QED theory of the specific mass shift in atoms

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The formalism of quantum electrodynamics for treating the interelectronic-interaction correction of first order in 1/Z to the two-electron part of the nuclear recoil effect on binding energies in atoms and ions is developed. The nonperturbative (in αZ) calculations of the corresponding contribution to the energies of the 1s2 state in He-like and the 1s22s and 1s22p1/2 states in Li-like ions are performed in the range Z = 5–100. The behavior of the two-electron part of the nuclear recoil effect beyond the lowest-order relativistic approximation as a function of Z is studied.

I. INTRODUCTION

Within the Breit approximation, the nuclear recoil effect on binding energies in atoms and ions can be treated by employing the mass shift (MS) Hamiltonian \( H_{\text{M}} = H_{\text{NMS}} + H_{\text{SMS}} \), which is given by [the relativistic units (\( \hbar = 1, c = 1 \)) are used throughout the paper]

\[
H_{\text{M}} = \frac{1}{2M} \sum_{i,j} \left\{ p_i \cdot p_j - \frac{\alpha Z}{r_i} \left[ \alpha_i + \frac{(\alpha \cdot r_i)r_i}{r_i^2} \right] \cdot p_i \right\},
\]

where the indices \( i \) and \( j \) enumerate the electrons, \( \alpha \) are the Dirac matrices, \( r \) is the position vector, \( r = |r| \), \( p \) is the momentum operator, \( \alpha \) is the fine-structure constant, \( Z \) and \( M \) are the nuclear charge number and nuclear mass, respectively. The first term in the curly braces in Eq. (1) represents the nonrelativistic recoil operator whereas the second term corresponds to the lowest-order relativistic correction. The Hamiltonian (1) can be written as a sum of its one- and two-electron parts

\[
H_{\text{M}} = H_{\text{NMS}} + H_{\text{SMS}},
\]

where

\[
H_{\text{NMS}} = \frac{1}{2M} \sum_i \left\{ p_i^2 - \frac{\alpha Z}{r_i} \left[ \alpha_i + \frac{(\alpha \cdot r_i)r_i}{r_i^2} \right] \cdot p_i \right\}
\]

is the normal mass shift (NMS) operator, and

\[
H_{\text{SMS}} = \frac{1}{2M} \sum_{i \neq j} \left\{ p_i \cdot p_j - \frac{\alpha Z}{r_i} \left[ \alpha_i + \frac{(\alpha \cdot r_i)r_i}{r_i^2} \right] \cdot p_i \right\}
\]

is the specific mass shift (SMS) operator. The terms “NMS” and “SMS” sometimes refer only to the nonrelativistic parts of the operators (3) and (4). In this case, the corresponding relativistic corrections given by the second terms in curly braces in Eqs. (3) and (4) are labeled with “RNMS” and “RSMS”, respectively, which denote the relativistic NMS and SMS operators. In the following, we will not separate these contributions employing, e.g., the term SMS for the whole operator (4).

The MS operator (1) is widely employed nowadays in relativistic calculations of the atomic electronic structure and, especially, isotope shifts (see, e.g., Refs. [12–15] and references therein). The Hamiltonian \( H_{\text{M}} \) allows one to take into account the nuclear recoil corrections within the \( (m/M)(\alpha Z)^4m^2c^2 \) approximation. The fully relativistic theory of the nuclear recoil effect in atoms in \( \alpha Z \) can be formulated only in the framework of quantum electrodynamics (QED) [1, 2, 16–18]. For the point-nucleus case, the calculations of the QED recoil contributions to the binding energies of few-electron ions to all orders in \( \alpha Z \) were performed in Refs. [13–21]. The finite nuclear size correction for these terms was partly taken into account for the 1s and 2s states of H-like ions in Refs. [22, 46]. We note that the rigorous treatment of the latter correction is currently accessible only within the lowest-order relativistic approximation [24, 26]. The most accurate to-date evaluation of the QED recoil effect for all of the \( n = 1 \) and \( n = 2 \) states of He-like ions was made in Ref. [27]. The results of the calculations for Be- and B-like ions were presented, e.g., in Refs. [9, 11]. It is worth noting that for high-\( Z \) systems the QED recoil corrections can be of comparable magnitude to the values obtained within the Breit approximation. For instance, the total nuclear recoil correction for the ground-state energy of H-like uranium constitutes 0.46 eV [22], and only about a half of this result comes from the MS operator (1).
All the previous calculations of the nuclear recoil contributions to all orders in \( \alpha Z \), see Refs. \[3, 11, 16, 23, 27\] and references therein, were limited by the independent-electron approximation, i.e., the interelectronic-interaction effects were treated only to zeroth order in \( 1/Z \). The present study aims at further development of the QED theory of the nuclear recoil effect in atoms. Namely, we derive the formalism for the QED evaluation of the interelectronic-interaction correction of first order in \( 1/Z \) to the two-electron part of the nuclear recoil effect on binding energies. The calculations of the two-electron contribution are generally more complicated than the evaluation of the one-electron part, which can be taken into account within the nonrelativistic approximation simply by replacing the electron mass \( m \) with the reduced one, \( m_e = mM/(m + M) \). In some sense, the contribution under consideration provides the QED correction for the SMS operator (4). In spite of the scaling factor of \( mM/\alpha Z \) electron mass \( m \) and charge \( e \), we employ the Furry picture of QED \[32\], where the electron-positron-field and electromagnetic-field moments are beyond the scope of the present study. For this reason, the nontrivial QED corrections to the SMS with increasing \( Z \) is analyzed. We note that for the \( S \) states, \( 1s^2 \) and \( 1s^22s \), the SMS vanishes to zeroth order in \( 1/Z \). Therefore, the correction of interest represents the leading two-electron contribution to the nuclear recoil effect for these states.

The paper is organized as follows. In Sec. II we remind the basic ideas of the QED theory of the nuclear recoil effect to zeroth order in \( 1/Z \). In Sec. III we consider the formulas derived for calculations within the rigorous QED approach of the first-order interelectronic-interaction correction to the two-electron part of the nuclear recoil effect on atomic binding energies. In Sec. IV the numerical results are presented and compared with the values obtained within the Breit approximation.

II. QED THEORY OF THE NUCLEAR RECOIL EFFECT TO ZEROTH ORDER IN \( 1/Z \)

In the present study we start with the QED theory of the nuclear recoil effect in atoms \[\frac{1}{2}\] which was generalized in Ref. \[10\]. The theory formulated in Ref. \[10\] leads to the diagram technique which represents a convenient approach for constructing the QED perturbation series. Within this approach, there is no need to sum infinite sequences of the Feynman diagrams describing the electron-nucleus interaction. This theory will be used in the next section in order to obtain formal expressions for the interelectronic-interaction correction to the two-electron part of the nuclear recoil effect. However, first, we briefly remind the basic formalism of the theory.

We consider the QED system which in addition to the electron-positron and electromagnetic fields includes also the nucleus. The latter one is assumed to be a nonrelativistic particle with mass \( M \) and charge \( Ze \) (\( e < 0 \) is the electron charge). Since the nuclear recoil effect on energy levels does not depend on the nuclear spin to first order in \( m/M \), we consider the nucleus to be spinless. Being an integral of motion, the total momentum of the whole system conserves. Therefore, in the center-of-mass frame the operator of the nuclear momentum can be expressed in terms of the electron-positron-field and electromagnetic-field momenta. Plugging the expression obtained into the Hamiltonian of the whole system, one can derive a field operator \( H_M \). This operator has to be added to the standard QED Hamiltonian of the electron-positron field interacting with the quantized electromagnetic field and with the classical Coulomb potential of the nucleus, \( V_{nucl} \), in order to take into account the nuclear recoil corrections to first order in \( m/M \) and to all orders in \( \alpha Z \). The contributions of first and higher orders in \( \alpha \) are beyond the scope of the present study. For this reason, the nontrivial terms involving the electromagnetic-field momentum \( P_f = \int dx [\mathcal{E}_i(x) \times \mathcal{H}_i(x)] \) contributing to these orders can be discarded in \( H_M \) actually, see the details in Ref. \[10\].

