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

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We perform *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 **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. Patkóš *et al.*, Phys. Rev. A **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 $\mathrm{Li}^+$, 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 $\ln(Z)$ and $\ln(\alpha)$ can be factorized out in terms of $\ln(Z\alpha)$ and $\ln^2(Z\alpha)$. The exact matching of coefficients at $\ln(Z)$ 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,

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

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

$$E^{(7,2)} = -\frac{1}{2\pi} Z^3\, Q_1 = -2Z^3\,\langle \delta^3(r_1)\rangle\,, \tag{2}$$

$$
\begin{aligned}
E^{(7,1)} = \frac{1}{3\pi}\bigg[& -8E_0E_4 - \frac{Z}{5}\Big(\frac{19}{3}+11Z\Big)Q_3 + \frac{11Z}{10}Q_4 - \frac{39}{10}Q_{6T} + 4E_4Q_7 \\
&+ Z\Big(-\frac{E_0}{5}+\frac{9Z^2}{8}+8Z^2\ln 2+Q_7\Big)Q_1 + \frac{26}{5}Q_{10} + 4E_0Z^2Q_{11} + 8E_0Z^2Q_{12} - 8E_0ZQ_{13} \\
&- 8Z^2Q_{14} + 8Z^3Q_{15} - 4Z^2Q_{16} + 4ZQ_{17} - \frac{38Z}{5}Q_{18} + 2Z^2Q_{21} + 2Z^2Q_{22} + 4ZQ_{24} - 2ZQ_{28} \\
&+ \frac{11Z}{10}Q_{51} + 4E_0^2ZQ_{53} - \frac{Z}{5}Q_{62} + 3Z^2\widetilde{Q}_{57} + 2\left\langle H_R'\frac{1}{(E_0-H_0)'}H_R\right\rangle\bigg], \qquad (3)
\end{aligned}
$$

$$
\begin{aligned}
E^{(7,0)} = \frac{1}{90\pi}\bigg\{& -8E_0E_4\big(19-30\ln 2\big) + Z\Big(-\frac{53183}{420}-\frac{2003Z}{140}+82\ln 2+66Z\ln 2\Big)Q_3 \\
&+ Z\Big(\frac{2003}{280}-33\ln 2\Big)Q_4 + \Big(\frac{14971}{70}+36\ln 2\Big)Q_{6T} + \Big(76E_4-120E_4\ln 2-105Q_9\Big)Q_7 \\
&+ \Big(\frac{9543}{20}-264\ln 2\Big)Q_{10} + 4E_0Z^2\Big(19-30\ln 2\Big)Q_{11} + 8E_0Z^2\Big(19-30\ln 2\Big)Q_{12} \\
&- 8E_0Z\Big(19-30\ln 2\Big)Q_{13} - 8Z^2\Big(19-30\ln 2\Big)Q_{14} + 8Z^3\Big(19-30\ln 2\Big)Q_{15} \\
&- 4Z^2\Big(19-30\ln 2\Big)Q_{16} + 4Z\Big(19-30\ln 2\Big)Q_{17} + Z\Big(-\frac{2757}{10}+288\ln 2\Big)Q_{18} \\
&+ 2Z^2\Big(19-30\ln 2\Big)Q_{21} + 2Z^2\Big(19-30\ln 2\Big)Q_{22} + 4Z\Big(19-30\ln 2\Big)Q_{24} + \frac{105}{8}Q_{25} \\
&- 2Z\Big(19-30\ln 2\Big)Q_{28} + Z\Big(\frac{3893}{280}-33\ln 2\Big)Q_{51} + Z\Big(76E_0^2-120E_0^2\ln 2+105Q_9\Big)Q_{53} \\
&- 105ZQ_{59} + \frac{105}{4}Q_{61} + 4Z\Big(\frac{7}{5}+3\ln 2\Big)Q_{62} + 88Z\widetilde{Q}_{52} - 72\widetilde{Q}_{54} - 297\widetilde{Q}_{55} \\
&+ Z^2\Big(\frac{513}{4}-90\ln 2\Big)\widetilde{Q}_{57} - 24Z\widetilde{Q}_{58} - 63\widetilde{Q}_{60} + 12Z\widetilde{Q}_{63} + Z\bigg[\frac{3317E_0}{140}+\frac{5755Z^2}{56} \\
&- \frac{85\pi^2Z^2}{6} + 6E_0\ln 2 - 362\,Z^2\ln 2 + 45\,Z^2\ln^2 2 + (19-30\ln 2)Q_7 + \frac{225Z^2}{2}\zeta(3)\bigg]\,Q_1\bigg\} \\
&+ \frac{Z^3}{2\pi}\beta_L\,Q_1 + \frac{Z^2}{2\pi^2}\,B_{50}\,Q_1 + \frac{Z}{2\pi^3}\,C_{40}\,Q_1 + E_{\rm sec}\,. \qquad (4)
\end{aligned}
$$

