QED $m\alpha^7$ effects for triplet states of helium-like ions

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We perform \textit{ab initio} calculations of the QED effects of order $m\alpha^7$ for the $2^3S$ and $2^3P$ states of He-like ions. The computed effects are combined with previously calculated energies from [V. A. Yerokhin and K. Pachucki, Phys. Rev. A \textbf{81}, 022507 (2010)], thus improving the theoretical accuracy by an order of magnitude. The obtained theoretical values for the $2^3S$-$2^3P_{0,2}$ transition energies are in good agreement with available experimental results and with previous calculations performed to all orders in the nuclear binding strength parameter $Z\alpha$. For the ionization energies, however, we find some inconsistency between the $Z\alpha$-expansion and all-order calculations, which might be related to a similar discrepancy between the theoretical and experimental results for the ionization energies of helium [V. Patkůš et al., Phys. Rev. A \textbf{103}, 042809 (2021)].

I. INTRODUCTION

Significant progress has recently been achieved in the theoretical description of the Lamb shift in the helium atom. After extensive efforts, a complete calculation of the QED effects of order $m\alpha^7$ has been accomplished for the triplet states of the helium atom [1–4]. This calculation improved the accuracy of the theoretical energies of the $2^3S$ and $2^3P$ states of helium by more than an order of magnitude and made the theoretical predictions sensitive to the nuclear charge radius on the 1% level. The theoretical result for the $2^3S$-$2^3P$ transition energy was found to be in excellent agreement with the experimental value [5]. However, the individual ionization energies of the $2^3S$ and $2^3P$ states were shown to deviate by $10\sigma$ from the experimental results [6].

In the present work we extend our calculations of the $m\alpha^7$ effects from helium to helium-like ions. The goal of this investigation is twofold. First, our calculations will improve the theoretical accuracy of the $2^3S$-$2^3P$ transition energies in light He-like ions. This is of particular importance in the case of Li$^7$, for which very precise experimental results are available [7]. Second, calculations of the $m\alpha^7$ effects for different nuclear charges $Z$ will allow us to study the $Z$-dependence of this correction (in particular, the high-$Z$ asymptotics) and to perform a cross-check against the hydrogen theory and independent calculations carried out to all orders in the nuclear binding strength parameter $Z\alpha$.

II. GENERAL FORMULAS

The QED effects of order $m\alpha^7$ for the centroid energy of triplet states of helium-like atoms were derived by us in a series of works [1–4]. In this paper we transform the obtained formulas to a form that is relatively compact and more suitable for studying the $Z$-dependence of these effects.

Formulas derived in previous works contained logarithmic contributions of two types, specifically, $\ln(Z\alpha)$ in the electron-nucleus terms and $\ln(\alpha)$ in the electron-electron terms. In addition, there were terms with $\ln(Z)$ implicitly present in matrix elements of individual operators and the Bethe-logarithm contributions. In the present work we show that the complete dependence of the $m\alpha^7$ correction on $\ln(Z\alpha)$ and $\ln(\alpha)$ can be factorized out in terms of $\ln(Z\alpha)$ and $\ln^3(Z\alpha)$. The exact matching of coefficients at $\ln(Z\alpha)$ and $\ln(\alpha)$ in the electron-electron terms served as an important cross-check of our derivation.

The QED correction of order $m\alpha^7$ for the centroid energy of triplet states of helium-like atoms is represented as a sum of the double-logarithmic, single-logarithmic, and non-logarithmic contributions,

$$E^{(7)} = E^{(7,2)} \ln^2(Z\alpha)^{-2} + E^{(7,1)} \ln(Z\alpha)^{-2} + E^{(7,0)} \quad (1)$$

where contributions $E^{(7,i)}$ do not contain any logarithms in their $1/Z$ expansion and are defined as follows,

$$E^{(7,2)} = -\frac{1}{2\pi} Z^3 Q_1 = -2Z^3 \langle \delta^3(r_1) \rangle, \quad (2)$$
\[ E^{(7,1)} = \frac{1}{3\pi} \left[ -8E_0 E_4 - \frac{Z}{5} \left( \frac{19}{3} + 11Z \right) Q_3 + \frac{11Z}{10} Q_4 - \frac{39}{10} Q_6 T + 4E_4 Q_7 + Z \left( - \frac{E_0}{5} + \frac{9Z^2}{8} + 8Z^2 \ln 2 + Q_7 \right) Q_1 + \frac{26}{5} Q_{10} + 4E_0 Z^2 Q_{11} + 8E_0 Z^2 Q_{12} - 8E_0 Z Q_{13} - 8Z^2 Q_{14} + 8Z^3 Q_{15} - 4Z^2 Q_{16} + 4Z Q_{17} - \frac{38Z^2}{5} Q_{18} + 2Z^2 Q_{21} + 2Z^2 Q_{22} + 4Z Q_{24} - 2Z Q_{28} + \frac{11Z}{10} Q_{31} + 4E_0^2 Z Q_{53} - \frac{Z}{5} Q_{62} + 3Z^2 \tilde{Q}_{57} + 2 \left\langle H_R \left( E_0 - H_0 \right) H_R \right\rangle \right], \tag{3} \]