Within this approximation, the operator \( H_M \) in the Schrödinger representation and the Coulomb gauge reads as follows

\[
H_M = \frac{1}{2M} \int dx \psi^\dagger(x)(-i\nabla_x)\psi(x) \int dy \psi^\dagger(y)(-i\nabla_y)\psi(y) - \frac{eZ}{M} \int dx \psi^\dagger(x)(-i\nabla_x)\psi(x) A(0) + \frac{e^2Z^2}{2M} A(0)^2, \tag{5}
\]

where \( \psi \) and \( A \) are the electron-positron and electromagnetic field operators, respectively.

Being interested in the QED theory to all orders in \( \alpha Z \), we employ the Furry picture of QED \[32\], where the interaction with the classical field of the nucleus is included in the unperturbed Hamiltonian. The perturbation
series are constructed by applying the two-times Green function (TTGF) method. In order to account for the nuclear recoil effect, we take the operator $H_M$ in the interaction representation and add it to the interaction part of the Hamiltonian. The Feynman rules for the theory without $H_M$ are given, e.g., in Ref. [33]. The inclusion of the term $H_M$ adds several new lines and vertices to the diagram technique, see Ref. [16] for the details. To introduce the notations employed in the following, we briefly discuss the new elements of the diagram technique by the example of the two-electron contribution.

To zeroth order in $1/Z$, the two-electron contribution to the nuclear recoil effect on binding energies of a few-electron atom is described by the diagrams shown in Fig. 1. As usual for bound-state QED, the double line denotes the electron propagator in the classical field of the nucleus. The vertex with a small black dot is the standard vertex of QED. The additional vertices with the bold dots come from the term $H_M$ and include the momentum operator $p = -i \nabla$. In accordance with Ref. [16], the dotted line ended by two bold dots in Fig. 1(a) designates the "Coulomb recoil" interaction. The dashed lines attached to a bold dot on one side in Figs. 1(b) and 1(c) denote the "one-transverse recoil" interaction, because these lines contain the transverse part of the photon propagator taken in the Coulomb gauge

$$D_{lk}(\omega, r) = \frac{1}{4\pi} \left[ \frac{\exp(i\sqrt{\omega^2 + i0} r)}{r} \delta_{lk} + \nabla_l \nabla_k \frac{\exp(i\sqrt{\omega^2 + i0} r) - 1}{\omega^2 r} \right],$$

where $r = |r|$ and the branch of the square root is fixed with the condition $\Im(\sqrt{\omega^2 + i0}) > 0$. Finally, the dashed line with a bold dot on it in Fig. 1(d) contains the product of two photon propagators (6) and, for this reason, corresponds to the "two-transverse recoil" interaction. We note that the employed separation of the terms as well as the terminology itself result from operating in the Coulomb gauge which is the most convenient one for dealing with the nuclear recoil effect, see, e.g., Refs. [1, 2, 18].

Applying the TTGF method, one can easily derive the formulas for the two-electron contribution. For simplicity, we consider a two-electron ion described by the one-determinant unperturbed wave function

$$u_{2el} = \frac{1}{\sqrt{2}} \sum_P (-1)^P \psi_P(a)e^{i}\nabla \psi_P(b)e^{-i}\nabla,$$

where $\psi_n$ are the solutions of the one-electron Dirac equation with the potential of the nucleus included

$$[-i\alpha \cdot \nabla + \beta m + V_{\text{nucl}}(r)] \psi_n(r) = \epsilon_n \psi_n(r),$$

$P$ is the permutation operator, and $(-1)^P$ is the sign of the permutation. A more general case of an $N$-electron atom described by a many-determinant wave function can be treated in the same manner. According to Ref. [33], the first-order correction to the energy of a single level is given by

$$\Delta E^{(1)}(E) = \frac{1}{2\pi i} \int_{\Gamma} \Delta E \Delta g_{uu}^{(1)}(E),$$

where $\Delta g_{uu}^{(1)}$ is the Fourier transform of the relevant first-order contribution to two-time Green’s function projected on the unperturbed state, $\Delta E = E - E_u^{(0)}$, and $E_u^{(0)}$ is the unperturbed energy. The contour $\Gamma$ oriented counterclockwise has to surround the point $E_u^{(0)}$. The derivation of the formulas for the two-electron part of the nuclear recoil effect to zeroth order in $1/Z$ is similar to that of the one-photon exchange correction, see, e.g., Ref. [34]. Employing the TTGF method, we obtain

$$\Delta E^{(1)} = \frac{1}{M} \sum_P (-1)^P \langle Pa | pk | a \rangle \langle Pb | pk | b \rangle,$
for the Coulomb contribution in Fig. 1(a),

$$\Delta E^{(1)}_{tr1} = -\frac{1}{M} \sum_{\rho} (-1)^\rho \left[ \langle Pa|p_k|a\rangle \langle Pb|D_k(\Delta)|b\rangle + \langle Pa|D_k(\Delta)|a\rangle \langle Pb|p_k|b\rangle \right]$$

(11)

for the one-transverse-photon contribution in Figs. 1(b) and 1(c), and

$$\Delta E^{(1)}_{tr2} = \frac{1}{M} \sum_{\rho} (-1)^\rho \langle Pa|D_k(\Delta)|a\rangle \langle Pb|D_k(\Delta)|b\rangle$$

(12)

for the two-transverse-photon contribution in Fig. 1(d). In Eqs. (10)-(12), the summation over the repeated indices is implied (this convention is held for the subsequent expressions as well), $\Delta = \varepsilon_{Pa} - \varepsilon_a$, and

$$D_k(\omega) = -4\pi\alpha Z\alpha_l D_{lk}(\omega),$$

(13)

where $\alpha_l$ ($l = 1, 2, 3$) are the Dirac matrices. The total two-electron contribution to the nuclear recoil effect to zeroth order in $1/Z$ is given by the sum of Eqs. (10)-(12),

$$\Delta E^{(1)}_{rec,2el} = \Delta E^{(1)}_c + \Delta E^{(1)}_{tr1} + \Delta E^{(1)}_{tr2}.$$  

(14)

Taking into account Eq. (9), the zero-energy-transfer limit $\omega \to 0$ of Eq. (13) reads as

$$D_k(0) = \frac{\alpha Z}{2r} \left[ \alpha_k + \frac{(\alpha_l r_k) r_k}{r^2} \right].$$

(15)

By discarding the two-transverse-photon contribution and considering the limit $\omega \to 0$ in the one-transverse-photon term in Eq. (14), one derives the effective two-electron operator which describes the nuclear recoil effect within the Breit approximation. Obviously, this procedure leads to the SMS operator given in Eq. (4). The Coulomb contribution (10) corresponds to the nonrelativistic two-electron recoil operator while its low-order relativistic correction arises from the one-transverse-photon contribution.

### III. INTERELECTRONIC-INTERACTION CORRECTION TO THE TWO-ELECTRON PART OF THE NUCLEAR RECOIL EFFECT

According to Ref. [32], the second-order correction for energy of a single level is given by

$$\Delta E^{(2)} = \frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g^{(2)}_{uu}(E) - \left( \frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g^{(1)}_{uu}(E) \right) \left( \frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g^{(1)}_{uu}(E) \right),$$

(16)

where the contour $\Gamma$ surrounds the pole of the level under consideration $E^{(0)}_u$ and keeps outside all the other singularities of Green’s function $\Delta g^{(2)}_{uu}$. The second term in Eq. (16), which we refer to as the disconnected one, usually can be fully canceled by separating the corresponding contributions in the most nontrivial first term. The procedure of the analytical cancellation of the disconnected contribution demands rather tedious manipulations and depends on the total number of electrons $N$. In this work, we consider the cases of heliumlike ($N = 2$) and lithiumlike ($N = 3$) ions and present the formulas only for single levels described by one-determinant unperturbed wave functions. The two-electron unperturbed wave function was given in Eq. (7) while in case of $N = 3$ the wave function can be written as

$$u_{3el} = \frac{1}{\sqrt{3!}} \sum_{\rho} (-1)^\rho \psi_{P1}(r_1)\psi_{P2}(r_2)\psi_{P3}(r_3),$$

(17)

where the one-electron states are labeled with the indices 1, 2, and 3. The generalization to the case of a many-determinant wave function is straightforward. Moreover, the derived formalism suits for any atomic systems actually and can be generalized to describe the nuclear recoil effect on energy levels of (quasi-)degenerate states [32].

