QED theory of the normal mass shift in few-electron atoms

A. V. Malyshev,1 I. S. Anisimova,1 D. A. Glazov,1 M. Y. Kaygorodov,1 D. V. Mironova,2 G. Plunien,3 and V. M. Shabaev1

1Department of Physics, St. Petersburg State University, Universitetskaya 7/9, 199034 St. Petersburg, Russia
2St. Petersburg Electrotechnical University, Prof. Popov 5, 197376 St. Petersburg, Russia
3Institut für Theoretische Physik, Technische Universität Dresden, Mommsenstraße 13, D-01062 Dresden, Germany

The electron-electron interaction correction of first order in $1/Z$ to the one-electron part of the nuclear recoil effect on binding energies in atoms and ions is considered within the framework of the rigorous QED approach. The calculations to all orders in $\alpha Z$ are performed for the $1s^2$ state in heliumlike ions and the $1s^22s$ and $1s^22p_{1/2}$ states in lithiumlike ions in the range $Z = 5–100$. The results obtained are compared with the Breit-approximation values. The performed calculations complete a systematic treatment of the QED nuclear recoil effect up to the first order in $1/Z$. The correction obtained is combined with the previously studied two-electron part as well as the higher-order electron-correlation corrections evaluated within the Breit approximation to get the total theoretical predictions for the mass shifts.

I. INTRODUCTION

It is well known that within the nonrelativistic approximation the effect of the nuclear motion on spectra of hydrogenlike ions is accounted for exactly by replacing the electron mass $m$ with the reduced mass $m_r = mM/(m + M)$ with $M$ being the mass of the nucleus. The lowest-order relativistic correction of first order in $m/M$ can be derived from the Breit equation for electron and nucleus [1]. For $N$-electron system, the corresponding one-electron contribution to the nuclear recoil effect can be described by the operator

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

(1)

where $p = -i\nabla$ is the momentum operator, $r$ is the position vector, $r = |r|$, $\alpha$ are the Dirac matrices, $\alpha$ is the fine-structure constant, and $Z$ is the nuclear charge number [the relativistic units ($\hbar = 1$, $c = 1$) are used throughout the paper]. The one-electron operator in Eq. (1) gives rise to the so-called normal mass shift (NMS). In the case of more than one electron, the NMS operator (1) does not provide the exhaustive description of the effect of the nuclear motion since there is also the two-electron contribution given by the specific mass shift (SMS) operator

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

(2)

The NMS and SMS operators add to the mass shift (MS) operator [2]

$$H_M = H_{\text{NMS}} + H_{\text{SMS}},$$  

(3)

which allows one to treat the nuclear recoil contribution within the $(m/M)(\alpha Z)^4mc^2$ approximation. To date, the MS operator (3) is used extensively in relativistic calculations of the atomic spectra and isotope shifts (see, e.g., Refs. [9, 20] and references therein).

The fully relativistic description of the nuclear recoil effect on binding energies requires application of the bound-state quantum electrodynamics (QED) beyond the Breit approximation. The corresponding theory to first order in $m/M$ and to all orders in $\alpha Z$ was developed in Refs. [2, 3, 21]; see also Refs. [22, 24]. Numerous QED evaluations of the nuclear recoil contribution to binding energies were performed over the past three decades [6, 13, 24–29]. However, all the previous nonperturbative (in $\alpha Z$) calculations were limited by the independent-electron approximation, i.e., the electron-electron interaction corrections to the nuclear recoil effect were neglected. It should be noted that the interelectronic-interaction effects were treated approximately in some cases by modifying the zeroth-order approximation and including it a local screening potential (see, e.g., Ref. [6]). In our recent work [28], we addressed the issue of 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 present paper focuses on deriving the rigorous QED formalism for calculations of the corresponding correction to the dominant one-electron part. The results obtained represent the nontrivial QED contribution to the NMS and complete the rigorous consideration of the first-order (in $1/Z$) nuclear recoil effect to all orders in $\alpha Z$.

The QED formalism worked out in the present work is illustrated by calculating the one-electron part of the nuclear recoil effect on binding energies of the $1s^2$ state in heliumlike ions and the $1s^22s$ and $1s^22p_{1/2}$ states in lithiumlike ions for the wide range of the nuclear charge number $Z = 5–100$. The behavior of the nontrivial QED contribution to the NMS as a function of $Z$ is studied. These calculations together with those performed in Ref. [20] provide a better understanding of the applicability limits for the MS operator (3). In particular, one can assume that the application of a rigorous
QED approach will resolve some discrepancies which take place nowadays between the preliminary calculations and the high-precision measurements of the isotope shifts of the fine-structure splittings in singly ionized argon (Ar$^+$) [31, 32] and calcium (Ca$^+$) [33]. We also stress that the effect under consideration may contribute significantly when specific differences of the energies or isotope shifts are studied (see, e.g., Ref. [34] for the related discussion in the case of the bound-electron $g$ factor).