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 $\widetilde{Q}_i$, which are free from $\ln(Z)$ and are defined by

$$Q_{52} = \widetilde{Q}_{52} + \frac{1}{2}\ln Z^{-2}\,Q_3\,, \qquad (5)$$

$$Q_{54} = \widetilde{Q}_{54} + \frac{1}{2}\ln Z^{-2}\,Q_{10}\,, \qquad (6)$$

$$Q_{55} = \widetilde{Q}_{55} + \frac{1}{6}\ln Z^{-2}\,Q_{6T}\,, \qquad (7)$$

$$Q_{56} = \widetilde{Q}_{56} + \frac{1}{2}\ln Z^{-2}\,Q_1\,, \qquad (8)$$

$$Q_{57} = \widetilde{Q}_{57} - Z\ln Z^{-2}\,Q_1\,, \qquad (9)$$

$$Q_{58} = \widetilde{Q}_{58} + \frac{1}{2}\ln Z^{-2}\,Q_{18}\,, \qquad (10)$$

$$Q_{60} = \widetilde{Q}_{60} + \frac{1}{2}\ln Z^{-2}\,Q_{6T}\,, \qquad (11)$$

$$Q_{63} = \widetilde{Q}_{63} + \frac{1}{2}\ln Z^{-2}\,Q_{62}\,. \qquad (12)$$

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], $B_{50} = -21.554\,47$ and $C_{40} = 0.417\,503\,770$ are the hydrogenic two-loop $(Z\alpha)^5$ and three-loop $(Z\alpha)^4$ expansion coefficients, respectively, see

Ref. [9], and $E_{\rm sec}$ is the second-order correction given by

$$E_{\rm sec} = 2\left\langle H_{\rm fs}^{(5)}\frac{1}{(E_0-H_0)'}H_{\rm fs}^{(4)}\right\rangle + \frac{1}{\pi}\Big(\frac{19}{45}-\frac{2}{3}\ln 2\Big)\left\langle H_R'\frac{1}{(E_0-H_0)'}H_R\right\rangle - \frac{7}{3\pi}\left\langle\frac{1}{r^3}\frac{1}{(E_0-H_0)'}H_R\right\rangle . \tag{13}$$

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

$$H_R|\phi\rangle = \left[-\frac{1}{2}(E-V)^2 - \frac{Z}{4}\frac{\vec r_1\cdot\vec\nabla_1}{r_1^3} - \frac{Z}{4}\frac{\vec r_2\cdot\vec\nabla_2}{r_2^3} + \frac{1}{4}\nabla_1^2\nabla_2^2 + \nabla_1^i\frac{1}{2r}\left(\delta^{ij}+\frac{r^ir^j}{r^2}\right)\nabla_2^j\right]|\phi\rangle , \tag{14}$$

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

$$H_R'|\phi\rangle = -2Z\left(\frac{\vec r_1\cdot\vec\nabla_1}{r_1^3}+\frac{\vec r_2\cdot\vec\nabla_2}{r_2^3}\right)|\phi\rangle . \tag{15}$$

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

$$H_{\rm fs} = \alpha^4 H_{\rm fs}^{(4)} + \alpha^5 H_{\rm fs}^{(5)} + O(\alpha^6) , \tag{16}$$

