{E}^{(6)}(\text{nlog})$, $G(0) = c_2$, for all states except $2\,^1P_1$ and $2\,^3P_1$. The values of c_2 obtained by fitting our numerical data are listed in Table VI. For the $2\,^1P_1$ and $2\,^3P_1$ states, the coefficient c_2 is not directly comparable with the all-order results because of the mixing effects.

TABLE VI. The $m\alpha^6$ corrections $\mathcal{E}_\infty^{(6)}(\log)$ and $\mathcal{E}_\infty^{(6)}(\text{nlog})$ and their $1/Z$-expansion coefficients. Atomic units are used.

Z	$1\,^1S$	$2\,^1S$	$2\,^3S$	$2\,^1P_1$	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$
$\mathcal{E}_\infty^{(6)}(\log)/[Z^3\ln(Z\alpha)^{-2}]$							
2	0.020 880 865	0.001 698 116	0	0.000 144 350	0	0	0
3	0.031 050 719	0.003 738 928	0	0.000 572 351	0	0	0
4	0.037 377 475	0.005 250 650	0	0.001 013 004	0	0	0
5	0.041 625 375	0.006 344 104	0	0.001 386 910	0	0	0
6	0.044 658 932	0.007 157 223	0	0.001 692 317	0	0	0
7	0.046 928 852	0.007 781 230	0	0.001 941 610	0	0	0
8	0.048 689 367	0.008 273 618	0	0.002 147 092	0	0	0
9	0.050 093 825	0.008 671 365	0	0.002 318 555	0	0	0
10	0.051 239 918	0.008 999 033	0	0.002 463 398	0	0	0
11	0.052 192 721	0.009 273 471	0	0.002 587 159	0	0	0
12	0.052 997 208	0.009 506 579	0	0.002 694 007	0	0	0
$1/Z$-expansion coefficients							
c_0	1/16	1/81	0	1/243	0	0	0
c_1	−0.121 468 0	−0.037 197 7	0	−0.019 997 1	0	0	0
c_2	0.091 963 7	0.038 711 4	0	0.037 995 7	0	0	0
c_3	−0.033 400 9	−0.014 283 2	0	−0.032 995 1	0	0	0
c_4	0.004 804 4	0.003 600 0	0	0.008 865 3	0	0	0
c_5	−0.000 487 4	−0.006 272 6	0	0.002 867 7	0	0	0
$\mathcal{E}_\infty^{(6)}(\text{nlog})/Z^6$							
2	2.181 233 3(1)	1.528 981(2)	1.536 593 1(1)	1.489 195(1)	1.459 456(1)	1.460 802(1)	1.466 251(1)
3	1.582 471 7(1)	1.016 337(1)	1.020 440 5(1)	0.977 073(1)	0.945 154(1)	0.937 827(1)	0.950 303(1)
4	1.224 451 9(8)	0.753 467(1)	0.754 660 8(1)	0.723 937(1)	0.691 625(1)	0.676 327(1)	0.696 280(1)
5	0.989 185 0(1)	0.592 746(1)	0.592 238 5(1)	0.574 526(1)	0.539 381(1)	0.517 140(1)	0.544 513(1)
6	0.823 348 1(1)	0.484 094(1)	0.482 626 2(4)	0.477 044(1)	0.437 493(1)	0.408 810(1)	0.443 440(1)
7	0.700 317 8(1)	0.405 658(1)	0.403 650 3(1)	0.409 248(1)	0.364 415(1)	0.329 514(1)	0.371 247(1)
8	0.605 469 6(1)	0.346 341(1)	0.344 035 2(1)	0.360 008(1)	0.309 399(1)	0.268 374(1)	0.317 082(1)
9	0.530 138 1(1)	0.299 896(1)	0.297 436 0(1)	0.323 136(1)	0.266 468(1)	0.219 353(1)	0.274 935(1)
10	0.468 871 6(1)	0.262 537(1)	0.260 008 6(1)	0.294 919(1)	0.232 024(1)	0.178 826(1)	0.241 202(1)
11	0.418 072 5(6)	0.231 831(1)	0.229 287 1(1)	0.272 996(1)	0.203 772(2)	0.144 482(4)	0.213 589(1)
12	0.375 272 1(1)	0.206 144(1)	0.203 617 0(4)	0.255 791(1)	0.180 178(2)	0.114 783(4)	0.190 568(1)
$1/Z$-expansion coefficients							
c_{-1}	0	0	0	729/114688	0	−729/114688	0
c_0	−1/8	−85/1024	−85/1024	−0.079 2398	−85/1024	−0.067 2446	−65/1024
c_1	6.342 8979	3.549 6121	3.487 5483	3.099 80	3.204 5132	3.119 05	3.059 7402
c_2	−4.261 9	−1.042 6	−0.590 0	0.068 6	−0.623 6	−0.260 9	−0.157 8
c_3	2.424 1	1.087 0	0.155 7	−0.039 0	0.833 4	0.328 9	0.271 4
c_4	−2.408 8	−0.815 7	0.053 9	−0.401 3	−0.210 5	0.071 7	0.101 0