The paper is organized as follows. The main aspects of the QED theory of the nuclear recoil effect on binding energies within the independent-electron approximation are outlined in Sec. II. The formulas for the first-order (in $1/Z$) correction to the one-electron part of the nuclear recoil effect valid to all orders in $\alpha Z$ are discussed in Sec. III. The numerical results and the comparison with the values obtained employing the MS Hamiltonian [9] are given in Sec. IV.

II. QED THEORY OF THE NUCLEAR RECOIL EFFECT WITHIN THE INDEPENDENT-ELECTRON APPROXIMATION

The QED theory of the nuclear recoil effect on atomic binding energies was worked out in Refs. [2, 3, 21]. The formulation of the theory presented in Ref. [21] is the most convenient for the needs of the present study. It reduces the problem of accounting for the nuclear recoil effect to a modification of the standard QED Hamiltonian of the electron-positron field interacting with the quantized electromagnetic field and the classical Coulomb potential of the nucleus $V_n$. The modification consists in an extra term to the interaction part of the QED Hamiltonian; see Ref. [21] for the details. As a result, the nuclear recoil effect to first order in $m/M$ and to all orders in $\alpha Z$ can be taken into account by perturbation theory in the interaction representation of the Furry picture [55]. For the construction of the perturbation series, we employ the two-time Green’s function (TTGF) method [36]. All the necessary Feynman rules can be found, e.g., in Ref. [36]. In order to describe the new elements of the diagram technique as compared to the standard bound-state QED, we discuss briefly the derivation of the formulas for the one-electron part of the nuclear recoil effect to zeroth order in $1/Z$ for the electron in the state $|\alpha\rangle$. The total one-electron contribution for a given many-electron state is obtained by adding the corresponding terms from all one-electron orbitals.

The one-electron part of the nuclear recoil effect is given by the diagrams depicted in Fig. 1. The double line denotes the propagator for an electron in the classical field of the nucleus. The vertex with a small black dot corresponds to the conventional QED vertex. The new vertex with a bold dot arises from the extra term to the QED Hamiltonian derived in Ref. [21]. It contains the momentum operator $\mathbf{p}$. Following the notations employed in Ref. [21], we refer to the dotted line joining two bold dots in Fig. 1(a) as to the “Coulomb recoil” interaction. The dashed line ended by a bold dot on one side in Figs. 1(b) and 1(c) designates the “one-transverse-photon recoil” interaction, since it includes the transverse part of the photon propagator in the Coulomb gauge

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

(4)

where we fix the branch of the square root by the condition $\operatorname{Im} \left( \sqrt{\omega^2 + \mathbf{p}^2} \right) > 0$. The dashed line with a bold dot on it in Fig. 1(d) corresponds to the “two-transverse-photon recoil” interaction, since it involves the product of two photon propagators [4]. The terminology used comes from operating in the Coulomb gauge which appears to be the most appropriate and convenient gauge for studying the nuclear recoil effect; see, e.g., Refs. [2, 3, 23].

Within the Furry picture, the zeroth-order approximation for one-electron energies and wave functions is determined by the Dirac equation with the binding potential of the nucleus $V_n$,

$$[-i\mathbf{\alpha} \cdot \nabla + \beta m + V_n(r)] \psi_n(r) = \varepsilon_n \psi_n(r).$$

(5)

The TTGF method prescribes that the first-order correction to the energy of an arbitrary single level $|u\rangle$ can be obtained according to the following formula:

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

(6)

Here $\Delta g_{uu}^{(1)}$ represents the Fourier transform of the contribution to the two-time Green’s function projected on the unperturbed state $|u^{(0)}\rangle$, $\Delta E = E - E_n^{(0)}$, $E_n^{(0)}$ is the unperturbed energy, and the oriented counterclockwise contour $\Gamma$ surrounds $E_n^{(0)}$ in the complex $E$ plane; see Ref. [36] for the details. For the one-electron nuclear recoil contribution under consideration, we assume that