$$\begin{aligned} H_{\rm fs} &= \frac{\alpha}{4\,m^2}\left(\frac{\vec\sigma_1\cdot\vec\sigma_2}{r^3} - 3\,\frac{\vec\sigma_1\cdot\vec r\,\vec\sigma_2\cdot\vec r}{r^5}\right)(1+\kappa)^2 \\ &+ \frac{Z\alpha}{4m^2}\left[\frac{1}{r_1^3}\,\vec r_1\times\vec p_1\cdot\vec\sigma_1 + \frac{1}{r_2^3}\,\vec r_2\times\vec p_2\cdot\vec\sigma_2\right](1+2\kappa) \\ &+ \frac{\alpha}{4\,m^2\,r^3}\Big[\big[(1+2\,\kappa)\,\vec\sigma_2 + 2\,(1+\kappa)\,\vec\sigma_1\big]\cdot\vec r\times\vec p_2 \\ &\quad - \big[(1+2\,\kappa)\,\vec\sigma_1 + 2\,(1+\kappa)\,\vec\sigma_2\big]\cdot\vec r\times\vec p_1\Big] , \end{aligned} \tag{17}$$

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,

$$E^{(8+)} = E_D^{(8)} + E_{\rm 1ph}^{(8)} + E_{\rm rad}^{(8+)} , \tag{18}$$

where $E_D^{(8+)}$ comes from the one-electron Dirac energy, $E_{\rm 1ph}^{(8+)}$ originates from the one-photon exchange correction, and $E_{\rm rad}^{(8+)}$ represents the radiative QED effects.

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

$$E_D^{(8)}(2s) = E_D^{(8)}(2p_{1/2}) = -\frac{429}{32768}\,Z^8 , \tag{19}$$

$$E_D^{(8)}(2p_{3/2}) = -\frac{5}{32768}\,Z^8 . \tag{20}$$

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

$$E_{\rm 1ph}^{(8)}\left(2^3S\right) = 0.0281\,Z^7 , \tag{21}$$

$$E_{\rm 1ph}^{(8)}\left(2^3P_0\right) = 0.1070\,Z^7 , \tag{22}$$

$$E_{\rm 1ph}^{(8)}\left(2^3P_2\right) = 0.0037\,Z^7 . \tag{23}$$

We note a relative large numerical contribution of the one-photon exchange correction for the $2^3P_0$ 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],

$$E_{\rm rad}^{(8+)} = \Big[E_{\rm rad,H}^{(8+)}(1s) + E_{\rm rad,H}^{(8+)}(nl)\Big]\,\frac{\langle\sum_i\delta^3(r_i)\rangle}{\frac{Z^3}{\pi}\left(1+\frac{\delta_{l,0}}{n^3}\right)} - E_{\rm rad,H}^{(8+)}(1s) , \tag{24}$$

where $E_{\rm rad,H}^{(8+)}(nl)$ is the hydrogenic QED contribution of order 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 $E_{\rm rad}^{(8+)}$, specifically,

$$\delta E_{\rm rad}^{(8+)} = \pm 0.75\,\Big[E_{\rm rad,H}^{(8+)}(1s) + E_{\rm rad,H}^{(8+)}(nl)\Big] \times\left[\frac{\langle\sum_i\delta^3(r_i)\rangle}{\frac{Z^3}{\pi}\left(1+\frac{\delta_{l,0}}{n^3}\right)} - 1\right] . \tag{25}$$

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 $Z\le 12$. The computation 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 $2^3P_{0,2}$ states are obtained by combining the $m\alpha^7$ correction for the $2^3P$ centroid

TABLE I. Definitions of elementary basic operators $Q_i$. Notations are: $r \equiv |\vec{r}_1 - \vec{r}_2|$, $\vec{P} = \vec{p}_1 + \vec{p}_2$, $\vec{p} = 1/2(\vec{p}_1 - \vec{p}_2)$.