The higher order remainder function $G(Z)$ inferred from the numerical results of Ref. [8] is plotted in Fig. 1, together with its limiting value at $Z = 0$ obtained by a fit of our numerical data. It should be stressed that the identification of the remainder implies a great deal of numerical cancellations, especially for the all-order results. The comparison drawn in Fig. 1 provides a stringent cross-check of the two complementary approaches. The visual agreement between the results is very good for the S states, whereas for the P states a slight disagreement seems to be present.

It is tempting to merge the all-order and the $Z\alpha$-expansion results by fitting the all-order data for $G(Z)$ toward lower values of Z. However, we do not attempt to do this in the present work because 1. the numerical accuracy of the all-order results is apparently not high enough and 2. the expansion of the remainder function $G(Z)$ contains terms $(Z\alpha)\ln^2(Z\alpha)$ and $(Z\alpha)\ln(Z\alpha)$, which cannot be reasonably fitted with numerical data available in the high-Z region only.

C. Total energies

Our total results for the ionization energy of the $n = 1$ and $n = 2$ states of helium-like atoms with the nuclear charge $Z = 2,\ldots,12$ are listed in Table VIII. The following values of fundamental constants were employed [19]: $R_\infty = 10\,973\,731.568\,527(73)$ m^{-1} and $\alpha^{-1} = 137.0359\,999\,679(94)$. The atomic masses were taken from Ref. [30].

The results for atomic helium presented in Table VIII differ from those reported previously only because of the different approximate treatment of the higher order ($m\alpha^7$ and higher) contribution employed in this work. For the S states of helium, the present values are practically equivalent to those of Refs. [6,7]. (The difference is that now we include some contributions of order $m\alpha^8$ and higher, which are negligible for helium but become noticeable for higher Z ions.) However, for the helium P states, our present estimate of the higher

TABLE VII. The finite-nuclear-size correction $E_{\rm fs}$ (with the used values of the root-mean-square nuclear charge radii being listed in Table VIII) and the higher order correction $\mathcal{E}^{(7+)} \equiv \mathcal{E}^{(7+)}_{\rm rad} + \mathcal{E}^{(7+)}_{\rm nrad}$. Contributions to the ionization energy are presented. Numerical values of the finite-nuclear-size correction are scaled by the same factor as for the higher order correction, in order to simplify the comparison between them.