\[ E^{(7,0)} = \frac{1}{90\pi} \left\{ -8E_0 E_4 \left( 19 - 30 \ln 2 \right) + Z \left( - \frac{53183}{420} - \frac{2003Z}{140} + 82 \ln 2 + 66Z \ln 2 \right) Q_3 + Z \left( \frac{2003}{280} - 33 \ln 2 \right) Q_1 + \left( \frac{14971}{70} + 36 \ln 2 \right) Q_6 T + \left( 76E_4 - 120E_4 \ln 2 - 105Q_9 \right) Q_7 + \left( \frac{9543}{20} - 264 \ln 2 \right) Q_{10} + 4E_0 Z^2 \left( 19 - 30 \ln 2 \right) Q_{11} + 8E_0 Z^2 \left( 19 - 30 \ln 2 \right) Q_{12} - 8E_0 Z \left( 19 - 30 \ln 2 \right) Q_{13} - 8Z^2 \left( 19 - 30 \ln 2 \right) Q_{14} + 8Z^3 \left( 19 - 30 \ln 2 \right) Q_{15} - 4Z^2 \left( 19 - 30 \ln 2 \right) Q_{16} + 4Z \left( 19 - 30 \ln 2 \right) Q_{17} + Z \left( - \frac{2757}{10} + 288 \ln 2 \right) Q_{18} + 2Z^2 \left( 19 - 30 \ln 2 \right) Q_{21} + 2Z^2 \left( 19 - 30 \ln 2 \right) Q_{22} + 4Z \left( 19 - 30 \ln 2 \right) Q_{24} + 105Q_{25} - 2Z \left( 19 - 30 \ln 2 \right) Q_{28} + Z \left( \frac{3893}{280} - 33 \ln 2 \right) Q_{51} + Z \left( 76E_0^2 - 120E_0^2 \ln 2 + 105Q_9 \right) Q_{53} - 105Z Q_{59} + \frac{105}{4} Q_{61} + 4Z \left( \frac{7}{5} + 3 \ln 2 \right) Q_{62} + 88Z \tilde{Q}_{52} - 72 \tilde{Q}_{54} - 297 \tilde{Q}_{55} + Z^2 \left( \frac{513}{4} - 90 \ln 2 \right) Q_{57} - 24Z \tilde{Q}_{58} - 63 \tilde{Q}_{60} + 12Z \tilde{Q}_{63} + Z \left[ \frac{3317E_0}{140} + \frac{5755Z^2}{56} - \frac{85\pi^2 Z^2}{6} + 6E_0 \ln 2 - 362Z^2 \ln 2 + 45Z^2 \ln^2 2 + 19 \left( 19 - 30 \ln 2 \right) Q_7 + \frac{225Z^2}{2} \zeta(3) \right] Q_1 \right\} + \frac{Z^3}{2\pi} \beta_L Q_1 + \frac{Z^2}{2\pi^2} B_{50} Q_1 + \frac{Z}{2\pi^3} C_{40} Q_1 + E_{sec}. \tag{4} \]

In the above formulas, \( Q_1 \ldots Q_{64} \) are the expectation values of the basic elementary operators defined in Table I. Some of \( Q_i \) contain implicitly terms with \( \ln(Z) \), which need to be separated out. We thus introduced expectation values \( \tilde{Q}_i \), which are free from \( \ln(Z) \) and are defined by

\[ Q_{52} = Q_{52} - 1 \ln Z^{-2} Q_3, \tag{5} \]

\[ Q_{54} = Q_{54} - 1 \ln Z^{-2} Q_{10}, \tag{6} \]

\[ Q_{55} = Q_{55} - 1 \frac{1}{6} \ln Z^{-2} Q_{6T}, \tag{7} \]

\[ Q_{56} = Q_{56} - 1 \frac{1}{2} \ln Z^{-2} Q_1, \tag{8} \]