| | | | |
|---|---|---|---|
| $Q_1$ | $4\pi\delta^3(r_1)$ | $Q_{33}$ | $\vec{p}_1 \cdot \vec{p}_2$ |
| $Q_2$ | $4\pi\delta^3(r)$ | $Q_{34}$ | $\vec{P}\,/r_1\,\vec{P}$ |
| $Q_3$ | $4\pi\delta^3(r_1)/r_2$ | $Q_{35}$ | $\vec{P}\,/r\,\vec{P}$ |
| $Q_4$ | $4\pi\delta^3(r_1)\,p_2^2$ | $Q_{36}$ | $\vec{P}\,/r_1^2\,\vec{P}$ |
| $Q_5$ | $4\pi\delta^3(r)/r_1$ | $Q_{37}$ | $\vec{P}\,/(r_1 r_2)\,\vec{P}$ |
| $Q_{6T}$ | $4\pi\,\vec{p}\,\delta^3(r)\,\vec{p}$ | $Q_{38}$ | $\vec{P}\,/(r_1 r)\,\vec{P}$ |
| $Q_7$ | $1/r$ | $Q_{39}$ | $\vec{P}\,/r^2\,\vec{P}$ |
| $Q_8$ | $1/r^2$ | $Q_{40}$ | $p_1^2\,p_2^2\,P^2$ |
| $Q_9$ | $1/r^3$ | $Q_{41}$ | $P^2\,p_1^i\,(r^i r^j + \delta^{ij} r^2)/r^3\,p_2^j$ |
| $Q_{10}$ | $1/r^4$ | $Q_{42}$ | $p_1^i\,(r_1^i r_1^j + \delta^{ij} r_1^2)/r_1^4\,P^j$ |
| $Q_{11}$ | $1/r_1^2$ | $Q_{43}$ | $p_1^i\,(r_1^i r_1^j + \delta^{ij} r_1^2)/(r_1^3 r_2)\,P^j$ |
| $Q_{12}$ | $1/(r_1 r_2)$ | $Q_{44}$ | $p_1^i\,p_2^k\,(r_1^i r_1^j + \delta^{ij} r_1^2)/r_1^3\,p_2^k\,P^j$ |
| $Q_{13}$ | $1/(r_1 r)$ | $Q_{45}$ | $p_2^i (r^i r^j + \delta^{ij} r^2)(r_1^j r_1^k + \delta^{jk} r_1^2)/(r_1^3 r^3)\,P^k$ |
| $Q_{14}$ | $1/(r_1 r_2 r)$ | $Q_{46}$ | $p_1^i (r_1^i r_1^j + \delta^{ij} r_1^2)(r_2^j r_2^k + \delta^{jk} r_2^2)/(r_1^3 r_2^3)\,p_2^k$ |
| $Q_{15}$ | $1/(r_1^2 r_2)$ | $Q_{47}$ | $(\vec{r}_1 \cdot \vec{r}_2)/(r_1^3 r_2^2)$ |
| $Q_{16}$ | $1/(r_1^2 r)$ | $Q_{48}$ | $r_1^i r^j\,(r_1^i r_1^j - 3\delta^{ij} r_1^2)/(r_1^4 r^3)$ |
| $Q_{17}$ | $1/(r_1 r^2)$ | $Q_{49}$ | $r_1^i r^j\,(r_2^i r_2^j - 3\delta^{ij} r_2^2)/(r_1^3 r_2 r^3)$ |
| $Q_{18}$ | $(\vec{r}_1 \cdot \vec{r})/(r_1^3 r^3)$ | $Q_{50}$ | $p_2^k\,r_1^i/r_1^3\,(\delta^{jk} r_2^i/r_2 - \delta^{ik} r_2^j/r_2 - \delta^{ij} r_2^k/r_2 - r_2^i r_2^j r_2^k/r_2^3)\,p_2^j$ |
| $Q_{19}$ | $(\vec{r}_1 \cdot \vec{r})/(r_1^3 r^2)$ | $Q_{51}$ | $4\pi\,\vec{p}_1\,\delta^3(r_1)\,\vec{p}_1$ |
| $Q_{20}$ | $r_1^i r_2^j (r^i r^j - 3\delta^{ij} r^2)/(r_1^3 r_2^3 r)$ | $Q_{52}$ | $4\pi\delta^3(r_1)/r_2\,(\ln r_2 + \gamma)$ |
| $Q_{21}$ | $p_2^2/r_1^2$ | $Q_{53}$ | $1/r_1$ |
| $Q_{22}$ | $\vec{p}_1/r_1^2\,\vec{p}_1$ | $Q_{54}$ | $1/r^4(\ln r + \gamma)$ |
| $Q_{23}$ | $\vec{p}_1/r^2\,\vec{p}_1$ | $Q_{55}$ | $1/r^5$ |
| $Q_{24}$ | $p_1^i\,(r^i r^j + \delta^{ij} r^2)/(r_1 r^3)\,p_2^j$ | $Q_{56}$ | $1/r_1^3$ |
| $Q_{25}$ | $P^i\,(3r^i r^j - \delta^{ij} r^2)/r^5\,P^j$ | $Q_{57}$ | $1/r_1^4$ |
| $Q_{26}$ | $p_2^k\,r_1^i\,/r_1^3(\delta^{jk} r^i/r - \delta^{ik} r^j/r - \delta^{ij} r^k/r - r^i r^j r^k/r^3)\,p_2^j$ | $Q_{58}$ | $(\vec{r}_1 \cdot \vec{r})/(r_1^3 r^3)(\ln r + \gamma)$ |
| $Q_{27}$ | $p_1^2\,p_2^2$ | $Q_{59}$ | $1/(r_1 r^3)$ |
| $Q_{28}$ | $p_1^2\,/r_1\,p_2^2$ | $Q_{60}$ | $\vec{p}\,/r^3\,\vec{p}$ |
| $Q_{29}$ | $\vec{p}_1 \times \vec{p}_2\,/r\,\vec{p}_1 \times \vec{p}_2$ | $Q_{61}$ | $\vec{P}\,/r^3\,\vec{P}$ |
| $Q_{30}$ | $p_1^k\,p_2^l\,(-\delta^{jl} r^i r^k/r^3 - \delta^{ik} r^j r^l/r^3 + 3r^i r^j r^k r^l/r^5)\,p_1^i\,p_2^j$ | $Q_{62}$ | $r^i r^j (\delta^{ij} r_1^2 - 3r_1^i r_1^j)/(r_1^5 r^3)$ |
| $Q_{31}$ | $4\pi\delta^3(r_1)\,\vec{p}_1 \cdot \vec{p}_2$ | $Q_{63}$ | $r^i r^j (\delta^{ij} r_1^2 - 3r_1^i r_1^j)/(r_1^5 r^3)(\ln r + \gamma)$ |
| $Q_{32}$ | $(\vec{r}_1 \cdot \vec{r}_2)/(r_1^3 r_2^3)$ | $Q_{64}$ | $p^i(\delta^{ij} r^2 - 3r^i r^j)/r^5 p^j$ |