Z	$1\,^1S$	$2\,^1S$	$2\,^3S$	$2\,^1P_1$	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$
$E_{\rm fs}/[m\alpha^7 Z^6]$							
2	3.41(1)	0.2346(5)	0.3039(7)	0.00735(2)	−0.0914(3)	−0.0914(3)	−0.0914(3)
3	4.5(1)	0.393(8)	0.47(1)	0.0166(4)	−0.110(3)	−0.110(3)	−0.110(3)
4	3.16(3)	0.305(3)	0.351(3)	0.0114(1)	−0.0623(6)	−0.0622(6)	−0.0623(6)
5	2.01(5)	0.206(5)	0.230(6)	0.0066(2)	−0.0327(8)	−0.0327(8)	−0.0327(8)
6	1.560(4)	0.1655(5)	0.1818(5)	0.00455(1)	−0.02150(6)	−0.02144(6)	−0.02150(6)
7	1.281(8)	0.1396(8)	0.1512(9)	0.00336(2)	−0.01528(9)	−0.01521(9)	−0.01528(9)
8	1.130(6)	0.1256(7)	0.1347(7)	0.00268(1)	−0.01187(6)	−0.01180(6)	−0.01187(6)
9	1.056(5)	0.1191(6)	0.1268(6)	0.00229(1)	−0.00990(5)	−0.00981(5)	−0.00990(5)
10	0.942(5)	0.1076(6)	0.1138(6)	0.00188(1)	−0.00797(4)	−0.00788(4)	−0.00797(4)
11	0.789(5)	0.0911(6)	0.0958(6)	0.00146(1)	−0.00608(4)	−0.00599(4)	−0.00608(4)
12	0.705(5)	0.0821(6)	0.0860(7)	0.001219(9)	−0.00499(4)	−0.00490(4)	−0.00499(4)
$\mathcal{E}^{(7+)}/Z^6$							
2	−8.2(4.1)	−0.43(22)	−0.59(30)	0.093(46)	0.37(18)	0.35(17)	0.31(15)
3	−9.5(3.2)	−0.72(24)	−0.89(30)	0.063(21)	0.37(12)	0.35(12)	0.31(10)
4	−9.6(2.4)	−0.83(21)	−0.97(24)	0.055(14)	0.312(78)	0.294(73)	0.261(65)
5	−9.4(1.9)	−0.86(17)	−0.98(20)	0.052(10)	0.266(53)	0.249(50)	0.219(44)
6	−9.0(1.5)	−0.87(14)	−0.96(16)	0.0510(85)	0.230(38)	0.214(36)	0.187(31)
7	−8.7(1.2)	−0.86(12)	−0.94(13)	0.0500(72)	0.202(29)	0.188(27)	0.162(23)
8	−8.3(1.0)	−0.84(11)	−0.91(11)	0.0490(62)	0.181(23)	0.167(21)	0.144(18)
9	−8.00(89)	−0.825(91)	−0.886(98)	0.0477(54)	0.163(18)	0.150(17)	0.129(14)
10	−7.70(77)	−0.806(80)	−0.859(85)	0.0463(48)	0.148(15)	0.136(14)	0.116(12)
11	−7.43(67)	−0.786(71)	−0.834(75)	0.0450(43)	0.135(13)	0.124(12)	0.1066(97)
12	−7.18(60)	−0.768(63)	−0.811(67)	0.0435(39)	0.124(11)	0.1132(99)	0.0984(82)

order contribution is about 1 MHz higher than that of Ref. [7]. The reason is that the one-electron radiative correction of the p electron state was previously not included in the approximation (25). It is included now [see Eq. (29)] in order to recover the correct asymptotic behavior of the radiative correction in the high-Z limit.