Further notations in Eqs. (3) and (4) are as follows: \( E_0 \) is the nonrelativistic energy, \( E_4 \) is the leading relativistic (Breit) correction of order \( m \alpha^4 \), \( \beta_L \) is the relativistic Bethe-logarithm correction defined as in Ref. [8], \( B_{50} = -21.55447 \) and \( C_{40} = 0.417503770 \) are the hydrogenic two-loop \((Z \alpha)^5\) and three-loop \((Z \alpha)^4\) expansion coefficients, respectively, see

\[ Q_{57} = Q_{57} - Z \ln Z^{-2} Q_1, \tag{9} \]

\[ Q_{58} = Q_{58} + \frac{1}{2} \ln Z^{-2} Q_{18}, \tag{10} \]

\[ Q_{60} = Q_{60} + \frac{1}{2} \ln Z^{-2} Q_{6T}, \tag{11} \]

\[ Q_{63} = Q_{63} + \frac{1}{2} \ln Z^{-2} Q_{62}. \tag{12} \]
Ref. [9], and $E_{\text{sec}}$ is the second-order correction given by

$$
E_{\text{sec}} = 2 \left( H_{fs}^{(5)} \right) \left( E_0 - H_0 \right) \frac{1}{H_{fs}^{(4)}} 
+ \frac{1}{\pi} \left( \frac{19}{45} - \frac{2}{3} \ln 2 \right) \left( H_{R}^{(4)} \right) \frac{1}{H_{fs}^{(4)}} H_{R}^{(4)} 
- \frac{7}{3\pi} \left( E_0 - H_0 \right) \frac{1}{H_{fs}^{(4)}} H_{R}^{(4)}.
$$

(13)

The effective Hamiltonians in the above formulas are defined as follows. $H_{R}$ is a regular part of the spin-independent Breit Hamiltonian and is defined by its action on a ket eigenstate $|\phi\rangle$ of the nonrelativistic Hamiltonian with the energy $E$ as

$$
H_{R}|\phi\rangle = \left[ -\frac{1}{2}(E-V)^2 - Z \frac{\vec{r}_1 \cdot \vec{\nabla}_1}{r_1^3} - Z \frac{\vec{r}_2 \cdot \vec{\nabla}_2}{r_2^3} 
+ \frac{1}{4} \nabla_1^2 \nabla_2^2 + \nabla_1 \frac{1}{2r} \left( \delta^{ij} + \frac{\vec{r}^i \vec{r}^j}{r^2} \right) \nabla_2^2 \right] |\phi\rangle,
$$

(14)

where $V = -Z/r_1 - Z/r_2 + 1/r$. The operator $H'_R$ is defined by its action on a ket $|\phi\rangle$ as

$$
H'_R|\phi\rangle = -2Z \left( \frac{\vec{r}_1 \cdot \vec{\nabla}_1}{r_1^3} + \frac{\vec{r}_2 \cdot \vec{\nabla}_2}{r_2^3} \right) |\phi\rangle.
$$

(15)

The operators $H_{fs}^{(4)}$ and $H_{fs}^{(5)}$ are the $m\alpha^4$ and $m\alpha^5$ parts of the spin-dependent Breit Hamiltonian $H_{fs}$ with anomalous magnetic moment, correspondingly,

$$
H_{fs} = \alpha^4 H_{fs}^{(4)} + \alpha^5 H_{fs}^{(5)} + O(\alpha^6),
$$

(16)

$$
H_{fs} = \frac{\alpha}{4m^2} \left( \frac{\vec{\sigma}_1 \cdot \vec{\sigma}_2}{r_3^3} - 3 \frac{\vec{\sigma}_1 \cdot \vec{r} \vec{\sigma}_2 \cdot \vec{r}}{r_5^5} \right) (1 + \kappa)^2 
+ \frac{Z\alpha}{4m^2} \left[ \frac{1}{r_1} \vec{r}_1 \times \vec{p}_1 \cdot \vec{\sigma}_1 + \frac{1}{r_2} \vec{r}_2 \times \vec{p}_2 \cdot \vec{\sigma}_2 \right] (1 + 2\kappa) 
+ \frac{\alpha}{4m^2 r_3^3} \left[ \left( 1 + 2\kappa \right) \vec{\sigma}_2 + 2(1 + \kappa) \vec{\sigma}_1 \right] \cdot \vec{r} \times \vec{p}_2 
- \left( 1 + 2\kappa \right) \vec{\sigma}_1 \cdot 2(1 + \kappa) \vec{\sigma}_2 \cdot \vec{r} \times \vec{p}_1,
$$

(17)

where $\kappa = \alpha/(2\pi) + O(\alpha^2)$ is the anomalous magnetic moment of the electron.