The example of diagrams describing the interelectronic-interaction correction to the two-electron part of the nuclear recoil effect is shown in Fig. 2. The wavy line denotes the photon propagator here. Other notations are the same as in Fig. 1. In Fig. 2 only the two-transverse-photon contribution is presented. One should consider also the diagrams with the two-transverse-photon recoil interaction replaced with the Coulomb and one-transverse-photon recoil interactions. As a result, the total number of the second-order diagrams is four times higher actually. We
FIG. 2. The second-order diagrams describing the interelectronic-interaction correction to the two-electron two-transverse-photon contribution to the nuclear recoil effect. The analogous diagrams with the Coulomb and one-transverse photon recoil interactions have to be taken into account as well. See the text and Ref. [16] for the description of the diagram technique.

FIG. 3. The one-photon exchange diagram which along with the first-order diagrams in Fig. 1 contributes to the second "disconnected" term in Eq. (16).

refer to the diagrams in Figs. 2(a) and 2(b) as the ladder contribution and to the diagrams in Figs. 2(c) and 2(d) as the crossed contribution. For heliumlike ions, only these two-electron diagrams contribute. For lithiumlike ions, the three-electron diagrams in Figs. 2(e) and 2(f) come into play as well. The list of diagrams, which have to be accounted for in the disconnected term in Eq. (16), includes the first-order diagrams in Fig. 1 and the one-photon-exchange diagram shown in Fig. 3.

For the subsequent consideration, it is convenient to introduce the following notations

\[ I(\omega) = e^2 \alpha_1^\mu \alpha_2^\nu D_{\mu\nu}(\omega), \]
\[ R_c = \frac{1}{M} p_1 \cdot p_2, \]
\[ R_{\text{tr}1}(\omega) = -\frac{1}{M} [p_1 \cdot D_2(\omega) + D_1(\omega) \cdot p_2], \]
\[ R_{\text{tr}2}(\omega) = \frac{1}{M} D_1(\omega) \cdot D_2(\omega), \]

where \( \alpha^\mu = (1, \alpha) \), \( D_{\mu\nu} \) is the photon propagator, and the vector \( D \) was defined in Eq. (13). We imply also that \( I'(\omega) = dI(\omega)/d\omega \) and \( R'(\omega) = dR(\omega)/d\omega \), where \( R \) means any of the operators (19)-(21). In the Coulomb gauge employed, Eq. (15) reads as follows

\[ I(\omega) = \alpha \left[ \frac{1}{r_{12}} - \frac{(\alpha_1 \cdot \alpha_2) \exp \left( i \sqrt{\omega^2 + i 0} r_{12} \right)}{r_{12}} + (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) \exp \left( i \sqrt{\omega^2 + i 0} r_{12} \right) - 1}{\omega^2 r_{12}^2} \right]. \]

From Eqs. (13) and (22), it is obvious that in the Coulomb gauge the following symmetry properties \( I(\omega) = I(-\omega) \) and \( R(\omega) = R(-\omega) \) are held. For brevity, we will designate the matrix elements of the operators (18) and (19).
as $I_{abcd}(\omega) = \langle ab|I(\omega)|cd \rangle$ and $R_{abcd}(\omega) = \langle ab|R(\omega)|cd \rangle$, respectively. The zero-energy-transfer limit $\omega \to 0$ of Eq. (22) which along with the MS operator $\tilde{I}$ can be employed to evaluate the effects of the interelectronic interaction on the nuclear recoil within the Breit approximation is given by

$$I = \alpha \left[ \frac{1}{r_{12}} - \frac{\langle \alpha_1 \cdot \alpha_2 \rangle}{r_{12}} - \frac{\langle \alpha_1 \cdot \nabla_1 (\alpha_2 \cdot \nabla_2) \rangle}{r_{12}} \right].$$  \hspace{1cm} (23)

The derivation of the formal expressions for the interelectronic-interaction correction to the two-electron part of the nuclear recoil effect within the TTGF method is very similar to the derivation of the corresponding formulas for the two-photon exchange contribution which was considered in details in Refs. 35, 36. We present only the final expressions omitting all the intermediate steps. First, we discuss the contribution of the two-electron diagrams presented in Figs. 2(a)-(d) and the related diagrams with the Coulomb and one-transverse-photon recoil interactions. As noted above, the two-electron contributions provide the total result in case of heliumlike ions. On the other hand, the three-electron problem with the unperturbed wave function $\tilde{\Psi}$ can be decomposed into three two-electron problems of the type $\tilde{\Psi}$. Therefore, the two-electron contribution has to be taken into account for all possible electron pairs $(ab) = (12), (13), \text{and} (23)$ in the three-electron state $u_{3\text{el}}$. The contribution of the ladder ("lad") diagrams in Figs. 2(a) and 2(b) is divided naturally into irreducible ("irr") and reducible ("red") parts. The reducible part covers the terms for which an intermediate-state energy coincides with the energy $E_0^{(3)} = \varepsilon_a + \varepsilon_b$ of the state under consideration whereas the irreducible part includes the remainder. The irreducible part of the ladder diagrams reads as

$$\Delta E_{\text{lad, irr}}^{(2)} = \frac{1}{2} \sum_p \sum_{n_1 n_2} \sum_{\mu \mu_1 \mu_2} \left( \frac{-i}{2\pi} \right) \int d\omega \left[ \frac{1}{(\omega + i0)^2} \right]$$

$$\times \left[ I_{P a P b \tilde{b} a}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P a} - \varepsilon_{P b}) R_{\tilde{b} a b}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P a} - \varepsilon_{P b}) + I_{P a P b \tilde{b} a}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P b} - \varepsilon_{P a}) R_{\tilde{b} a b}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P b} - \varepsilon_{P a}) \right] \hspace{1cm} (24)$$

where $u = (1 - i0)$ provides the proper treatment of the poles in the electron propagator, and the prime on the sum indicates that the intermediate states with $\varepsilon_{n_1} + \varepsilon_{n_2} = \varepsilon_a + \varepsilon_b$ are excluded. As to the reducible part, the condition $\varepsilon_{n_1} + \varepsilon_{n_2} = \varepsilon_a + \varepsilon_b$ generally restricts the summation over $n_1$ and $n_2$ to the terms with $(\varepsilon_{n_1}, \varepsilon_{n_2}) = (\varepsilon_a, \varepsilon_b)$. However, since the matrix elements of the operators $P$ and $D$ are equal to zero for states which have the same parity, one can conclude that only one of these possibilities contributes. For the same reason, the reducible part of the ladder diagrams does not vanish identically as a whole only if the electrons $a$ and $b$ belong to different electron shells having the opposite parity. The reducible part of the ladder diagram can be expressed as

$$\Delta E_{\text{lad, red}}^{(2)} = \frac{1}{2} \sum_p \sum_{\mu \mu_1 \mu_2} \left( \frac{-i}{2\pi} \right) \int d\omega \left[ \frac{1}{(\omega + i0)^2} \right]$$

$$\times \left[ I_{P a P b \tilde{b} a}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P a} - \varepsilon_{P b}) R_{\tilde{b} a b}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P a} - \varepsilon_{P b}) + I_{P a P b \tilde{b} a}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P b} - \varepsilon_{P a}) R_{\tilde{b} a b}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P b} - \varepsilon_{P a}) \right] \hspace{1cm} (25)$$

where it is assumed that $\varepsilon_{\tilde{a}} = \varepsilon_a$ and $\varepsilon_{\tilde{b}} = \varepsilon_b$. Finally, the contribution of the crossed ("cr") diagrams in Figs. 2(c) and 2(d) is given by

$$\Delta E_{\text{cr}}^{(2)} = \sum_p \sum_{n_1 n_2} \sum_{\mu \mu_1 \mu_2} \left( \frac{-i}{2\pi} \right) \int d\omega \left[ \frac{1}{(\omega + i0)^2} \right]$$

$$\times \left[ I_{P_{n_1} P_{n_2} \tilde{b} a}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P_{n_1} P_{n_2}} - \varepsilon_{\tilde{b} a}) R_{\tilde{b} a b}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P_{n_1} P_{n_2}} - \varepsilon_{\tilde{b} a}) + I_{P_{n_1} P_{n_2} \tilde{b} a}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P_{n_1} P_{n_2}} - \varepsilon_{\tilde{b} a}) R_{\tilde{b} a b}^{\mu \mu_1 \mu_2} (\omega + \varepsilon_{P_{n_1} P_{n_2}} - \varepsilon_{\tilde{b} a}) \right] \hspace{1cm} (26)$$