![FIG. 1. One-electron nuclear recoil diagrams to zeroth order in $1/Z$: the Coulomb (a), one-transverse (b) and (c), and two-transverse (d) contributions. See the text and Ref. [21] for the description of the Feynman rules.](attachment:fig1.png)
the unperturbed wave function $|\psi_{el}(0)\rangle$ is given by the solution $\psi_{el}$ of the Dirac equation $[1]$, and the unperturbed energy coincides with the corresponding energy $\varepsilon_{el}$. The diagrams shown in Fig. 1 are similar to the first-order self-energy diagram; see, e.g., Refs. [37–39]. For this reason, the derivation of the formulas does not cause any problems, and by applying the TTGF method one readily obtains

$$\Delta E^{(1)}_{c} = \frac{1}{M} \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_{n} \frac{\langle a|p_{k}|n\rangle\langle n|p_{k}|a\rangle}{\omega + \varepsilon_{a} - \varepsilon_{n}}$$  \hspace{1cm} (7)

for the Coulomb contribution in Fig. 1(a),

$$\Delta E^{(1)}_{tr1} = -\frac{1}{M} \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_{n} \left[ \frac{\langle a|p_{k}|n\rangle\langle n|D_{k}(\omega)|a\rangle}{\omega + \varepsilon_{a} - \varepsilon_{n}} + \frac{\langle a|D_{k}(\omega)|n\rangle\langle n|p_{k}|a\rangle}{\omega + \varepsilon_{a} - \varepsilon_{n}} \right]$$  \hspace{1cm} (8)

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

$$\Delta E^{(1)}_{tr2} = \frac{1}{M} \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_{n} \frac{\langle a|D_{k}(\omega)|n\rangle\langle n|D_{k}(\omega)|a\rangle}{\omega + \varepsilon_{a} - \varepsilon_{n}}$$  \hspace{1cm} (9)

for the two-transverse-photon contribution in Fig. 1(d). In Eqs. (7)–(9) and below, the summation over the repeated indices is implied, $u = 1 - i0$ provides the proper treatment of the poles in the electron propagator, and

$$D_{k}(\omega) = -4\pi\alpha Z \alpha_{l} D_{kl}(\omega),$$  \hspace{1cm} (10)

where $\alpha_{l}$ ($l = 1, 2, 3$) are the Dirac matrices. For the following, it is convenient to introduce the notations

$$R_{c} = \frac{1}{M} p_{1} \cdot p_{2},$$  \hspace{1cm} (11)

$$R_{tr1}(\omega) = -\frac{1}{M} [p_{1} \cdot D_{2}(\omega) + D_{1}(\omega) \cdot p_{2}],$$  \hspace{1cm} (12)

$$R_{tr2}(\omega) = \frac{1}{M} D_{1}(\omega) \cdot D_{2}(\omega),$$  \hspace{1cm} (13)

for the Coulomb, one-transverse-photon, and two-transverse-photon interactions, respectively. By analogy with the self-energy operator $\Sigma(E)$, we also introduce the operator $P(E)$ for the nuclear recoil effect to zeroth order in $1/Z$ is given by the sum of Eqs. (7)–(9),

$$\Delta E^{(1)}_{el} = \Delta E^{(1)}_{c} + \Delta E^{(1)}_{tr1} + \Delta E^{(1)}_{tr2}.$$  \hspace{1cm} (15)

The integration over $\omega$ in the Coulomb contribution (7) can be evaluated analytically using the standard identity ($\omega_{1} < 0 < \omega_{2}$):

$$\int_{\omega_{1}}^{\omega_{2}} d\omega \frac{f(\omega)}{\omega + i0} = \mp i\pi f(0) + \mathcal{P} \int_{\omega_{1}}^{\omega_{2}} d\omega \frac{f(\omega)}{\omega},$$  \hspace{1cm} (16)

where $\mathcal{P}$ means the principal value integral. Indeed, applying the formula (16) to Eq. (7) and taking into account that all the principal value integrals vanish, one obtains

$$\Delta E^{(1)}_{c} = \frac{1}{2M} \sum_{n} \langle a|p_{k}|n\rangle\langle n|p_{k}|a\rangle$$

$$- \frac{1}{2M} \sum_{n} \langle a|p_{k}|n\rangle\langle n|p_{k}|a\rangle,$$  \hspace{1cm} (17)

where the first and second summations run over the positive- and negative-energy parts of the spectrum, respectively. It is useful to compare this expression with the formula which can be obtained by employing the nonrelativistic part of the NMS operator (1):