### III. HIGHER-ORDER EFFECTS

The effects of order $m\alpha^8$ and higher cannot be calculated rigorously at present and need to be estimated. Our approximation for these effects is represented as a sum of three terms,

$$
E_{\text{rad}}^{(8+)} = E_{D}^{(8)} + E_{\text{ph}}^{(8)} + E_{\text{rad}}^{(8+)},
$$

(18)

where $E_{D}^{(8)}$ comes from the one-electron Dirac energy, $E_{\text{ph}}^{(8)}$ originates from the one-photon exchange correction, and $E_{\text{rad}}^{(8+)}$ represents the radiative QED effects.

The Dirac contribution to the ionization energy of an 1s$n$l state comes from the valence electron, $E_D = E_D(nl)$ and is given by

$$
E_{D}^{(8)}(2s) = E_{D}^{(8)}(2p_{1/2}) = -\frac{429}{32768} Z^8,
$$

(19)

$$
E_{D}^{(8)}(2p_{3/2}) = -\frac{5}{32768} Z^8.
$$

(20)

The one-photon exchange correction of order $m\alpha^8$ was calculated in Ref. [10], with the result

$$
E_{\text{ph}}^{(8)}(23S) = 0.0281 Z^7,
$$

(21)

$$
E_{\text{ph}}^{(8)}(23P_1) = 0.1070 Z^7,
$$

(22)

$$
E_{\text{ph}}^{(8)}(23P_2) = 0.0037 Z^7.
$$

(23)

We note a relative large numerical contribution of the one-photon exchange correction for the $2^3H_0$ state.

An approximation for the radiative QED contribution of order $m\alpha^8$ and higher is obtained by scaling the hydrogenic results with the expectation value of the $\delta$-function [11, 12],

$$
E_{\text{rad}}^{(8+)} = \left[ E_{\text{rad},H}(1s) + E_{\text{rad},H}(nl) \right] \frac{\langle \sum_i \delta^3(r_i) \rangle}{Z^3} \left( 1 + \frac{\delta_{\text{QED}}}{n^3} \right)
$$

(24)

$$
- E_{\text{rad},H}(1s),
$$

where $E_{\text{rad},H}(nl)$ is the hydrogenic QED contribution of order $m\alpha^8$ and higher of an $nl$ state. This contribution consists of the one-loop and two-loop effects, which are reviewed in Ref. [9]. We estimate the uncertainty of this approximation for He-like ions as 75% of the few-body part of $E_{\text{rad}}^{(8+)}$, specifically,

$$
\delta E_{\text{rad}}^{(8+)} = \pm 0.75 \left[ E_{\text{rad},H}(1s) + E_{\text{rad},H}(nl) \right] \times \left[ \frac{\langle \sum_i \delta^3(r_i) \rangle}{Z^3} \left( 1 + \frac{\delta_{\text{QED}}}{n^3} \right) - 1 \right].
$$

(25)

In addition we include the finite nuclear size correction, which is obtained from the corresponding hydrogenic corrections analogously to Eq. (24), see Ref. [12] for details.

### IV. NUMERICAL RESULTS

In this work we performed calculations of the $m\alpha^7$ effects for the centroid energies of the $2^3S$ and $2^3P$ states of helium-like ions with $Z \leq 12$. The computations followed the numerical approach developed in our previous investigations [4, 12] and used results for the relativistic Bethe-logarithm correction obtained in Ref. [8].

Numerical values for the $m\alpha^7$ corrections to energies of the $2^3S$, $2^3P_0$, and $2^3P_2$ states of helium and helium-like ions are presented in Table II. Results for the $2^3P_{1/2}$ states are obtained by combining the $m\alpha^7$ correction for the $2^3P_1$ centroid
TABLE I. Definitions of basic elementary operators $Q_i$. Notations are: $r \equiv |r_1 - r_2|$, $\vec{P} = \vec{p}_1 + \vec{p}_2$, $\vec{p} = \frac{1}{2} (\vec{p}_1 - \vec{p}_2)$.