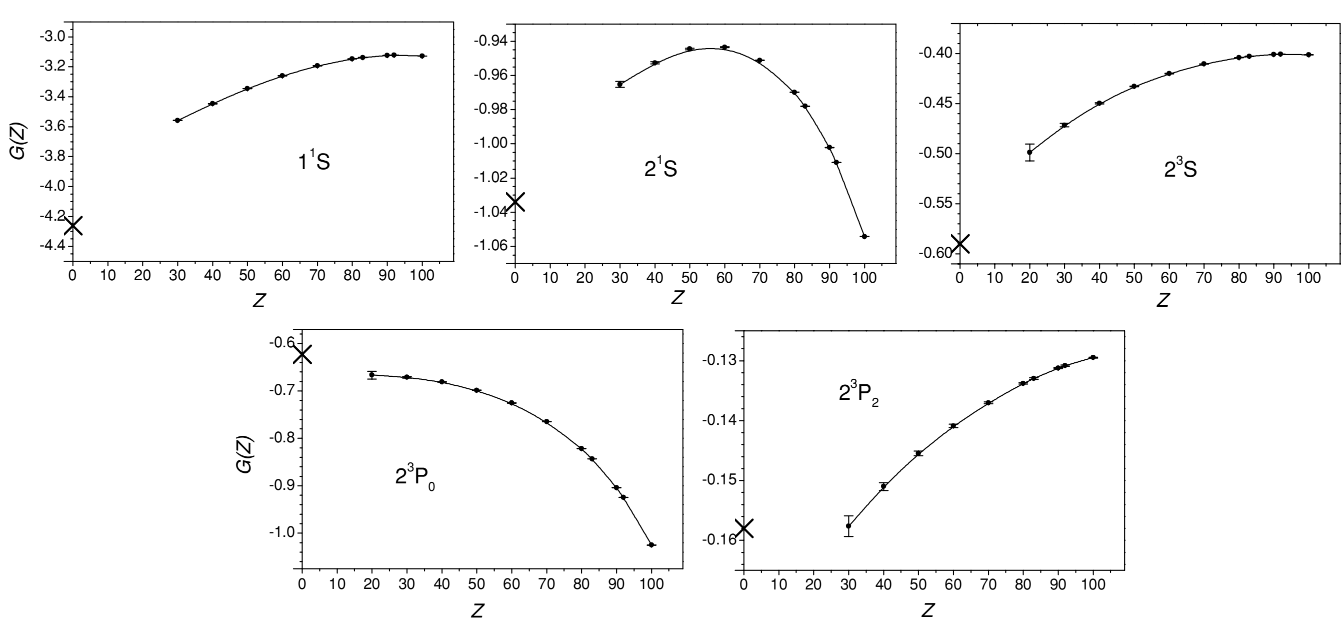

FIG. 1. The higher order remainder function $G(Z)$ from Eq. (35) inferred from the all-order numerical results of Ref. [8] for the two-electron QED correction, in comparison with the $Z = 0$ limit obtained by fitting the $1/Z$ expansion of the $m\alpha^6$ correction calculated in this work (denoted by the cross on the y axis). The all-order results for Z smaller than 30 (in some cases, 20) were left out since their numerical accuracy turns out to be not high enough.

TABLE VIII. Total theoretical ionization energies of $n = 1$ and $n = 2$ states in light helium-like ions, in cm^{-1}. A is the nuclear mass number and R_{ch} is the root-mean-square nuclear charge radius.

Z	A	R_{ch}[fm]	$1\,^1S$	$2\,^1S$	$2\,^3S$
2	4	1.676(3)	−198 310.665 1(12)	−32 033.228 734(63)	−38 454.694 593(86)
3	7	2.43(3)	−610 078.549(11)	−118 704.799 71(79)	−134 044.256 96(98)
4	9	2.52(1)	−1 241 256.625(45)	−260 064.342 7(38)	−284 740.785 8(45)
5	11	2.41(3)	−2 091 995.58(13)	−456 261.994(12)	−490 434.928(14)
6	12	2.470(2)	−3 162 423.60(32)	−707 370.691(31)	−751 130.806(34)
7	14	2.558(7)	−4 452 723.93(66)	−1 013 458.475(66)	−1 066 874.012(72)
8	16	2.701(6)	−5 963 074.2(1.2)	−1 374 588.68(13)	−1 437 720.48(14)
9	19	2.898(2)	−7 693 708.5(2.1)	−1 790 837.48(22)	−1 863 745.75(24)
10	20	3.005(2)	−9 644 843.7(3.5)	−2 262 278.68(36)	−2 345 025.61(39)
11	23	2.994(2)	−11 816 821.8(5.4)	−2 789 016.99(57)	−2 881 669.22(60)
12	24	3.057(2)	−14 209 915.2(8.1)	−3 371 143.82(86)	−3 473 772.54(90)

Z	$2\,^1P_1$	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$
2	−27 175.771 929(13)	−29 222.838 110(54)	−29 223.826 028(51)	−29 223.902 466(45)
3	−108 270.881 302(69)	−115 812.954 89(40)	−115 818.148 68(38)	−115 816.058 08(34)
4	−243 787.567 65(25)	−257 876.174 4(14)	−257 887.732 4(14)	−257 872.840 8(12)
5	−434 000.421 29(74)	−455 041.300 3(37)	−455 057.499 0(35)	−455 004.840 0(31)
6	−679 022.761 7(18)	−707 232.019 2(81)	−707 244.528 3(76)	−707 108.731 2(66)
7	−978 929.118 5(39)	−1 014 453.504(15)	−1 014 444.829(14)	−1 014 153.830(12)
8	−1 333 765.988 7(74)	−1 376 741.630(27)	−1 376 682.831(25)	−1 376 131.273(22)
9	−1 743 582.370(13)	−1 794 154.597(44)	−1 794 003.382(41)	−1 793 045.585(35)
10	−2 208 407.741(22)	−2 266 761.636(70)	−2 266 460.989(65)	−2 264 903.347(54)
11	−2 728 303.815(35)	−2 794 653.26(11)	−2 794 130.721(97)	−2 791 723.350(82)
12	−3 303 295.620(52)	−3 377 923.51(15)	−3 377 091.31(14)	−3 373 518.82(12)

TABLE IX. Comparison of theoretical and experimental transition energies. Units are MHz for He and Li^+ and cm^{-1} for other ions. Results by Drake are from 2005 for He [31], from 1994 for Li^+ [37], and from 1988 for other ions [5].