Now, we consider the contribution of the three-electron diagrams in Figs. 2(e) and 2(f). As in case of the ladder diagrams, one can divide the three-electron contribution into the irreducible and reducible parts. The irreducible contribution of the three-electron diagrams reads as

$$\Delta E_{\text{3el, irr}}^{(2)} = \sum_{PQ} \sum_{n_1 n_2} \sum_{\mu \mu_1 \mu_2} \left[ \frac{I_{P_{n_2} Q_{n_1}} (\Delta_{P_{n_2} Q_{n_1}}) R_{P_{n_2} Q_{n_1} Q_{2}} (\Delta_{Q_{n_1} Q_{2}})}{\varepsilon_{Q_{n_1} Q_{2}} - \varepsilon_{P_{n_1} P_{n_2}}} + \{ I \leftrightarrow R \} \right] \hspace{1cm} (27)$$

where the prime on the sum indicates that the terms with vanishing denominator have to be omitted in the summation. The contribution of the reducible part of the three-electron diagrams in Figs. 2(e) and 2(f) can be expressed as

$$\Delta E_{\text{3el, red}}^{(2)} = \frac{1}{2} \sum_{PQ} \sum_{\mu \mu_1 \mu_2} \left[ \frac{I_{P_{n_2} Q_{n_1}} (\Delta_{P_{n_2} Q_{n_1}}) R_{P_{n_2} Q_{n_1} Q_{2}} (\Delta_{Q_{n_1} Q_{2}})}{\varepsilon_{Q_{n_1} Q_{2}} - \varepsilon_{P_{n_1} P_{n_2}}} + \{ I \leftrightarrow R \} \right] \hspace{1cm} (28)$$
To summarize, in case of a single level in heliumlike ion the QED interelectron-interaction correction of first order in 1/Z to the two-electron part of the nuclear recoil effect is given by the sum of Eqs. (24)-(26). For lithiumlike ions, in order to take into account the corresponding correction one has to calculate Eqs. (24)-(26) for all possible pairs of electrons present in the unperturbed three-electron state and then add the contribution of Eqs. (27) and (28). The calculations have to be performed for all the operators (19)-(21),

\[
\Delta E_{rec,2el}^{(2)} = \Delta E_{c}^{(2)} + \Delta E_{tr1}^{(2)} + \Delta E_{tr2}^{(2)}.
\]

Finally, we note that the formalism presented in this section reproduces the expressions for the interelectronic-interaction correction to the SMS within the Breit approximation if one neglects the energy dependence in the operators \( D(\omega) \) and \( I(\omega) \) in Eqs. (13) and (22), respectively, and introduces projectors on the positive-energy part of the spectrum. As previously, the Coulomb gauge is implied for the interelectronic-interaction operator \( I(\omega) \), so that within the zero-energy-transfer limit one comes to the operator \( I \) in Eq. (28). On these assumptions, all the reducible contributions vanish since \( I'(0) = 0 \) and \( R'(0) = 0 \), and the \( \omega \) integrations in the two-electron terms can be carried out analytically employing Cauchy’s residue theorem. The contribution of the crossed diagram vanishes because all the zeros of the denominators in Eq. (26) lie in the upper half-plane and, therefore, the integration contour can be closed in the lower half-plane avoiding the singularities. Therefore, the irreducible part of the ladder contribution yields the total two-electron correction within the Breit approximation:

\[
\Delta E_{rec,2el}^{(2)} = \sum_{P} (-1)^P \sum_{n_1 n_2} \left[ \sum_{\mu_{n_1} \mu_{n_2}} I_{P a P b n_1 n_2}(0) R_{n_1 n_2 \mu_{n_1} \mu_{n_2}}(0) \right] \frac{\epsilon_a + \epsilon_b - \epsilon_{n_1} - \epsilon_{n_2}}{\epsilon_a + \epsilon_b - \epsilon_{n_1} - \epsilon_{n_2}} + \{ I \leftrightarrow R \}.
\]

where the summation over \( n_1 \) and \( n_2 \) is restricted by the conditions \( \epsilon_{n_1} > 0, \epsilon_{n_2} > 0 \), and \( \epsilon_{n_1} + \epsilon_{n_2} \neq \epsilon_a + \epsilon_b \).

The three-electron contribution within the Breit approximation is readily obtained from Eq. (27) by discarding the negative-energy part of the spectrum \( \epsilon < 0 \) and replacing \( \Delta_{P 3Q3} \) and \( \Delta_{Q1P1} \) with zeros. The contribution of the two-transverse-photon operator (21) has to be omitted within this approximation.

### IV. NUMERICAL RESULTS AND DISCUSSION

In the present section, the formalism derived in Secs. I1 and II is applied to the all-order (in \( \alpha Z \)) evaluation of the two-electron contribution to the nuclear recoil effect on the binding energies of the 1s\(^2\) state in heliumlike ions and the 1s\(^2\)2s and 1s\(^2\)2p\(_{1/2}\) states in lithiumlike ions. In Ref. 16, it was shown that the nuclear size correction to the nuclear recoil effect can be partially taken into account by replacing the pure Coulomb potential \( V_{nucl} = -\alpha Z/r \) with the potential of an extended nucleus. Following this prescription, we employ the Fermi model to describe the nuclear charge distribution for all ions except for the ones with \( Z = 5 \) and \( Z = 10 \). For the latter nuclei, the homogeneously-charged-sphere model is used instead. The nuclear charge radii are taken from Refs. 37, 38.

The summation over intermediate electron states is performed employing the finite basis sets constructed from the B-splines 39, 40 within the dual kinetic balance approach 41.

For states under consideration, to zeroth order in 1/Z the two-electron recoil contribution does not vanish only for the state 1s\(^2\)2p\(_{1/2}\). The results of our calculations expressed in terms of the dimensionless function \( A(\alpha Z) \),

\[
\Delta E_{rec,2el}^{(1)} = \frac{m}{M} (\alpha Z)^2 A(\alpha Z) mc^2,
\]

are given in Table II. We stress that the index “(1)” in the left part of Eq. (31) designates that the corresponding energy shift is obtained as the first-order perturbation within the TTGF method. For each \( Z \), the values evaluated according to Eqs. (10)–(12) are shown in the first line. The results obtained within the lowest-order relativistic approximation employing the SMS operator \( H_{SMS} \) are displayed in the second lines. The functions \( A_c \), \( A_{tr1} \), and \( A_{tr2} \) correspond to the terms \( \Delta E_{c}^{(1)} \), \( \Delta E_{tr1}^{(1)} \), and \( \Delta E_{tr2}^{(1)} \), respectively. One can see that to zeroth order in 1/Z the Coulomb contribution \( A_c \) has the same value within both approaches. The deviation of the one-transverse-photon term is determined by the frequency-dependent correction in the operator \( D(\omega) \) in Eq. (15). The two-transverse-photon contribution is absent in the Breit approximation. From Table II it is seen that the terms of the higher orders in \( \alpha Z \) can significantly alter the total values, especially, for high-Z ions, where the contribution of the nonrelativistic part of the SMS operator (1) is canceled considerably by the contribution due to the low-order relativistic correction for it, see, e.g., the relevant discussion in Ref. 4. For the point-nucleus case, the corresponding correction was considered previously in Ref. 21. We note that in Ref. 20 the two-electron...
contribution for the $1s^22p_{1/2}$ was presented in terms of the dimensionless function $Q(\alpha Z)$ which differs from the function $A(\alpha Z)$ by the factor of $-3^8/2^9$, see Eq. (74) in Ref. [20]. For comparison, the point-nucleus results from Ref. [21] expressed in terms of the function $A(\alpha Z)$ are given in the last column of Table [I].