| $Q_1$ | $4\pi \delta^3(r_1)$ |
| $Q_2$ | $4\pi \delta^3(r)$ |
| $Q_3$ | $4\pi \delta^3(r_1)/r_2$ |
| $Q_4$ | $4\pi \delta^3(r_1)\vec{p}_2^2$ |
| $Q_5$ | $4\pi \delta^3(r)/r_1$ |
| $Q_{6T}$ | $4\pi \vec{p} \delta^3(r) \vec{p}$ |
| $Q_7$ | $1/r$ |
| $Q_8$ | $1/r^2$ |
| $Q_9$ | $1/r^3$ |
| $Q_{10}$ | $1/r^4$ |
| $Q_{11}$ | $1/r^2_1$ |
| $Q_{12}$ | $1/(r_1r_2)$ |
| $Q_{13}$ | $1/(r_1r)$ |
| $Q_{14}$ | $1/(r_1r_2r)$ |
| $Q_{15}$ | $1/(r_1^2r_2)$ |
| $Q_{16}$ | $1/(r_1r_2^2)$ |
| $Q_{17}$ | $1/(r_1r^2)$ |
| $Q_{18}$ | $(r_1^2 - r_2^2)/(r_1^2r_2^2)$ |
| $Q_{19}$ | $(r_1^2 - r_2^2)/(r_1^2r_2^2)$ |
| $Q_{20}$ | $r_1^2r_2^2(r^2 - 3\delta^2 r^2)/(r_1^2r_2^2)$ |
| $Q_{21}$ | $p_1^2(\vec{r})^2$ |
| $Q_{22}$ | $p_1^2(\vec{r})^2$ |
| $Q_{23}$ | $p_1^2(\vec{r})^2$ |
| $Q_{24}$ | $p_1^2(r^2 + \delta^2 r^2)/(r_1r^2) p_1^2$ |
| $Q_{25}$ | $p^6(3r^2 - \delta^2 r^2)/r_1^2 p^3$ |
| $Q_{26}$ | $p^2(\vec{r})^2(r^2_1 r^2_2 - \delta^2 r^2_1 r^2_2 - 3\delta^2 r^2_1 r^2_2 + 3\delta^2 r^2_1 r^2_2)/(r_1^2r_2^2)$ |
| $Q_{27}$ | $p^2(\vec{r})^2$ |
| $Q_{28}$ | $p^2(\vec{r})^2$ |
| $Q_{29}$ | $p_1^2(\vec{r})^2$ |
| $Q_{30}$ | $p_1^2(\vec{r})^2$ |
| $Q_{31}$ | $4\pi \delta^3(r_1) \vec{p}_1 \cdot \vec{p}_2$ |
| $Q_{32}$ | $(r_1^2 - r_2^2)/(r_1^2r_2^2)$ |
| $Q_{33}$ | $\vec{p}_1 \cdot \vec{p}_2$ |
| $Q_{34}$ | $\vec{P}/r_1 \vec{P}$ |
| $Q_{35}$ | $\vec{P}/r_2 \vec{P}$ |
| $Q_{36}$ | $\vec{P}/r^2_1 \vec{P}$ |
| $Q_{37}$ | $\vec{P}/(r_1r_2) \vec{P}$ |
| $Q_{38}$ | $\vec{P}/(r_1r) \vec{P}$ |
| $Q_{39}$ | $\vec{P}/r^2 \vec{P}$ |
| $Q_{40}$ | $p^2(\vec{r})^2$ |
| $Q_{41}$ | $P^2 p_1^2(\vec{r}^2 + \delta^2 r^2)/(r^3 p_1^2$ |
| $Q_{42}$ | $p_1^2(\vec{r})^2(\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/r_1^2 p^3$ |
| $Q_{43}$ | $p_1^2(\vec{r})^2(\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/r_1^2 p^3$ |
| $Q_{44}$ | $p_1^2(\vec{r})^2(\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/r_1^2 p^3$ |
| $Q_{45}$ | $p_1^2(\vec{r})^2(\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/r_1^2 p^3$ |
| $Q_{46}$ | $p_1^2(\vec{r})^2(\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/r_1^2 p^3$ |
| $Q_{47}$ | $(\vec{r}_1 \cdot \vec{r}_2)/(\vec{r}_1^2 r_2^2)$ |
| $Q_{48}$ | $r_1^2 r_2^2(\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/(\vec{r}_1^2 r_2^2)$ |
| $Q_{49}$ | $r_1^2 r_2^2(\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/(\vec{r}_1^2 r_2^2)$ |
| $Q_{50}$ | $p^2(\vec{r})^2(\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/(\vec{r}_1^2 r_2^2)$ |
| $Q_{51}$ | $4\pi \vec{p}_1 \delta^3(r_1) \vec{p}_1$ |
| $Q_{52}$ | $4\pi \delta^3(r_1)/r_2 (\ln r + \gamma)$ |
| $Q_{53}$ | $1/r_1$ |
| $Q_{54}$ | $1/r^2(\ln r + \gamma)$ |
| $Q_{55}$ | $1/r^3$ |
| $Q_{56}$ | $1/r_1^3$ |
| $Q_{57}$ | $1/r_1^3$ |
| $Q_{58}$ | $(\vec{r}_1 - \vec{r}_2)/(\vec{r}_1^2 r_2^3) \ln r + \gamma$ |
| $Q_{59}$ | $1/(\vec{r}_1 r_2)$ |
| $Q_{60}$ | $\vec{p}/r^3 \vec{p}$ |
| $Q_{61}$ | $\vec{P}/r^3 \vec{P}$ |
| $Q_{62}$ | r_1 r_2 (\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/(\vec{r}_1^2 r_2^3)$ |
| $Q_{63}$ | r_1 r_2 (\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/(\vec{r}_1^2 r_2^3)$ |
| $Q_{64}$ | p^i (\vec{r}_1^2 + \delta^2 \vec{r}_1^2)/(\vec{r}_1^2 r_2^3)$ |