$$\Delta E^{(1)}_{c,\text{Breit}} = \left\langle a \left[ \frac{p^{2}}{2M} \right] a \right\rangle = \frac{1}{2M} \sum_{n} \langle a|p_{k}|n\rangle\langle n|p_{k}|a\rangle,$$  \hspace{1cm} (18)

where the summation runs over all the states. One can see that introducing the projectors on the positive-energy part of the spectrum in Eqs. (7) or (17) leads to the result which differs from the value (18) by the contribution of the negative-energy continuum, being of order $(m/M)(\alpha Z)^{5} mc^{2}$, i.e., beyond the Breit approximation. The expression (18) is implied to be the lowest-order approximation of the Coulomb contribution (7). One should note that Eq. (18) contains actually some terms of the higher orders in $\alpha Z$ as well, since it is evaluated with the Dirac wave functions. The nontrivial QED Coulomb contribution, which can not be obtained from the Breit equation, reads [25]

$$\Delta E^{(1)}_{c,QED} = \Delta E^{(1)}_{c} - \Delta E^{(1)}_{c,\text{Breit}}$$

$$- \frac{1}{M} \sum_{n, \varepsilon_{n} < 0} \langle a|p_{k}|n\rangle\langle n|p_{k}|a\rangle.$$  \hspace{1cm} (19)

In order to obtain the lowest-order relativistic approximation to the one-transverse-photon contribution [8], one has to consider the zero-energy-transfer limit $\omega \rightarrow 0$ of Eq. (10) given by

$$D_{k}(0) = \frac{\alpha Z}{2r} \left[ \frac{\varepsilon_{a} + \langle \alpha_{l} r \rangle p_{k}}{r^{2}} \right].$$  \hspace{1cm} (20)
By neglecting the energy dependence of the vector $D(\omega)$ in Eq. (5), we come to the integral which is similar to the Coulomb case (7). One should take care defining its Breit approximation, since discarding the negative-energy part of the spectrum in Eq. (5) leads once again to a slightly different result. As in the Coulomb case, we consider the expression arising from the NMS operator, $\Delta E_{1el} = \frac{1}{2M} [a|p\cdot D(0) + D(0)\cdot p)|a]$, (21)

as the lowest-order relativistic approximation to Eq. (8), and the nontrivial QED part of the one-transverse-photon contribution is

$$\Delta E_{tr1,QED}^{(1)} = \Delta E_{1el} - \Delta E_{1el,\text{Breit}}.$$  

(22)

We note, finally, that the two-transverse-photon contribution $\Delta E_{tr2}^{(1)}$ is completely beyond the Breit approximation. Thus, we relegate it to the nontrivial QED part.

The total one-electron nuclear recoil contribution (15) can be conveniently represented as a sum of the Breit-approximation term and the nontrivial QED term,

$$\Delta E_{1el}^{(1)} = \Delta E_{1el,\text{Breit}} + \Delta E_{1el,QED}^{(1)},$$  

(23)

$$\Delta E_{1el,\text{Breit}} = \Delta E_{1el}^{(1)} + \Delta E_{tr1,\text{Breit}}^{(1)} = \frac{1}{2M} [a|p^2 - (p\cdot D(0) + D(0)\cdot p)|a]$$  

(24)

$$\Delta E_{1el,QED}^{(1)} = \Delta E_{c,QED}^{(1)} + \Delta E_{tr1,QED}^{(1)} + \Delta E_{tr2}^{(1)} = \frac{1}{M} \int_{-\infty}^{\infty} d\omega \langle a| \frac{[p_k, V_1]}{\omega + i0} \rangle D_k(\omega) \langle a| \frac{[p_k, V_1]}{\omega + i0} \rangle,'$$  

(25)

where $G(\omega) = \sum_n |n\rangle\langle n| \omega - \epsilon_n |^{-1}$ is the Dirac-Coulomb Green’s function and $[A, B] = AB - BA$. The formalism for treating the nuclear recoil effect to all orders in $\alpha Z$ was initially derived in Ref. [2] in the form given by the Eqs. (23)–(25).

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

One set of Feynman diagrams contributing to the first order (in $1/Z$) electron-electron interaction correction to the one-electron part of the nuclear recoil effect is shown in Fig. 2. The wavy line corresponds to the photon propagator, while all the other notations are the same as in Fig. 1. The two-transverse-photon contribution presented in Fig. 2 has to be complemented by the corresponding Coulomb and one-transverse-photon contributions. Therefore, the total number of the second-order diagrams is four times higher.