energy calculated in this work and the corresponding corrections to the fine structure from Ref. [13]. We do not present results for the $2^3P_1$ state because it mixes with the $2^1P_1$ 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,

$$E^{(7,i)} = Z^6\left(c_0^{(7,i)} + \frac{c_1^{(7,i)}}{Z} + \frac{c_2^{(7,i)}}{Z^2} + \ldots\right). \tag{26}$$

The leading coefficients $c_0^{(7,i)}$ are known from the hydrogen theory. They are induced by the one-loop QED correction of order $\alpha(Z\alpha)^6$. Specifically, for the $1snl_j$ state, we have

$$c_0^{(7,i)} = \frac{1}{\pi}\left[A_{6i}(1s) + \frac{A_{6i}(nl_j)}{n^3}\right], \tag{27}$$

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 $G^{(7+)}_{\rm 2elQED}(Z\alpha) = \delta E^{(7+)}/[m\alpha^2(Z\alpha)^5]$ is defined by Eqs. (21)-(23) of Ref. [14]. In the limit $Z\alpha \to 0$, $G^{(7+)}_{\rm 2elQED}(Z\alpha)$ 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

$$c_1^{(7,0)}(\text{2loop}) = \frac{B_{50}}{\pi^2}\left(1+\frac{\delta_{l,0}}{n^3}\right), \tag{28}$$

where $B_{50} = -21.554\,47$, 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 $G^{(7+)}_{\text{2elQED}}$ 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 $G^{(7+)}_{\text{nlog}}$ that has a smooth behaviour in the region $Z \approx 0$,

$$G^{(7+)}_{\text{nlog}}(Z\alpha) = G^{(7+)}_{\text{2elQED}}(Z\alpha) - c_1^{(7,2)}\,\ln^2(Z\alpha)^{-2} - c_1^{(7,1)}\,\ln(Z\alpha)^{-2} - c_1^{(8,1)}\,(Z\alpha)\ln(Z\alpha)^{-2}\,. \tag{29}$$

The logarithmic coefficient in the order $m\alpha^8$ comes from the one-loop self-energy and vacuum-polarization contribution $\propto \alpha(Z\alpha)^6\ln(Z\alpha)$. 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,

$$c_1^{(8,1)} = \left(\frac{427}{192} - \ln 2\right)\delta_1\,, \tag{30}$$

where $\delta_1$ is the $1/Z^1$ coefficient of the $1/Z$ expansion of the matrix element of the Dirac $\delta$ function, $\delta_1(2^3S) = -0.211\,484$ and $\delta_1(2^3P) = -0.085\,951$ [11].