energy calculated in this work and the corresponding corrections to the fine structure from Ref. [13]. We do not present results for the $2^3 P_3$ state because it mixes with the $2^1 P_1$ state and thus requires a separate treatment [14]. Results for helium listed in Table II are in full agreement with those reported by us previously [4].

Table II also presents results for the coefficients of the $1/Z$ expansion of the $m\alpha^7$ contributions,

$$E_{(7,i)} = Z^6 \left( c_0^{(7,i)} + \frac{c_1^{(7,i)}}{Z} + \frac{c_2^{(7,i)}}{Z^2} + \ldots \right).$$

The leading coefficients $c_0^{(7,i)}$ are known from the hydrogen theory. They are induced by the one-loop QED correction of order $\alpha(Z\alpha)^0$. Specifically, for the $1snl_j$ state, we have

$$c_0^{(7,i)} = \frac{1}{\pi} \left[ A_{6i} (1s) + A_{6i} (nl_j)^2 \right],$$

where the coefficients $A_{6i} (nl_j)$ are listed in Ref. [9].

We checked that our formulas for $E_{(7,i)}$ are reduced to $Z^6 c_0^{(7,i)}$ in the large-$Z$ limit, see Appendix A for details. We also checked this correspondence for our numerical results, by fitting the numerical data from Table II to the form (26) and comparing the fitted values of the coefficients $c_0^{(7,i)}$ with the analytical result of Eq. (27). In this way we confirmed that our calculations of the $m\alpha^7$ effects are correct to the leading (zeroth) order in $1/Z$.

As a further test, we will compare the next term of the $1/Z$ expansion of $E_{(7)}$ with results of the all-order (in $Z\alpha$) calculations performed recently in Ref. [14]. In that work results were obtained for the higher-order two-electron QED remainder function that contains contributions of order $m\alpha^7$ and is linear in $1/Z$. The remainder function $G_{2eQED}(Z\alpha) = \delta E_{(7,i)}/[m\alpha^2(Z\alpha)^5]$ is defined by Eqs. (21)-(23) of Ref. [14]. In the limit $Z\alpha \rightarrow 0$, $G_{2eQED}(Z\alpha)$ should approach the linear in $1/Z$ part of $E_{(7)}$, if one removes the two-loop part that is not included into the all-order calculations.

The linear in $1/Z$ part of $E_{(7)}$ is induced by the coefficients $c_1^{(7,i)}$. The two-loop effects influence only the nonlogarithmic coefficient $c_1^{(7,0)}$. The corresponding contribution comes from
the hydrogenic correction $\propto \alpha^2 (Z\alpha)^5$ and is given by
\begin{equation}
\epsilon_1^{(7,0)}(2\text{loop}) = \frac{B_{50}}{\pi^2} \left( 1 + \frac{\delta_{1,0}}{n^3} \right),
\end{equation}
where $B_{50} = -21.55447$, see Ref. [14]. It is interesting that the two-loop part of $c_1$ is much larger than the total values of $c_1$ in Table II, which means that the corresponding one-loop and two-loop contributions largely cancel each other.

The function $G_{2e0\text{QED}}^{(7+)\text{Z}}$ was calculated for $Z \geq 10$ in Ref. [14]. The extrapolation of the numerical values towards smaller values of $Z$ is complicated by presence of logarithms. In order to make an extrapolation possible, we subtract all known logarithms, introducing a new function $G_{\text{log}}^{(7+)}$ that has a smooth behaviour in the region $Z \approx 0$,
\begin{equation}
G_{\text{log}}^{(7+)}(Z\alpha) = G_{2e0\text{QED}}^{(7+)\text{Z}}(Z\alpha) - \epsilon_1^{(7,2)}(Z\alpha)^{-2} - c_1^{(7,1)}(Z\alpha)^{-2} - c_1^{(8,1)}(Z\alpha) \ln(Z\alpha)^{-2}.
\end{equation}

The logarithmic coefficient in the order $m\alpha^8$ comes from the one-loop self-energy and vacuum-polarization contributions $\propto \alpha(Z\alpha)^6 \ln(Z\alpha)$. It is known for hydrogen [15, 16]. Since it is proportional to the Dirac $\delta$ function, the result can be immediately generalized to the few-electron case,
\begin{equation}
\epsilon_1^{(8,1)} = \left( \frac{247}{192} - \ln 2 \right) \delta_1,
\end{equation}
where $\delta_1$ is the $1/Z^1$ coefficient of the $1/Z$ expansion of the matrix element of the Dirac $\delta$ function, $\delta_1(2^3S) = -0.211484$ and $\delta_1(2^3P) = -0.085951$ [11].