**FIG. 2.** The second-order diagrams describing the electron-electron interaction correction to the one-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. [21] for the description of the diagram technique.

The second-order correction to energy of a single level $|u\rangle$ is given by (36)

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

$$- \left[ \frac{1}{2\pi i} \int_{\Gamma} dE \Delta E \Delta g_{uu}^{(1)}(E) \right] \left[ \frac{1}{2\pi i} \int_{\Gamma} dE \Delta g_{uu}^{(1)}(E) \right],$$  

(26)

where the contour $\Gamma$ surrounds the unperturbed energy $E_u^{(0)}$ and keeps outside all the other singularities of the Green’s function. In this paper we are interested in the two-electron corrections presented in Fig. 2. An arbitrary many-electron problem can be easily decomposed into the set of two-electron problems. For this reason, it is sufficient to assume the unperturbed wave function $|u^{(0)}\rangle$ in Eq. (26) to be represented by the one-determinant two-electron wave function,

$$|u_{(2el)}^{(0)}\rangle = \frac{1}{\sqrt{2}} \sum_P (-1)^P \psi_\alpha(r_1)\psi_\beta(r_2),$$  

(27)

where $\psi_\alpha$ and $\psi_\beta$ are the solutions of the Dirac equation (5), $P$ is the permutation operator, and $(-1)^P$ is the sign of the permutation. The unperturbed energy is given by the sum of the one-electron Dirac energies: $E_u^{(0)} = \epsilon_\alpha + \epsilon_\beta$. The generalization to the case of a many-determinant wave function is straightforward and can be done in the final expressions.

The second term in Eq. (26), given by the product of the first-order contributions to the Green’s function, is usually referred to as the “disconnected” one. The relevant diagrams are shown in Figs. 1 and 3. The disconnected term is to be considered together with the...
The operator (30) can be used to evaluate the interelectronic-interaction correction to the MS operator (3) within the Breit approximation.

\[
\Delta E^{(2) \text{vert}} = \sum_p (-1)^p \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_{n_1 n_2} \left[ \langle Pa n_2 | R(\omega) | n_1 a \rangle \langle n_1 Pb | I(\Delta) | n_2 b \rangle \right. \\
\left. \frac{1}{(\omega + \varepsilon_{n_1} - u\varepsilon_{n_2})} \frac{1}{(\omega + \varepsilon_a - u\varepsilon_{n_1})} \right] + \langle Pa n_1 | I(\Delta) | an_2 \rangle \langle Pb n_2 | R(\omega) | n_1 b \rangle \\
\left. \frac{1}{(\omega + \varepsilon_{n_1} - u\varepsilon_{n_2})} \frac{1}{(\omega + \varepsilon_b - u\varepsilon_{n_1})} \right].
\]

To summarize, within the rigorous QED approach the interelectronic-interaction correction of first order in \(1/Z\) to the one-electron part of the nuclear recoil effect is given by the sum of Eqs. (31), (34), and (35). The calculations are to be performed for all the operators (11)-(13).
Concluding this section, we note that the Breit-approximation results for the electron-electron correction to the NMS can be obtained from the QED formulas derived in the present work. To do so, one has to neglect the energy dependence in the operators \( D(\omega) \) and \( I(\omega) \) in Eqs. \( (10) \) and \( (29) \), respectively, and introduce the projectors on the positive-energy part of the spectrum in Eqs. \( (32), (33) \), and \( (35) \). In addition, the lowest-order relativistic limit of the operator \( P \) in Eq. \( (14) \) has to be treated as discussed in Sec. \( III \). On these assumptions, the integration over \( \omega \) in all the expressions can be performed analytically by employing Eq. \( (16) \) and Cauchy’s residue theorem. As a result, the reducible and vertex contributions vanish identically, and the irreducible contribution reproduces the interelectronic-interaction correction to the nuclear recoil effect on binding energies of low-lying states in hydrogen-like ions can be found in the literature; see Refs. \( [24–26, 29] \). Nevertheless, for the sake of completeness, we summarize our results for the one-electron contribution to zeroth order in \( 1/Z \) to the one-electron part of the nuclear recoil within the Breit approximation. Obviously, the two-transverse-photon contribution has to be omitted in this approximation.