In the $Z \to 0$ limit, the function $G^{(7+)}_{\text{nlog}}$ should coincide with the $c_1^{(7,0)}$ coefficient from our $m\alpha^7$ calculations, after subtraction of the two-loop part. Specifically,

$$G^{(7+)}_{\text{nlog}}(Z=0) = c_1^{(7,0)} - c_1^{(7,0)}(\text{2loop})\,. \tag{31}$$

In Fig. 1 we present a comparison of numerical values of the function $G^{(7+)}_{\text{nlog}}(Z)$ extracted from the all-order calculations of Ref. [14] and our present results for the $Z=0$ limiting value (31). The all-order data were fitted by a polynomial to yield results for the $Z=0$ limit. As can be seen from the figure, a small inconsistency between the all-order and our present $\alpha$-expansion results at $Z=0$ is observed. While the deviations are only slightly larger than the estimated uncertainties of the fit, it is remarkable that for all three states studied they are of the same sign and of comparable magnitude. These deviations might be related to the 0.4 MHz difference between the theoretical and experimental $2^3S$ and $2^3P$ ionization energies of helium reported in Refs. [4, 6]. Similarly to the helium case, the deviations largely cancels in the $2^3S$-$2^3P$ difference.

## 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 $m\alpha^6$ 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 $\ln(Z)$ 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 $m\alpha^7$ corrections for energies of triplet states of He-like atoms.

| $Z$ | $2^3S$ | | | $2^3P$ | $2^3P_0$ | | $2^3P_2$ | |
|---|---|---|---|---|---|---|---|---|
| | $E^{(7,2)}/Z^6$ | $E^{(7,1)}/Z^6$ | $E^{(7,0)}/Z^6$ | $E^{(7,2)}/Z^6$ | $E^{(7,1)}/Z^6$ | $E^{(7,0)}/Z^6$ | $E^{(7,1)}/Z^6$ | $E^{(7,0)}/Z^6$ |
| 2 | −0.330 089 | 1.725 409 | −11.343 605 (7) | −0.314 715 | 1.649 911 | −10.825 73 (8) | 1.648 886 | −10.826 25 (8) |
| 3 | −0.338 059 | 1.775 871 | −11.290 585 (7) | −0.313 708 | 1.645 555 | −10.458 59 (6) | 1.647 921 | −10.470 69 (6) |
| 4 | −0.342 592 | 1.805 773 | −11.283 785 (7) | −0.313 991 | 1.650 084 | −10.314 51 (6) | 1.653 032 | −10.329 21 (6) |
| 5 | −0.345 472 | 1.825 149 | −11.285 055 (7) | −0.314 440 | 1.655 751 | −10.242 46 (6) | 1.658 167 | −10.256 15 (6) |
| 6 | −0.347 456 | 1.838 657 | −11.287 954 (7) | −0.314 856 | 1.660 905 | −10.200 67 (6) | 1.662 493 | −10.212 27 (6) |
| 7 | −0.348 903 | 1.848 593 | −11.290 984 (7) | −0.315 211 | 1.665 302 | −10.173 90 (6) | 1.666 033 | −10.183 22 (6) |
| 8 | −0.350 005 | 1.856 203 | −11.293 764 (7) | −0.315 508 | 1.669 005 | −10.155 55 (6) | 1.668 938 | −10.162 68 (6) |
| 9 | −0.350 872 | 1.862 214 | −11.296 219 (11) | −0.315 757 | 1.672 131 | −10.142 32 (6) | 1.671 348 | −10.147 44 (6) |
| 10 | −0.351 571 | 1.867 082 | −11.298 368 (14) | −0.315 967 | 1.674 790 | −10.132 38 (6) | 1.673 370 | −10.135 70 (6) |
| 11 | −0.352 148 | 1.871 104 | −11.300 241 (14) | −0.316 147 | | | | |
| 12 | −0.352 630 | 1.874 482 | −11.301 910 (18) | −0.316 302 | | | | |
| $1/Z$-expansion coefficients | | | | | | | | |
| $c_0$ | −0.358 099 | 1.913 246 | −11.324 577 | −0.318 310 | 1.705 367 | −10.069 396 | 1.695 420 | −10.047 690 |
| $c_1$ | 0.067 317 | −0.482 89 (4) | 0.3211 (4) | 0.027 359 | −0.368 03 (5) | −0.3888 (4) | −0.25568 (5) | −0.7262 (10) |
| $c_2$ | −0.020 020 | 0.213 6 (15) | −0.562 (11) | −0.038 518 | 0.6445 (14) | −2.4326 (33) | 0.3565 (12) | −1.4937 (80) |