In the $Z \to 0$ limit, the function $G_{\text{log}}^{(7+)}$ should coincide with the $c_1^{(7,0)}$ coefficient from our $m\alpha^7$ calculations, after subtraction of the two-loop part. Specifically,
\begin{equation}
G_{\text{log}}^{(7+)}(Z = 0) = c_1^{(7,0)}(Z\alpha)^{-2} - c_1^{(7,0)}(2\text{loop}).
\end{equation}

V. TRANSITION ENERGIES

We are now in a position to collect all available theoretical contributions for the transition energies between the $n = 2$ triplet states in light He-like ions. A systematic calculation of all QED effects up to order $m\alpha^8$ has been already performed in our previous investigation [12]. We now add the $m\alpha^7$ correction tabulated in Table II and estimations of higher-order corrections summarized in Sec. III.

Our theoretical results for the $2^3S-2^3P_{0,2}$ transition energies are presented in Table III, in comparison with available experimental data and previous theoretical values. We observe very good agreement with the experimental results for Li$^+$ [7] and B$^{3+}$ [17], but a significant deviation in the case of Be$^{2+}$ [18]. It should be noted that the measurement of Ref. [18] was already reported to disagree with theoretical predictions for the fine structure [13], which calls for an independent verification of this experiment.

The comparison with our previous calculations of Ref. [12] shows an excellent consistency of the results and of the uncertainty estimates. It can be seen that our present calculation of the $m\alpha^7$ effects improves the theoretical accuracy by an order of magnitude.

It can be seen from Table III that for $Z = 5$ our present theoretical values are fully consistent with our recent results obtained in Ref. [14]. It is important that Ref. [14] utilized a different approach for calculating the effects of order $m\alpha^7$ and higher. In that work, the higher-order effects were obtained from the all-order (in $Z\alpha$) calculations, whereas in the present study we calculate the $m\alpha^7$ effects rigorously with the $\alpha$ expansion and estimate the $m\alpha^{8+}$ effects from the hydrogenic theory. The comparison with results of Ref. [14] thus confirms the consistency of two different approaches for the $2^3S-2^3P$ transition energies.

In summary, we reported calculations of the $m\alpha^7$ QED effects for the $2^3S$ and $2^3P$ states of He-like ions. The $Z$-dependence of the obtained corrections was studied. It was demonstrated that all terms containing $\ln(Z\alpha)$ and $\ln(\alpha)$ in general formulas can be combined together and expressed in terms of $\ln(Z\alpha)$. The high-$Z$ limit of the calculated $m\alpha^7$ correction was cross-checked against the analytical results derived from the hydrogen theory. The linear term of the $1/Z$ expansion of the $m\alpha^7$ correction was cross-checked against previous calculations performed to all orders in $Z\alpha$. The consistency of the two approaches was demonstrated for the $2^3S-2^3P$ transition energies but a small deviation was found for the ionization energies. In the result, we obtain the most accurate theoretical predictions for the $2^3S-2^3P_{0,2}$ transition energies in He-like Li, Be, and B, which are in good agreement with previous theoretical values and the experimental data for Li and B.

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TABLE II. The $\alpha_7$ corrections for energies of triplet states of He-like atoms.

| $Z$  | $2^3S$ | $2^3P_0$ | $2^3P_2$ |
|------|--------|----------|----------|
|      | $E^{(7,2)}/Z^6$ | $E^{(7,1)}/Z^6$ | $E^{(7,0)}/Z^6$ |
| 2    | -0.335089 | 1.725409 | -11.343605 (7) |
| 3    | -0.338059 | 1.775817 | -11.290585 (7) |
| 4    | -0.342592 | 1.805773 | -11.283785 (7) |
| 5    | -0.345472 | 1.825149 | -11.285055 (7) |
| 6    | -0.347456 | 1.838657 | -11.287954 (7) |
| 7    | -0.348903 | 1.848593 | -11.290984 (7) |
| 8    | -0.350005 | 1.856203 | -11.293764 (7) |
| 9    | -0.350872 | 1.862214 | -11.296219 (11) |
| 10   | -0.351571 | 1.867082 | -11.298368 (14) |
| 11   | -0.352148 | 1.871104 | -11.300241 (14) |
| 12   | -0.352630 | 1.874482 | -11.301910 (18) |

1/Z-expansion coefficients

$c_0 = -0.358099$, $c_1 = 0.067317$, $c_2 = -0.020020$.