### IV. NUMERICAL RESULTS AND DISCUSSION

In this work, the formalism derived in Sec. \( III \) is employed for nonperturbative (in \( \alpha Z \)) calculations of the one-electron contribution to the nuclear recoil effect on binding energies of the \( 1s^2 \) state in heliumlike ions and the \( 1s^22s \) and \( 1s^22p_{1/2} \) states in lithiumlike ions. By evaluating the differences of the results obtained for the binding energies, one can calculate the corresponding contributions to the ionization energies of the \( 1s^22s \) and \( 1s^22p_{1/2} \) states and to the \( 2p_{1/2} - 2s \) transition energy in Li-like ions. The calculations are performed in the range \( Z = 5–100 \). As noted in Sec. \( III \) for the Coulomb contributions the integration over \( \omega \) can be performed analytically. For the one-transverse-photon and two-transverse-photon contributions, the corresponding integrals are calculated numerically employing Wick’s rotation of the integration contour to the complex plane; see Ref. \( [41] \) for the details. The summation over the one-electron states in the electron propagator is carried out using the finite basis set of the Dirac-equation eigenfunctions constructed from the B-splines \( [12, 43] \) by means of the dual-kinetic-balance approach \( [14] \).

#### A. One-electron part of the nuclear recoil effect

We start with the results obtained within the independent-electron approximation. As noted above, numerous calculations of the one-electron contribution to the nuclear recoil effect on binding energies of low-lying states in hydrogen-like ions can be found in the literature; see Refs. \( [24–26, 29] \). Nevertheless, for the sake of completeness, we summarize our results for the one-electron contribution to zeroth order in \( 1/Z \) in Table \( \ref{tab:1} \). The results for the \( 1s, 2s, \) and \( 2p_{1/2} \) states are given in terms of the dimensionless function \( \mathcal{A}(\alpha Z) \) defined by

\[
\Delta E^{(1)} = \frac{m}{M} (\alpha Z)^2 \mathcal{A}(\alpha Z) mc^2.
\]

To avoid misunderstanding, we note that the index “(1)” here (and analogous indices below) refers to the perturbation-theory order in the framework of the TTGF method, and it is equal to the order in \( 1/Z \) plus one. For each \( Z \) (in Table \( \ref{tab:1} \)), the values calculated within the rigorous QED formalism employing Eqs. \( \ref{eq:7}–\ref{eq:9} \) are displayed in the first line, while the results obtained by means of the NMS operator \( (1) \) are shown in

\[
\Delta E^{(2)}_{\text{c,vert}} = \frac{1}{M} \sum_{P} (-1)^P \left\{ \sum_{\varepsilon_2 < 0} \sum_{\varepsilon_n > 0} \left[ \frac{\langle Pa|p_k|n_2\rangle\langle n_2|p_k|a\rangle\langle n_1Pb|I(\Delta)|n_2b\rangle}{\varepsilon_n - \varepsilon_2 - \Delta} + \frac{\langle Pa|n_1|I(\Delta)|an_2\rangle\langle Pb|p_k|n_1\rangle\langle n_2|p_k|b\rangle}{\varepsilon_{n_2} - \varepsilon_{n_1} - \Delta} \right] \right. 
\]

\[
+ \left. \sum_{\varepsilon_2 < 0} \sum_{\varepsilon_n > 0} \left[ \frac{\langle Pa|p_k|n_1\rangle\langle n_2|p_k|a\rangle\langle n_1Pb|I(\Delta)|n_2b\rangle}{\varepsilon_{n_1} - \varepsilon_2 - \Delta} + \frac{\langle Pa|n_1|I(\Delta)|an_2\rangle\langle Pb|p_k|n_1\rangle\langle n_2|p_k|b\rangle}{\varepsilon_{n_1} - \varepsilon_{n_2} + \Delta} \right] \right\}. \quad (37)
\]
TABLE I. The nuclear recoil contribution to binding energies of the 1s, 2s, and 2p_{1/2} states expressed in terms of the function $A(\alpha Z)$ defined by Eq. (36). 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 normal mass shift (NMS) operator given in Eq. (1). The individual contributions, the Coulomb ($c$), the one-transverse-photon (tr1), and the two-transverse-photon (tr2) ones, are shown only for the 1s state.