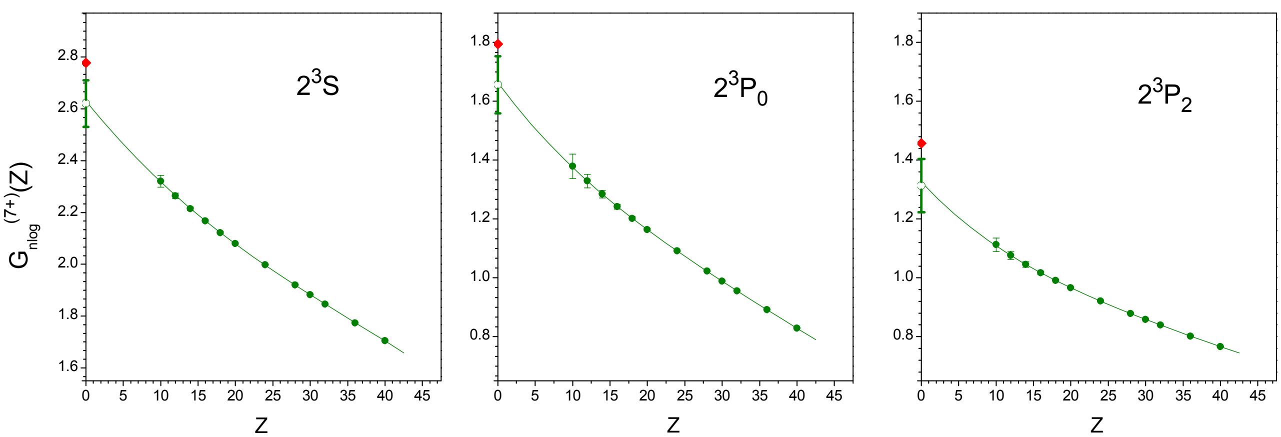


FIG. 1. The nonlogaritmic $m\alpha^{(7+)}$ contribution defined by Eq. (29) as a function of the nuclear charge $Z$, for the $2^3S$, $2^3P_0$, and $2^3P_2$ states of He-like ions. Filled green dots denote results of all-order numerical calculations, open green dots show fitting results at $Z = 0$, red diamonds display the $\alpha$-expansion results.

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

| $Z$ | $A$ | Theory | Experiment | Difference | Ref. |
|---|---|---|---|---|---|
| $2\,^3S_1$–$2\,^3P_0$ | | | | | |
| 3 | 7 | 18 231.30193 (10) | 18 231.301972 (14) | −0.00004 (10) | [7] |
| | | 18 231.3021 (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) | 35 393.627 (13) | −0.003 (13) | [17] |
| | | 35 393.6211 (49)[b] | | | |
| | | 35 393.628 (14)[a] | | | |
| $2\,^3S_1$–$2\,^3P_2$ | | | | | |
| 3 | 7 | 18 228.19893 (10) | 18 228.198963 (15) | −0.00003 (10) | [7] |
| | | 18 228.1989 (10)[a] | | | |
| 4 | 9 | 26 867.94512(54) | 26 867.9484 (3) | −0.0033 (6) | [18] |
| | | 26 867.9450(47)[a] | | | |
| 5 | 11 | 35 430.0880(20) | 35 430.084 (9) | 0.004 (9) | [17] |
| | | 35 430.0876 (22)[b] | | | |
| | | 35 430.088 (14)[a] | | | |

[a] Yerokhin and Pachucki 2010 [12];
[b] Yerokhin, Patkóš, and Pachucki 2022 [14];

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## Appendix A: Large-$Z$ limit