FIG. 1. The nonlogarithmic $\alpha_7$ contribution defined by Eq. (29) as a function of the nuclear charge $Z$, for the $2^3S$, $2^3P_0$, and $2^3P_2$ states of He-like ions. Filled green dots denote results of all-order numerical calculations, open green dots show fitting results at $Z = 0$, red diamonds display the $\alpha$-expansion results.

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TABLE III. Theoretical and experimental $2^3S - 2^3P$ transition energies, in cm$^{-1}$. $A$ is the mass number of the isotope.

| $Z$ | $A$ | Theory | Experiment | Difference | Ref. |
|-----|-----|--------|------------|------------|-----|
| 2 | 3 | $18 231.30193$ (10) | $18 231.301972$ (14) | $0.00004$ (10) | [7] |
| | | $18 231.30211$ (11)$^a$ | | | |
| 4 | 9 | $26 864.61052$ (54) | $26 864.6120$ (4) | $0.0015$ (7) | [18] |
| | | $26 864.6114$ (47)$^a$ | | | |
| 5 | 11 | $35 393.6244$ (20) | $35 393.6267$ (13) | $0.003$ (13) | [17] |
| | | $35 393.6211$ (49)$^b$ | | | |
| | | $35 393.628$ (14)$^a$ | | | |

$^a$ Yerokhin and Pachucki 2010 [12];
$^b$ Yerokhin, Patkős, and Pachucki 2022 [14];

where the plus sign stands for the singlet and the minus sign, for the triplet states, and $\psi_{nl}(r)$ are the hydrogenic radial wave functions with the principal quantum number $n$ and the orbital momentum $l$. The expectation value of an arbitrary operator $O$ with the triple-state wave function is

$$
\langle O \rangle = \frac{1}{2} \langle (1, 0), (n, l) | O | (1, 0), (n, l) \rangle + \frac{1}{2} \langle (n, l), (1, 0) | O | (n, l), (1, 0) \rangle
\langle (n, l), (1, 0) | O | (1, 0), (n, l) \rangle - \frac{1}{2} \langle (1, 0), (n, l) | O | (n, l), (1, 0) \rangle,
$$

(A2)

where $\langle (m, l_1), (n, l_2) | \psi_{nl_1}(r_1) \psi_{nl_2}(r_2) \rangle$.

If the operator $O$ is a sum of one-electron operators $O = O'(r_1) + O'(r_2)$, the first two terms in the right-hand-side of Eq. (A2) are reduced to the sum of two one-electron matrix elements, $\langle (10) | O' | (10) \rangle + \langle (n) | O' | (n) \rangle$. The last two terms in the right-hand-side of Eq. (A2) are of a different form. It can be shown that for the large-$Z$ limit of the total $ma^7$ correction such “mixing” terms from the first-order operators cancel identically with the corresponding terms in the second-order contribution.

For evaluating the large-$Z$ limit of various operators contributing to the $ma^7$ correction, we make use of the following results for the one-electron matrix elements,

$$
\langle nl | \frac{1}{r} | nl \rangle = \frac{Z}{n^2},
$$

(A3)

$$
\langle nl | \frac{1}{r^2} | nl \rangle = \frac{Z^2}{n^3(l + \frac{7}{2})},
$$

(A4)

$$
\langle nl | p^2 | nl \rangle = 2E_n + \langle nl | \frac{2Z}{r} | nl \rangle = \frac{Z^2}{n^2},
$$

(A5)

$$
\langle nl | 4\pi\delta^3(r) | nl \rangle = \frac{4Z^3}{n^3} \delta_0,
$$

(A6)

$$
\langle nl | \frac{\vec{p} \cdot 4\pi\delta^3(r) \vec{p}}{r^2} | nl \rangle = \frac{4Z^4}{3} \left( -\frac{1}{n^6} + \frac{1}{n^3} \right) \delta_{l1},
$$

(A7)

where $\delta_0 = 2(1 - \delta_{l0}) \left( \frac{1}{2l - 1} + \frac{2}{2l + 1} \right)$. The last two terms in the right-hand-side of Eq. (A2) are of a different form. It can be shown that for the large-$Z$ limit of the total $ma^7$ correction such “mixing” terms from the first-order operators cancel identically with the corresponding terms in the second-order contribution.

For evaluating the large-$Z$ limit of various operators contributing to the $ma^7$ correction, we make use of the following results for the one-electron matrix elements,