Z	This work	Drake	Experiment	Reference
$2\,^3P_0$–$2\,^3S_1$ transition:				
2	276 764 094.7(3.0)	276 764 099(17)	276 764 094.678 8(21)	[1]
3	546 560 686(32)	546 560 627	546 560 683.07(42)	[37]
4	26 864.6114(47)	26 864.64(3)	26 864.612 0(4)	[38]
5	35 393.628(14)	35 393.70(8)	35 393.627(13)	[39]
8	60 978.85(14)	60 979.6(5)	60 978.44(52)	[40]
10	78 263.98(39)	78 265.9(1.2)	78 265.0(1.2)	[40]
$2\,^3P_1$–$2\,^3S_1$ transition:				
2	276 734 477.7(3.0)	276 734 476(17)	276 764 477.724 2(20)	[1]
3	546 404 980(31)	546 404 885	546 404 978.80(51)	[37]
4	26 853.0534(47)	26 852.04(3)	26 853.053 4(3)	[38]
5	35 377.429(14)	35 377.40(8)	35 377.424(13)	[39]
8	61 037.65(14)	61 037.7(5)	61 037.62(93)	[40]
$2\,^3P_2$–$2\,^3S_1$ transition:				
2	276 732 186.1(2.9)	276 732 183(17)	276 732 186.593(15)	[1]
3	546 467 655(31)	546 467 553	546 467 657.21(44)	[37]
4	26 867.9450(47)	26 867.92(3)	26 867.948 4(3)	[38]
5	35 430.088(14)	35 430.02(8)	35 430.084(9)	[39]
8	61 589.21(14)	61 589.0(5)	61 589.70(53)	[40]
10	80 122.3(4)	80 121.6(1.2)	80 121.53(64)	[41]
$2\,^1P_1$–$2\,^1S_0$ transition:				
4	16 276.775(4)	16 276.77(3)	16 276.774(9)	[42]
$2\,^3P_1$–$2\,^1S_0$ transition:				
7	986.36(7)	986.6(3)	986.3180(7)	[43]

A selection of our theoretical results for transition energies is compared with the theory by Drake [5,31] and with experimental data in Table IX. Agreement between theory and experiment is excellent in all cases studied. We observe a distinct improvement in theoretical accuracy as compared to the previous results by Drake. This improvement is due to the complete treatment of the corrections of order $m\alpha^6$ and $m^2/M\alpha^5$ accomplished in this work.

Theoretical results for the fine-structure splitting intervals $2\,^3P_0$–$2\,^3P_1$ and $2\,^3P_1$–$2\,^3P_2$ are not analyzed in the present work. This is because these intervals can nowdays be calculated more accurately (complete up to order $m\alpha^7$), as was recently done for helium [15]. We intend to perform such a calculation in a subsequent investigation.

Among the results listed in Table VIII for helium-like ions, the ground-state energy of the carbon ion is of particular importance, because it is used in the procedure of the adjustment of fundamental constants [32] for the determination of the mass of $^{12}C^{4+}$ and, consequently, of the proton mass from the Penning trap measurement by Van Dyck *et al.* [33]. Our result for the ground-state ionization energy of helium-like carbon is

$$E(^{12}\mathrm{C}^{4+}) = -3\,162\,423.60(32)\ \mathrm{cm}^{-1}, \tag{36}$$

which is in agreement with the previous result by Drake [5] of $-3\,162\,423.34(15)\ \mathrm{cm}^{-1}$. We note that, despite our calculation being an additional order of α more complete than that by Drake, our estimate of uncertainty is more conservative.

In summary, significant progress has been achieved during the past few decades in both experimental technique and theoretical calculations of helium-like atoms. In the present investigation, we performed a calculation of the energy levels of the $n = 1$ and $n = 2$ states of light helium-like atoms with the nuclear charge $Z = 2, \ldots, 12$, within the approach complete up to orders $m\alpha^6$ and $m^2/M\alpha^5$. An extensive analysis of the $1/Z$ expansion of individual corrections was carried out and comparison with results of the complementary approach was made whenever possible. Our general conclusion is that the results obtained within the approaches based on the $Z\alpha$ and the $1/Z$ expansion are consistent with each other up to a high level of precision. However, further improvement of numerical accuracy of the all-order, $1/Z$-expansion results and their extension into the lower Z region is needed in order to safely merge the two complementary approaches.