| Z | Approach | $A_{1s}^c(\alpha Z)$ | $A_{1s}^{tr1}(\alpha Z)$ | $A_{1s}^{tr2}(\alpha Z)$ | $A_{1s}(\alpha Z)$ | $A_{2s}(\alpha Z)$ | $A_{2p_{1/2}}(\alpha Z)$ |
|---|---------|----------------------|--------------------------|--------------------------|------------------------|------------------------|--------------------------|
| 5 | QED     | 0.501315             | -0.001201                | -0.000047                | 0.500066               | 0.125051               | 0.125041               |
|    | NMS     | 0.501333             | -0.001334                | -                         | 0.499999               | 0.125042               | 0.125042               |
| 10 | QED     | 0.505223             | -0.000502                | -0.00253                 | 0.500468               | 0.125237               | 0.125163               |
|    | NMS     | 0.505363             | -0.000536                | -                         | 0.499995               | 0.125166               | 0.125167               |
| 20 | QED     | 0.520945             | -0.016490                | -0.001206                | 0.503248               | 0.126176               | 0.125656               |
|    | NMS     | 0.521953             | -0.021999                | -                         | 0.499544               | 0.125667               | 0.125673               |
| 30 | QED     | 0.548214             | -0.035322                | -0.002787                | 0.510105               | 0.128157               | 0.126517               |
|    | NMS     | 0.551392             | -0.051594                | -                         | 0.499798               | 0.126508               | 0.126534               |
| 40 | QED     | 0.589533             | -0.061804                | -0.004789                | 0.529240               | 0.131600               | 0.127850               |
|    | NMS     | 0.596793             | -0.097421                | -                         | 0.499373               | 0.127698               | 0.127781               |
| 50 | QED     | 0.649386             | -0.098199                | -0.006909                | 0.544277               | 0.137127               | 0.129846               |
|    | NMS     | 0.663456             | -0.165147                | -                         | 0.498309               | 0.129224               | 0.129456               |
| 60 | QED     | 0.735510             | -0.148884                | -0.008655                | 0.577971               | 0.145734               | 0.132852               |
|    | NMS     | 0.760401             | -0.264500                | -                         | 0.495901               | 0.131033               | 0.131619               |
| 70 | QED     | 0.860884             | -0.221722                | -0.009082                | 0.630080               | 0.150089               | 0.137493               |
|    | NMS     | 0.902512             | -0.412217                | -                         | 0.490294               | 0.132886               | 0.134339               |
| 80 | QED     | 1.049608             | -0.331694                | -0.006266                | 0.711648               | 0.180304               | 0.144991               |
|    | NMS     | 1.117655             | -0.639407                | -                         | 0.478248               | 0.134239               | 0.137667               |
| 90 | QED     | 1.343409             | -0.506445                | 0.004025                 | 0.840989               | 0.215024               | 0.157885               |
|    | NMS     | 1.453046             | -1.002570                | -                         | 0.450476               | 0.133231               | 0.141468               |
| 95 | QED     | 1.420806             | -0.553271                | 0.007663                 | 0.875198               | 0.224427               | 0.161526               |
|    | NMS     | 1.541376             | -1.099804                | -                         | 0.441572               | 0.132411               | 0.142324               |
| 100| QED     | 1.553578             | -0.634200                | 0.014619                 | 0.933997               | 0.240743               | 0.167966               |
|    | NMS     | 1.693024             | -1.267592                | -                         | 0.425432               | 0.130603               | 0.143340               |
|    |         | 1.831537             | -0.805924                | 0.031669                 | 1.057282               | 0.275548               | 0.182201               |
|    |         | 2.010789             | -1.622347                | -                         | 0.388442               | 0.125349               | 0.144890               |

The first-order (in $1/Z$) electron-electron interaction correction to the nuclear recoil effect can be conveniently expressed in terms of the dimensionless function $B(\alpha Z)$ defined by

$$\Delta E^{(2)} = \frac{m (\alpha Z)^2}{2} B(\alpha Z) mc^2.$$  \hspace{1cm} (39)$$

Our results for the interelectronic-interaction correction to the one-electron part of the nuclear recoil effect on the binding energies of the $1s^2$, $1s^22s$, and $1s^22p_{1/2}$ states are shown in Tables II, III, and IV respectively. As in Table I for each $Z$ we present two values. The first value is evaluated within the framework of the \textit{ab initio} approach derived in the preceding section, whereas the second one is obtained within the Breit approximation via the NMS operator (1). The functions $B_c$, $B_{tr1}$, and $B_{tr2}$ correspond to the contributions of the Coulomb (11), the one-transverse-photon (12), and the two-transverse-photon (13) interactions, respectively. The uncertainties given in the parentheses are due to the numerical errors only. They are estimated by studying the convergence of the results with respect to the size of the basis set as well as the number of points in the quadrature formula for the integration over $\omega$.