The interelectronic-interaction correction of first order in $1/Z$ to the two-electron part of the nuclear recoil effect is conveniently represented via the dimensionless function $B(\alpha Z)$ defined by

$$\Delta E^{(2)}_{\text{rec,2el}} = \frac{m}{M}(\alpha Z)^2 B(\alpha Z) mc^2,$$

(32)

The results of the calculations for the $1s^2$, $1s^22s$, and $1s^22p_{1/2}$ states expressed in terms of the function $B(\alpha Z)$ are presented in Tables [I] [III] and [IV] respectively. As in Table [I] for each $Z$ the results of the QED calculations to all orders in $\alpha Z$ as well as the values obtained employing the SMS operator $H_{\text{SMS}}$ are given. The functions $B_C$, $B_{11}$, and $B_{22}$ correspond to the contributions of the Coulomb [19], the one-transverse-photon [20], and the two-transverse-photon [21] operators, respectively. The uncertainties given in the tables correspond only to errors of the numerical calculations. They were estimated by increasing the size of the employed basis set and also by studying how the integrations over the energy parameter $\omega$ in Eq. (24) and the other related contributions converge. When the uncertainty is not specified, all the digits presented should be correct. Except for the heaviest ions with $Z \geq 92$, the uncertainties due to varying the nuclear charge distribution model as well as the nuclear charge radii are below the number of digits shown. For the heaviest ions, this varying may alter the last digit. In addition, we should stress once more that the calculations with the wave functions evaluated for the extended nucleus correspond to a partial treatment of the nuclear size corrections to the recoil effect. The uncertainty due to this approximation can be estimated in accordance with the prescription given, e.g., in Ref. [27].

As noted at the end of the previous section, the calculation formulas which are valid within the lowest-order relativistic approximation can be obtained from the general QED expressions if we neglect the energy dependence of the transverse part of the photon propagator in the Coulomb gauge in Eq. (4), restrict the consideration to the positive-energy part of the Dirac spectrum, and omit the two-transverse-photon contribution. As an independent check, we evaluated the two-electron part of the nuclear recoil effect in the Breit approximation employing the numerical code for the QED calculations and compared the results obtained with the direct application of the SMS operator [4]. The two calculations were found to be in agreement with each other.

From Tables [I] [IV] one can note that, compared to the independent-electron approximation, the Coulomb correction acquires the correction to the Breit-approximation result due to the higher orders in $\alpha Z$. The alteration of the one-transverse-photon contribution is also more pronounced than it takes place to zeroth order in $1/Z$, since the corresponding correction is not limited to the simple inclusion of the frequency-dependent correction. In addition, the two-transverse-photon contribution increases rapidly with increasing $Z$. As a result, the total QED values may drastically differ from the approximate ones evaluated to lowest orders in $\alpha Z$ employing the operator $H_{\text{SMS}}$. In order to illustrate the behavior of the interelectronic-interaction correction to the two-electron part of the nuclear recoil effect, we plot the total contributions to the binding energies of the states under consideration in Figs. [4]-[6].

The data given in the last columns of Tables [I] [IV] are presented. The results obtained employing the SMS operator [I] are shown with dashed lines. The values calculated by means of $ab\ initio$ approach derived in the previous section are displayed with solid lines. It is worth noting that for the $1s^22p_{1/2}$ state the interelectronic-interaction correction to the two-electron recoil within the Breit approximation tends to zero as it was found for the leading in $1/Z$ contribution. From Fig. [6] one can see that the effects of higher orders in $\alpha Z$ changes the situation. Finally, we should note also that by combining the data presented in Tables [II] [IV] one can readily obtain the interelectronic-interaction correction to the two-electron part of the nuclear recoil effect on the ionization potentials of the $1s^22s$ and $1s^22p_{1/2}$ states as well as the $2p_{1/2} - 2s$ transition energy in lithiumlike ions.

The total two-electron nuclear recoil contribution to the energy shift can be expressed as

$$\Delta E_{\text{rec,2el}} = \frac{m}{M}(\alpha Z)^2 F(\alpha Z, Z) mc^2,$$

(33)

where, in accordance with the definitions given in Eqs. (31) and (32), one obtains

$$F(\alpha Z, Z) = A(\alpha Z) + \frac{1}{Z} B(\alpha Z) + \cdots,$$

(34)

and an elipsis in Eq. (34) corresponds to the terms of the second and higher orders in $1/Z$. As noted above, for the $S$ states, $1s^2$ and $1s^22s$, the $1/Z$ perturbation theory starts from the first-order correction $B(\alpha Z)$, and the contribution of interest represents the leading two-electron term. For the $1s^22p_{1/2}$ state, it is not the case. Therefore, in Table [IV] we compare the zeroth- and first-order contributions to the corresponding function $F(\alpha Z, Z)$. The term $A(\alpha Z)$ is taken from the penultimate column in Table [I] while the function $B(\alpha Z)$ is from the last column in Table [IV]. For illustrative purposes, the data given in Table [V] are plotted also in Fig. [7]. As in Figs. [4]-[6], the
dashed lines correspond to the calculations with the SMS operator \( \mathbb{I} \), and the solid lines represent the QED results. The zeroth-order contributions to the function \( F(\alpha Z, Z) \) are indicated with the blue lines with circles on them. The next-to-leading approximations to the function \( F(\alpha Z, Z) \), given by the sums of zeroth and first orders in \( 1/Z \), are shown with the red lines with squares on them. Naturally, for low-\( Z \) ions the \( 1/Z \) perturbation theory may converge slowly. From Fig. 7 it is seen that the interelectronic-interaction correction to the SMS is comparable in magnitude with the leading contribution. For this reason, our calculations taken alone do not pretend to provide the best possible theoretical predictions for the two-electron part of the nuclear recoil effect for low-\( Z \) ions. If needed, the results obtained for these systems can be further improved by considering within the Breit approximation the second- and higher-order contributions to Eq. (33) by means of, e.g., the configuration interaction \( \mathbb{I} \) or the recursive perturbation theory \( \mathbb{I} \) methods. In the present work, we pursue the aim to study the influence of the nontrivial QED effects on the two-electron recoil contribution. In this regard, one can see from Table VI and Fig. 7 that taking into account of the terms of higher orders in \( \alpha Z \) considerably changes the behavior of the function \( F(\alpha Z, Z) \) as a function of \( Z \). The calculations based on the SMS operator \( H_{\text{SMS}} \) lead to an underestimation of the two-electron contribution for high-\( Z \) ions. Moreover, the dashed lines in Fig. 7 lie much closer to each other than the solid ones for high-\( Z \) ions. This designates once again that the nontrivial QED contribution of first order in \( 1/Z \) represents the significant effect.