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APPENDIX A: BETHE LOGARITHM

Following the approach of Refs. [34,35], the Bethe logarithm (13) is expressed in terms of an integral over the momentum of the virtual photon,

$$\ln(k_0) = \frac{1}{D}\lim_{K\to\infty}\left[\langle\vec{\nabla}^2\rangle K + D\ln(2K) + \int_0^K dk\,k\,J(k)\right], \tag{A1}$$

where $D = 2\pi Z\langle\delta^3(r_1)+\delta^3(r_2)\rangle$, $\vec{\nabla} \equiv \vec{\nabla}_1 + \vec{\nabla}_2$, and

$$J(k) = \left\langle \vec{\nabla}\frac{1}{E_0 - H_0 - k}\vec{\nabla}\right\rangle. \tag{A2}$$

For the purpose of numerical evaluation, the integration over the photon momentum k is divided into two regions by introducing the auxiliar parameter κ,

$$\ln(k_0) = R(\kappa) + \frac{1}{D}\int_0^\kappa dk\,k\,J(k) + \int_\kappa^\infty dk\,\frac{w(k)}{k^2}, \tag{A3}$$

where the function $w(k)$ represents the residual obtained from $J(k)$ by removing all known terms of the large-k asymptotics,

$$w(k) = \frac{k^3}{D}J(k) + \frac{k^2}{D}\langle\vec{\nabla}^2\rangle + k - 2\sqrt{2}Zk^{1/2} + 2Z^2\ln k, \tag{A4}$$

and $R(\kappa)$ is a simple function obtained by integrating out the separated asymptotic expansion terms,

$$R(\kappa) = \kappa\frac{\langle\vec{\nabla}^2\rangle}{D} + \ln(2\kappa) + \frac{4\sqrt{2}Z}{\kappa^{1/2}} - \frac{2Z^2(\ln\kappa + 1)}{\kappa}. \tag{A5}$$

The calculational scheme employed for the evaluation of Eq. (A3) is similar to that previously used [15] for the relativistic corrections to the Bethe logarithm. At the first step, a careful optimization of nonlinear basis-set parameters was carried out for a sequence of scales of the photon momentum: $k_i = 10^i$ and $i = 1, \ldots, i_{\max}$, with $i_{\max} = 5$ for the S states and $i_{\max} = 4$ for the P states. The optimization was performed with incrementing the size of the basis until the prescribed level of convergence is achieved for the function $w(k)$. At the second step, the integrations of the photon momentum k were performed. For a given value of k, the function $J(k)$ was calculated with a basis obtained by merging together the optimized bases for the two closest k_i points, thus essentially doubling the number of the basis functions. The function $w(k)$ was obtained from $J(k)$ according to Eq. (A4).

The integral over $k \in [0,\kappa]$ was calculated analytically, by diagonalizing the Hamiltonian matrix and using the spectral representation of the propagator. The value of the auxiliary parameter κ was set to $\kappa = 100$. The integral over $k \in [\kappa,\infty)$ was separated into two parts, $k < 10^{i_{\max}}$ and $k > 10^{i_{\max}}$. The first part was evaluated numerically by using Gauss-Legendre quadratures, after the change of variables $t = 1/k^2$. The second part was obtained by integrating the asymptotic expansion of the function $w(k)$. The coefficients of this expansion were obtained by fitting the numerical data for $w(k)$ to the form

$$w(k) = \mathrm{pol}\left(\frac{1}{\sqrt{k}}\right) + \frac{\ln k}{k}\mathrm{pol}\left(\frac{1}{k}\right), \tag{A6}$$

where $\mathrm{pol}(x)$ denotes a polynomial of x. The total number of fitting parameters was about 9–11. The range of k to be fitted and the exact form of the fitting function were optimized so as to yield the best possible results for the known asymptotic expansion terms of $J(k)$.