To the leading order in the large-$Z$ expansion we can omit all operators containing the electron-electron radial distance and keep only the electron-nucleus operators containing $r_1$ and $r_2$. The spatial part of the wave function in the large-$Z$ limit is given by an (anti-) symmetrized product of two hydrogenic wave functions,

$$\psi(r_1,r_2) = \frac{1}{\sqrt{2}}\big[\psi_{10}(r_1)\,\psi_{nl}(r_2)\pm\psi_{nl}(r_1)\,\psi_{10}(r_2)\big]\,, \quad \text{(A1)}$$

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 triplet-state wave function is

$$\begin{aligned}\langle O\rangle = {} & \frac{1}{2}\langle(1,0),(n,l)|O|(1,0),(n,l)\rangle \\ & +\frac{1}{2}\langle(n,l),(1,0)|O|(n,l),(1,0)\rangle \\ & -\frac{1}{2}\langle(n,l),(1,0)|O|(1,0),(n,l)\rangle \\ & -\frac{1}{2}\langle(1,0),(n,l)|O|(n,l),(1,0)\rangle\,, \end{aligned} \quad \text{(A2)}$$

where $|(m,l_1),(n,l_2)\rangle = \psi_{ml_1}(r_1)\,\psi_{nl_2}(r_2)$.

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, $\langle 10|\,O'\,|10\rangle + \langle nl|\,O'\,|nl\rangle$. 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 $m\alpha^7$ 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 $m\alpha^7$ correction, we make use of the following results for the one-electron matrix elements,

$$\langle nl|\,\frac{1}{r}\,|nl\rangle = \frac{Z}{n^2}, \quad \text{(A3)}$$

$$\langle nl|\,\frac{1}{r^2}\,|nl\rangle = \frac{Z^2}{n^3(l+\frac{1}{2})}, \quad \text{(A4)}$$

$$\langle nl|\,p^2\,|nl\rangle = 2E_n + \langle nl|\,\frac{2Z}{r}\,|nl\rangle = \frac{Z^2}{n^2}, \quad \text{(A5)}$$

$$\langle nl|\,4\pi\delta^3(r)\,|nl\rangle = \frac{4Z^3}{n^3}\delta_{l0}, \quad \text{(A6)}$$

$$\langle nl|\,\vec{p}\,4\pi\,\delta^3(r)\,\vec{p}\,|nl\rangle = \frac{4Z^5}{3}\bigg(-\frac{1}{n^5}+\frac{1}{n^3}\bigg)\delta_{l1}\,, \quad \text{(A7)}$$

$$\langle nl|\,\frac{1}{r^3}\,|nl\rangle = \frac{4Z^3}{n^3}\bigg(\ln\frac{n}{2Z} - \Psi(n) - \gamma + \frac{1}{2} - \frac{1}{2n}\bigg)\delta_{l,0} + \frac{2Z^3}{n^3}\,\frac{1-\delta_{l,0}}{l(l+1)(2l+1)}, \quad \text{(A8)}$$

$$\begin{aligned}\langle nl|\,\frac{1}{r^4}\,|nl\rangle = {} & \frac{8Z^4}{n^3}\bigg(-\ln\frac{n}{2Z} + \Psi(n) + \gamma - \frac{5}{3} + \frac{1}{2n} + \frac{1}{6n^2}\bigg)\delta_{l,0} \\ & +(1-\delta_{l,0})\frac{4Z^4\big(3n^2 - l(1+l)\big)}{(2l-1)l(2l+1)(l+1)(2l+3)n^5}, \end{aligned} \quad \text{(A9)}$$

$$\langle nl|\,p^2\frac{1}{r}\,|nl\rangle = 2E_n\,\langle nl|\,\frac{1}{r}\,|nl\rangle + 2Z\,\langle nl|\,\frac{1}{r^2}\,|nl\rangle = -\frac{Z^3}{n^4} + \frac{2Z^3}{n^3(l+\frac{1}{2})}, \quad \text{(A10)}$$

$$\langle nl|\,\vec{p}\,\frac{1}{r^2}\vec{p}\,|nl\rangle = Z^4\bigg[\delta_{l0}\bigg(-\frac{2}{3n^5}+\frac{8}{3n^3}\bigg) + \frac{2(1-\delta_{l0})}{(2l-1)(2l+1)(2l+3)}\bigg(\frac{\big(1-4l(l+1)\big)}{n^5}+\frac{8}{n^3}\bigg)\bigg]. \quad \text{(A11)}$$