Finally, we consider the two-electron part of the nuclear recoil effect on the \( 2p_{1/2} \rightarrow 2s \) transition energy in lithiumlike ions. For the point-nucleus case, the one-electron contribution arising from the NMS operator \( \mathbb{I} \) can be evaluated analytically to zeroth order in \( 1/Z \) \( \mathbb{I} \):

\[
\Delta E_{\text{1el},\text{1st}}^{(p)} = \frac{m^2 - \varepsilon^2}{2M},
\]

where \( \varepsilon \) is the Dirac energy. Since \( \varepsilon_{2s} = \varepsilon_{2p_{1/2}} \) for the pure Coulomb potential \( V_{\text{nucl}} = -\alpha Z/r \), the one-electron contribution within the Breit approximation vanishes in this limit. Therefore, the total mass shift for this transition is determined by the finite-nuclear-size, one-electron QED as well as two-electron recoil effects. In Fig. 8 we plot the two-electron nuclear recoil contribution to the \( 2p_{1/2} \rightarrow 2s \) transition energy evaluated by means of the \( 1/Z \) perturbation theory up to the first order. The notations are the same as in Fig. 7 for the binding energy of the \( 1s^22p_{1/2} \) state. Since the two-electron recoil term for the \( 1s^22s \) state is equal to zero within the independent-electron approximation, to zeroth order in \( 1/Z \) the corresponding contributions to the transition and \( 1s^22p_{1/2} \) state coincide with each other (the blue lines in Figs. 7 and 8 are the same). The first-order interelectronic-interaction correction can be obtained by taking the difference of the results presented in Tables VII and VIII, respectively. From Figs. 7 and 8 one can conclude that, in principle, the behavior of the total two-electron nuclear recoil effect with the growth of \( Z \) is rather similar in these two cases. Compared to the binding energy of the \( 1s^22p_{1/2} \) state, the nontrivial QED part of the interelectronic-interaction correction is reduced slightly for the \( 2p_{1/2} \rightarrow 2s \) transition. Nevertheless, it notably contributes. For instance, in Refs. 7, 8 the nuclear recoil correction for the \( 2p_{1/2} \rightarrow 2s \) transition energy was studied. The approach employed there merges the calculations based on the MS operator \( \mathbb{I} \) within the Breit approximation to all orders in \( 1/Z \) with the QED contributions evaluated within the independent-electron approximation 20. The nuclear recoil corrections were presented in terms of the mass shift coefficient \( K \) defined according to

\[
\Delta E_{\text{rec}} = \frac{K}{M}.
\]

In Refs. 7, 8, the mass shift coefficients for the \( 2p_{1/2} \rightarrow 2s \) transition energy in lithiumlike thorium and uranium were found to be (in units of 1000 GHz amu) \( K_{\text{Th}} = -3441(57) \) and \( K_{\text{U}} = -3734(65) \), respectively. As noted in Ref. 8, the uncertainties specified are mainly due to the estimation of the uncalculated QED contributions of first order in \( 1/Z \). Based on the results obtained in this work for the interelectronic-interaction correction to the two-electron recoil effect which are presented in Tables VIII and IX one can extract the nontrivial QED part of first order in \( 1/Z \). This two-electron QED correction constitutes (in units of 1000 GHz amu) \( \delta K_{\text{QED},2\text{el}}^{\text{Th}} = 51 \) and \( \delta K_{\text{QED},2\text{el}}^{\text{U}} = 60 \) for thorium and uranium ions, respectively. The theoretical accuracy of the mass shift calculations for the \( 2p_{1/2} \rightarrow 2s \) transition can be significantly improved, provided the one-electron QED correction of first order in \( 1/Z \) is calculated. We should stress that, to zeroth order in \( 1/Z \), the one- and two-electron QED recoil corrections contribute to the total mass shift for the \( 2p_{1/2} \rightarrow 2s \) transition with the same sign enhancing each other, see Ref. 8. If this trend persists in first order in \( 1/Z \), one may expect that the effect of the uncalculated QED contributions is probably underestimated in Ref. 7, 8.

V. SUMMARY

To summarize, we have derived the formalism for \textit{ab initio} calculations of the interelectronic-interaction correction to the two-electron part of the nuclear recoil effect on binding energies in atoms and ions to all orders in \( \alpha Z \). The
technique developed was applied to evaluate the two-electron recoil contributions for the $1s^2$ state in heliumlike ions and the $1s^22s$ and $1s^22p_{1/2}$ states in lithiumlike ions in the wide range $Z = 5–100$. The corresponding contribution to the $2p_{1/2} - 2s$ transition energy in lithiumlike ions was investigated as well. The results of the QED calculations to zeroth and first orders in $1/Z$ were compared with their counterparts obtained by employing the specific mass shift operator $H_{\text{SMS}}$ given by Eq. (4). The behavior of the nontrivial two-electron QED contribution with increasing nuclear charge number $Z$ was discussed. The obtained all-order (in $\alpha Z$) results allow one to estimate in a more rigorous way the accuracy of the calculations based on the mass shift Hamiltonian $H_M$ in Eq. (1) which describes the nuclear recoil effects only within the $(m/M)(\alpha Z)^4mc^2$ approximation.

In the future, we plan to extend the QED formalism developed in order to study the interelectronic-interaction correction to the one-electron part of the nuclear recoil effect on binding energies in atoms. In particular, this will allow one to improve the theoretical accuracy of the mass shift calculations in highly charged ions. We note also that the largest contribution to the theoretical uncertainty of the isotope shift of the $g$ factor in lithiumlike calcium is currently determined by the screened QED contributions of first order in $1/Z$ [43]. In view of the experiments presently implemented at the Max-Planck-Institut für Kernphysik (MPIK) in Heidelberg [44] and at GSI in Darmstadt [45, 46], which are aimed at further improvement of the experimental precision of the $g$ factor itself as well as the isotope shifts of the $g$ factor, the QED calculations of the nuclear recoil effect on the $g$ factor of highly charged ions turn out to be urgent. In this connection, the QED theory of the nuclear recoil effect on binding energies developed represents a good starting point for the corresponding theory for the $g$ factor.

Finally, the nonperturbative (in $\alpha Z$) calculations of the nuclear recoil contributions of first order in $\alpha$ for hydrogen and light hydrogenlike ions are also of great interest. The comparison between the nonperturbative numerical approach and the analytical perturbative techniques may provide important data for the remaining higher-order contributions beyond the known $\alpha Z$-expansion terms, see the related discussion about the contribution of the nuclear recoil effect on the Lamb shift to zeroth order in $\alpha$ in Refs. [47, 48].

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TABLE I: The two-electron recoil contribution of zeroth order in $1/Z$ to the binding energy of the $1s^22p_{1/2}$ state expressed in terms of the dimensionless function $A(\alpha Z)$ defined by Eq. 31. For each $Z$, the first line shows the results of the QED calculations to all orders in $\alpha Z$, whereas the second line displays the values obtained within the Breit approximation employing the specific mass shift (SMS) operator given in Eq. 31. The results by Artemyev et. al [20] for point-nucleus case expressed in terms of $A(\alpha Z)$ are in the last column.