The first-order perturbation of the Bethe logarithm by the mass-polarization operator can be represented as [10]

$$\ln(k_0)_M = \frac{m}{M}\left[R_M(\kappa) + \frac{1}{D}\int_0^\kappa dk\, k\, J_M(k) + \int_\kappa^\infty dk\, \frac{w_M(k)}{k^2}\right], \tag{A7}$$

where

$$J_M(k) = 2\langle\phi|\vec{\nabla}\frac{1}{E_0 - H_0 - k}\vec{\nabla}|\delta\phi\rangle + \langle\phi|\vec{\nabla}\frac{1}{E_0 - H_0 - k}[\delta E - \vec{p}_1\cdot\vec{p}_2]\frac{1}{E_0 - H_0 - k}\vec{\nabla}|\phi\rangle \tag{A8}$$

and $\delta E = \langle \vec{p}_1 \cdot \vec{p}_2\rangle$. The perturbed wave function $\delta\phi$ is defined by

$$|\delta\phi\rangle = |\delta_M\phi\rangle - |\phi\rangle\frac{\delta_M D}{D}, \tag{A9}$$

where δ_M stands for the first-order perturbation induced by the operator $\vec{p}_1 \cdot \vec{p}_2$. The asymptotic expansion of $J_M(k)$ is much simpler than that of $J(k)$ and $w_M(k)$ is just

$$w_M(k) = \frac{k^3}{D}J_M(k) + \frac{k^2}{D}2\langle\phi|\vec{\nabla}^2|\delta\phi\rangle. \tag{A10}$$

Correspondingly, the function $R_M(\kappa)$ is

$$R_M(\kappa) = \frac{2\kappa}{D}\langle\phi|\vec{\nabla}^2|\delta\phi\rangle. \tag{A11}$$

The numerical evaluation of Eq. (A7) was performed in a way similar to that for the plain Bethe logarithm. In particular, the same sets of optimized nonlinear parameters were used. Since a high accuracy is not needed for this correction, a somewhat simplified calculational scheme was used in this case. The high-energy part of the photon-momentum integral, $k \in [100, \infty)$, was evaluated by integrating the fitted asymptotic expansion for $w_M(k)$, which was taken to be of the form (A6) with 6–9 fitting parameters.

APPENDIX B: EXPECTATION VALUE OF $1/r^3$

The definition of the expectation value of the regularized operator $1/r^3$ is given by Eq. (12). With the basis-set representation of the wave function employed in this work, a typical singular integral to be calculated is

$$I_\epsilon = \frac{1}{16\pi^2}\int d^3r_1 d^3r_2 \frac{\exp(-\alpha r_1 - \beta r_2 - \gamma r)}{r^3}\Theta(r-\epsilon). \tag{B1}$$

The straightforward way is to evaluate this integral analytically for a finite value of the regulator ϵ and then expand it in small ϵ. This way is possible, but we prefer to use a simpler procedure, which is also the closest to the method of evaluation of the regular integrals.

We recall that all regular integrals are immediately obtained from the master integral

$$\frac{1}{16\pi^2}\int d^3r_1 d^3r_2 \frac{\exp(-\alpha r_1 - \beta r_2 - \gamma r)}{r_1 r_2 r} = \frac{1}{(\alpha+\beta)(\beta+\gamma)(\alpha+\gamma)} \tag{B2}$$

by formal differentiation or integration with respect to the corresponding parameters. The differentiation over α and β and an integration over γ delivers a result for the integral of the type $1/r^2$. This integral is convergent, so the result is exact. The second integration over γ (which would yield an integral of the type $1/r^3$) is divergent. The simplest way to proceed is as follows. We introduce a cutoff parameter for large values of γ, evaluate the integral over γ, and drop all cutoff-dependent terms. The expression obtained in this way differs from the correct one by a γ-independent constant only, which can be proved by differentiating with respect to γ.

The missing constant is most easily recovered by considering the behavior of the integral I when $\gamma \to \infty$. For very large γ, only the region of very small r contributes and we have

$$I_\epsilon = 2\int_\epsilon^\infty dr\, r \int_0^\infty dr_1 r_1 \int_{|r_1-r|}^{r_1+r} dr_2 r_2 \frac{e^{-\alpha r_1 - \beta r_2 - \gamma r}}{r^3} \approx \frac{2}{(\alpha+\beta)^3}\int_\epsilon^\infty dr\, \frac{e^{-\gamma r}}{r}. \tag{B3}$$

Therefore,

$$I_{\rm reg} \equiv \lim_{\epsilon\to 0}[I_\epsilon + \gamma + \ln\epsilon] \overset{\gamma\to\infty}{=} -\frac{2}{(\alpha+\beta)^3}\ln\gamma. \tag{B4}$$

This equation yields the necessary condition for determining the missing constant term in the general expression for the regularized integral $I_{\rm reg}$.

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