| $Z$ | Approach | $A_c(\alpha Z)$ | $A_{131}(\alpha Z)$ | $A_{132}(\alpha Z)$ | $A(\alpha Z)$ | $A^{(b)}(\alpha Z)$ [20] |
|-----|----------|-----------------|---------------------|---------------------|----------------|--------------------------|
| 5   | QED      | -0.078 168     | 0.000 182           | 0.000 000           | -0.077 986     | -0.077 986               |
|     | HMS      | -0.078 168     | 0.000 182           | —                   | -0.077 986     | —                        |
| 10  | QED      | -0.078 565     | 0.000 732           | -0.000 002          | -0.077 835     | -0.077 835               |
|     | RMS      | -0.078 565     | 0.000 732           | —                   | -0.077 833     | —                        |
| 20  | QED      | -0.080 186     | 0.002 989           | -0.000 028          | -0.077 225     | -0.077 225               |
|     | RMS      | -0.080 186     | 0.002 990           | —                   | -0.077 196     | —                        |
| 30  | QED      | -0.083 015     | 0.006 960           | -0.000 145          | -0.076 199     | -0.076 199               |
|     | RMS      | -0.083 015     | 0.006 969           | —                   | -0.076 046     | —                        |
| 40  | QED      | -0.087 267     | 0.013 008           | -0.000 482          | -0.074 741     | -0.074 741               |
|     | RMS      | -0.087 267     | 0.013 033           | —                   | -0.074 234     | —                        |
| 50  | QED      | -0.093 301     | 0.021 735           | -0.001 254          | -0.072 820     | -0.072 819               |
|     | RMS      | -0.093 301     | 0.021 795           | —                   | -0.071 506     | —                        |
| 60  | QED      | -0.101 698     | 0.034 138           | -0.002 828          | -0.070 388     | -0.070 385               |
|     | RMS      | -0.101 698     | 0.034 256           | —                   | -0.067 442     | —                        |
| 70  | QED      | -0.113 418     | 0.051 891           | -0.005 840          | -0.067 367     | -0.067 361               |
|     | RMS      | -0.113 418     | 0.052 091           | —                   | -0.061 327     | —                        |
| 80  | QED      | -0.130 121     | 0.077 941           | -0.011 452          | -0.063 632     | -0.063 623               |
|     | RMS      | -0.130 121     | 0.078 235           | —                   | -0.051 886     | —                        |
| 90  | QED      | -0.154 856     | 0.117 812           | -0.021 945          | -0.058 988     | -0.058 972               |
|     | RMS      | -0.154 856     | 0.118 162           | —                   | -0.036 694     | —                        |
| 92  | QED      | -0.161 216     | 0.128 274           | -0.024 984          | -0.057 926     | -0.057 908               |
|     | RMS      | -0.161 216     | 0.128 619           | —                   | -0.032 597     | —                        |
| 95  | QED      | -0.171 943     | 0.146 083           | -0.030 375          | -0.056 235     | -0.056 214               |
|     | RMS      | -0.171 943     | 0.146 407           | —                   | -0.025 536     | —                        |
| 100 | QED      | -0.193 788     | 0.182 924           | -0.042 259          | -0.053 123     | -0.053 097               |
|     | RMS      | -0.193 788     | 0.183 143           | —                   | -0.010 645     | —                        |
TABLE II: The interelectronic-interaction correction of first order in $1/Z$ to the two-electron part of the nuclear recoil contribution to the binding energy of the $1s^2$ state expressed in terms of the dimensionless function $B(\alpha Z)$ defined by Eq. (32).

| $Z$ | Approach | $B_1(\alpha Z)$ | $B_{11}(\alpha Z)$ | $B_{12}(\alpha Z)$ | $B(\alpha Z)$ |
|-----|----------|------------------|---------------------|---------------------|--------------|
| 5   | QED      | 0.13333          | −0.00025            | 0.00000             | 0.13368      |
|     | SMS      | 0.13394          | −0.00029            | —                   | 0.13366      |
| 10  | QED      | 0.13578          | −0.00092            | 0.00000             | 0.13466      |
|     | SMS      | 0.13589          | −0.00116            | —                   | 0.13473      |
| 20  | QED      | 0.14297          | −0.00326            | 0.0007              | 0.13977      |
|     | SMS      | 0.14381          | −0.00494            | —                   | 0.13888      |
| 30  | QED      | 0.15481          | −0.00678            | 0.00034             | 0.14837      |
|     | SMS      | 0.15748          | −0.01216            | —                   | 0.14532      |
| 40  | QED      | 0.17169          | −0.01151            | 0.00107             | 0.16125      |
|     | SMS      | 0.17774          | −0.02422            | —                   | 0.15352      |
| 50  | QED      | 0.19453          | −0.01779            | 0.00262             | 0.17936      |
|     | SMS      | 0.20603          | −0.04322            | —                   | 0.16281      |
| 60  | QED      | 0.22495          | −0.02633            | 0.00556             | 0.20418      |
|     | SMS      | 0.24477          | −0.07234            | —                   | 0.17242      |
| 70  | QED      | 0.26574          | −0.03850            | 0.01081             | 0.23805      |
|     | SMS      | 0.29790          | −0.11662            | —                   | 0.18128      |
| 80  | QED      | 0.32176          | −0.05694            | 0.01994             | 0.28476      |
|     | SMS      | 0.37224          | −0.18457            | —                   | 0.18767      |
| 90  | QED      | 0.40176          | −0.08701            | 0.03591             | 0.35067      |
|     | SMS      | 0.48001          | −0.29167            | —                   | 0.18833      |
| 92  | QED      | 0.42192          | −0.09527            | 0.04039             | 0.36704      |
|     | SMS      | 0.50733          | −0.32006            | —                   | 0.18727      |
| 95  | QED      | 0.45562          | −0.10967            | 0.04821             | 0.39415      |
|     | SMS      | 0.55314          | −0.36854            | —                   | 0.18460      |
| 100 | QED      | 0.52333          | −0.140771           | 0.06509             | 0.44764(2)   |
|     | SMS      | 0.64543          | −0.46918            | —                   | 0.17625      |
TABLE III: The interelectronic-interaction correction of first order in $1/Z$ to the two-electron part of the nuclear recoil contribution to the binding energy of the $1s^22s$ state expressed in terms of the dimensionless function $B(\alpha Z)$ defined by Eq. (32).

| Z  | Approach | $B_1(\alpha Z)$ | $B_{11}(\alpha Z)$ | $B_{12}(\alpha Z)$ | $B(\alpha Z)$ |
|----|----------|-----------------|-------------------|-------------------|-------------|
| 5  | QED      | 0.156 55        | -0.000 28         | 0.000 00          | 0.156 27    |
|    | $H_{SM}$ | 0.156 57        | -0.000 32         | -                  | 0.156 25    |
| 10 | QED      | 0.158 85        | -0.001 04         | 0.000 00          | 0.157 82    |
|    | $H_{SM}$ | 0.158 99        | -0.001 31         | -                  | 0.157 68    |
| 20 | QED      | 0.167 82        | -0.003 72         | 0.000 08          | 0.164 18    |
|    | $H_{SM}$ | 0.168 82        | -0.005 58         | -                  | 0.163 24    |
| 30 | QED      | 0.182 64        | -0.007 78         | 0.000 38          | 0.175 23    |
|    | $H_{SM}$ | 0.185 81        | -0.013 84         | -                  | 0.171 97    |
| 40 | QED      | 0.203 86        | -0.013 34         | 0.001 18          | 0.191 69    |
|    | $H_{SM}$ | 0.211 07        | -0.027 82         | -                  | 0.183 25    |
| 50 | QED      | 0.232 68        | -0.020 85         | 0.002 90          | 0.214 73    |
|    | $H_{SM}$ | 0.246 47        | -0.050 14         | -                  | 0.196 33    |
| 60 | QED      | 0.271 24        | -0.031 23         | 0.006 18          | 0.246 19    |
|    | $H_{SM}$ | 0.295 14        | -0.084 81         | -                  | 0.210 32    |
| 70 | QED      | 0.323 19        | -0.046 22         | 0.012 06          | 0.289 02    |
|    | $H_{SM}$ | 0.362 21        | -0.138 25         | -                  | 0.223 96    |
| 80 | QED      | 0.394 89        | -0.069 22         | 0.022 36          | 0.348 03    |
|    | $H_{SM}$ | 0.456 57        | -0.221 39         | -                  | 0.235 18    |
| 90 | QED      | 0.497 92        | -0.107 13         | 0.040 57          | 0.431 35    |
|    | $H_{SM}$ | 0.594 22        | -0.354 26         | -                  | 0.239 95    |
| 92 | QED      | 0.523 97        | -0.117 61         | 0.045 70          | 0.452 07    |
|    | $H_{SM}$ | 0.629 27        | -0.389 76         | -                  | 0.239 50    |
| 95 | QED      | 0.567 62        | -0.135 92         | 0.054 72          | 0.486 41    |
|    | $H_{SM}$ | 0.688 12        | -0.450 62         | -                  | 0.237 50    |
| 100| QED      | 0.655 56        | -0.175 64(2)      | 0.074 32          | 0.554 24(2) |
|    | $H_{SM}$ | 0.807 08        | -0.577 69         | -                  | 0.229 39    |
TABLE IV: The interelectronic-interaction correction of first order in $1/Z$ to the two-electron part of the nuclear recoil contribution to the binding energy of the $1s^22p_{1/2}$ state expressed in terms of the dimensionless function $B(\alpha Z)$ defined by Eq. (32).

| $Z$ | Approach | $B_1(\alpha Z)$ | $B_{\text{tr}1}(\alpha Z)$ | $B_{\text{tr}2}(\alpha Z)$ | $B(\alpha Z)$ |
|-----|-----------|------------------|----------------------------|----------------------------|---------------|
| 5   | QED       | 0.44462          | -0.00107                   | 0.00000                    | 0.44355       |
|     | $H_{\text{SMS}}$ | 0.44464          | -0.00111                   | —                          | 0.44353       |
| 10  | QED       | 0.44941          | -0.00423                   | 0.00001                    | 0.44519       |
|     | $H_{\text{SMS}}$ | 0.44953          | -0.00448                   | —                          | 0.44505       |
| 20  | QED       | 0.46862          | -0.01693                   | 0.00022                    | 0.45191       |
|     | $H_{\text{SMS}}$ | 0.46956          | -0.01872                   | —                          | 0.45084       |
| 30  | QED       | 0.50159          | -0.03924                   | 0.00112                    | 0.46348       |
|     | $H_{\text{SMS}}$ | 0.50458          | -0.04513                   | —                          | 0.45946       |
| 40  | QED       | 0.55062          | -0.07389                   | 0.00373                    | 0.48046       |
|     | $H_{\text{SMS}}$ | 0.55745          | -0.08810                   | —                          | 0.46936       |
| 50  | QED       | 0.61988          | -0.12587                   | 0.00977                    | 0.50378       |
|     | $H_{\text{SMS}}$ | 0.63305          | -0.15488                   | —                          | 0.47816       |
| 60  | QED       | 0.71645          | -0.20385                   | 0.02235                    | 0.53496       |
|     | $H_{\text{SMS}}$ | 0.73944          | -0.25740                   | —                          | 0.48204       |
| 70  | QED       | 0.85244          | -0.32319                   | 0.04716                    | 0.57640       |
|     | $H_{\text{SMS}}$ | 0.89029          | -0.41588                   | —                          | 0.47441       |
| 80  | QED       | 1.04942          | -0.51252                   | 0.09534                    | 0.63224       |
|     | $H_{\text{SMS}}$ | 1.10983          | -0.66686                   | —                          | 0.44267       |
| 90  | QED       | 1.34832          | -0.82896                   | 0.19041                    | 0.70977       |
|     | $H_{\text{SMS}}$ | 1.44375          | -1.08121                   | —                          | 0.36255       |
| 92  | QED       | 1.42653          | -0.91650                   | 0.21890                    | 0.72893       |
|     | $H_{\text{SMS}}$ | 1.53116          | -1.19463                   | —                          | 0.33653       |
| 95  | QED       | 1.55969          | -1.06934                   | 0.27034                    | 0.76069       |
|     | $H_{\text{SMS}}$ | 1.67995          | -1.39154                   | —                          | 0.28841       |
| 100 | QED      | 1.83558          | -1.39931(2)                | 0.38725(1)                 | 0.82352(2)    |
|     | $H_{\text{SMS}}$ | 1.98799          | -1.81228                   | —                          | 0.17571       |
TABLE V: The two-electron part of the nuclear recoil contribution to the binding energy of the 1s^22p_{1/2} state. The values obtained within the independent electron approximation (to zeroth order in 1/Z) are given in terms of the dimensionless function \( A(\alpha Z) \) defined by Eq. (31).

The interelectronic-interaction correction of first order in 1/Z is given in terms of the dimensionless function \( B(\alpha Z)/Z \) defined by Eq. (32).

| Z | Approach | \( A \) | \( B/Z \) | \( A + B/Z \) |
|---|----------|------|--------|--------|
| 5 | QED      | -0.077 986 | 0.088 710 | 0.010 723 |
|   | \( H_{\text{SMS}} \) | -0.077 986 | 0.088 706 | 0.010 719 |
| 10 | QED      | -0.077 835 | 0.044 519 | -0.033 316 |
|   | \( H_{\text{SMS}} \) | -0.077 833 | 0.044 505 | -0.033 328 |
| 20 | QED      | -0.077 225 | 0.022 595 | -0.054 630 |
|   | \( H_{\text{SMS}} \) | -0.077 196 | 0.022 542 | -0.054 654 |
| 30 | QED      | -0.076 199 | 0.015 449 | -0.060 750 |
|   | \( H_{\text{SMS}} \) | -0.076 046 | 0.015 315 | -0.060 731 |
| 40 | QED      | -0.074 741 | 0.012 011 | -0.062 729 |
|   | \( H_{\text{SMS}} \) | -0.074 234 | 0.011 734 | -0.062 500 |
| 50 | QED      | -0.072 820 | 0.010 076 | -0.062 744 |
|   | \( H_{\text{SMS}} \) | -0.071 506 | 0.009 563 | -0.061 943 |
| 60 | QED      | -0.070 388 | 0.008 916 | -0.061 472 |
|   | \( H_{\text{SMS}} \) | -0.067 442 | 0.008 034 | -0.059 408 |
| 70 | QED      | -0.067 367 | 0.008 234 | -0.059 133 |
|   | \( H_{\text{SMS}} \) | -0.061 327 | 0.006 777 | -0.054 549 |
| 80 | QED      | -0.063 632 | 0.007 903 | -0.055 729 |
|   | \( H_{\text{SMS}} \) | -0.051 886 | 0.005 537 | -0.046 349 |
| 90 | QED      | -0.058 988 | 0.007 886 | -0.051 102 |
|   | \( H_{\text{SMS}} \) | -0.036 694 | 0.004 028 | -0.032 666 |
| 92 | QED      | -0.057 926 | 0.007 923 | -0.050 003 |
|   | \( H_{\text{SMS}} \) | -0.032 597 | 0.003 658 | -0.028 939 |
| 95 | QED      | -0.056 235 | 0.008 007 | -0.048 227 |
|   | \( H_{\text{SMS}} \) | -0.025 536 | 0.003 036 | -0.022 500 |
| 100 | QED    | -0.053 123 | 0.008 235 | -0.044 887 |
|    | \( H_{\text{SMS}} \) | -0.010 645 | 0.001 757 | -0.008 888 |
FIG. 4. The first-order in $1/Z$ interelectronic-interaction correction to the two-electron part of the nuclear recoil effect on the binding energy of the $1s^2$ state expressed in terms of the dimensionless function $B(\alpha Z)$ defined by Eq. (32). The solid line represents the results of the QED calculations to all orders in $\alpha Z$ whereas the dashed line stands for the calculations based on the specific mass shift (SMS) operator given by Eq. (4).

FIG. 5. The first-order in $1/Z$ interelectronic-interaction correction to the two-electron part of the nuclear recoil effect on the binding energy of the $1s^22s$ state expressed in terms of the dimensionless function $B(\alpha Z)$ defined by Eq. (32). Notations are the same as in Fig. 4.
Contribution to the binding energy of the $1s^22p_{1/2}$ state

FIG. 6. The first-order in $1/Z$ interelectronic-interaction correction to the two-electron part of the nuclear recoil effect on the binding energy of the $1s^22p_{1/2}$ state expressed in terms of the dimensionless function $B(\alpha Z)$ defined by Eq. (32). Notations are the same as in Fig. 4.
FIG. 7. The two-electron part of the nuclear recoil effect on the binding energy of the 1s2p1/2 state expressed in terms of the dimensionless function $F(\alpha Z, Z)$ defined by Eqs. (33) and (34). The solid lines represent the results of the QED calculations to all orders in $\alpha Z$ while the dashed lines stand for the calculations based on the specific mass shift (SMS) operator given by Eq. (34). The contributions of zeroth order in $1/Z$, $F_0(\alpha Z) = A(\alpha Z)$, and the sums of zeroth and first orders in $1/Z$, $F_{01}(\alpha Z, Z) = A(\alpha Z) + B(\alpha Z)/Z$, are shown with blue (circles) and red (squares) lines, respectively.

FIG. 8. The two-electron part of the nuclear recoil effect on the 2p1/2 − 2s transition energy in Li-like ions expressed in terms of the dimensionless function $F(\alpha Z, Z)$ defined by Eqs. (33) and (34). Notations are the same as in Fig. 7.