From Tables II, III, and IV one can see that the results of the QED calculations tend to the Breit-approximation values when $\alpha Z \to 0$. This behavior is what one can expect, having in mind that the NMS operator (1) provides the lowest-order relativistic approximation to the
theory worked out. On the other hand, due to the energy dependence of the vector \( D(\omega) \) in the integration over \( \omega \) in Eq. (14) and analogous expressions, the one-transverse-photon contribution acquires the considerable correction compared to the Breit approximation for high-\( Z \) ions. The nontrivial QED Coulomb contribution as well as the two-transverse-photon contribution also grow rapidly with increasing \( Z \). As a result, the higher orders (in \( \alpha Z \)) modify the behavior of the function \( B(\alpha Z) \) significantly. Indeed, the function \( B(\alpha Z) \) calculated to all orders in \( \alpha Z \) may differ by several times from the approximate one obtained by means of the NMS operator. In order to illustrate this fact, the interelectronic-interaction correction to the one-electron part of the nuclear recoil effect on the binding energy of the \( 1s^2 \) state is plotted in Fig. [4] where the data given in the last column of Table [I] are presented. The Breit-approximation values and the \textit{ab initio} QED results are shown with the dashed and solid lines, respectively. It is seen that the NMS operator leads to the strong underestimation of the nuclear recoil effect at the high-\( Z \) region. The similar situation takes place for binding energies of the \( 1s^22s \) and \( 1s^22p_{1/2} \) states. However, it is not always the case. For instance, the contribution under consideration to the \( 2p_{1/2} \rightarrow 2s \) transition energy in Li-like ions is presented in Fig. [5]. In this transition energy, the interelectronic-interaction correction to the one-electron part of the nuclear recoil effect obtained by means of the rigorous QED approach appears to be less pronounced than the one evaluated within the lowest-order relativistic approximation.

| \( Z \) | Approach | \( B_a(\alpha Z) \) | \( B_{a1}(\alpha Z) \) | \( B_{a2}(\alpha Z) \) | \( B(\alpha Z) \) |
|-------|----------|----------------|----------------|----------------|----------------|
| 5     | QED      | \(-0.1027\)   | \(-0.0274\)   | \(-0.00008\)  | \(-1.02460\)  |
|       | \( H_{NMS} \) | \(-0.1027\)   | \(-0.00303\)  | \(-1.02442\)  |               |
| 10    | QED      | \(-1.0412\)   | \(-0.01360\)  | \(-0.00041\)  | \(-1.03049\)  |
|       | \( H_{NMS} \) | \(-1.0415\)   | \(-0.01224\)  | \(-1.02927\)  |               |
| 20    | QED      | \(-1.0979\)   | \(-0.03996\)  | \(-0.00851\)  | \(-1.05297\)  |
|       | \( H_{NMS} \) | \(-1.0983\)   | \(-0.05122\)  | \(-1.04861\)  |               |
| 30    | QED      | \(-1.1989\)   | \(-0.08672\)  | \(-0.00399\)  | \(-1.10820\)  |
|       | \( H_{NMS} \) | \(-1.2049\)   | \(-0.12427\)  | \(-1.10807\)  |               |
| 40    | QED      | \(-1.3564\)   | \(-0.15948\)  | \(-0.00614\)  | \(-1.13982\)  |
|       | \( H_{NMS} \) | \(-1.3708\)   | \(-0.25454\)  | \(-1.12530\)  |               |
| 50    | QED      | \(-1.5927\)   | \(-0.26916\)  | \(-0.00717\)  | \(-1.31638\)  |
|       | \( H_{NMS} \) | \(-1.6221\)   | \(-0.44013\)  | \(-1.18206\)  |               |
| 60    | QED      | \(-1.9467\)   | \(-0.43776\)  | \(-0.00484\)  | \(-1.50415\)  |
|       | \( H_{NMS} \) | \(-2.0024\)   | \(-0.75257\)  | \(-1.24992\)  |               |
| 70    | QED      | \(-2.4879\)   | \(-0.70598\)  | \(-0.00556\)  | \(-1.78748\)  |
|       | \( H_{NMS} \) | \(-2.5861\)   | \(-1.26394\)  | \(-1.32467\)  |               |
| 80    | QED      | \(-3.3500\)   | \(-1.15466\)  | \(-0.03461\)  | \(-2.29295\)  |
|       | \( H_{NMS} \) | \(-3.5302\)   | \(-2.13366\)  | \(-1.39663\)  |               |
| 90    | QED      | \(-4.7904\)   | \(-1.94762\)  | \(-0.10743\)  | \(-2.95022\)  |
|       | \( H_{NMS} \) | \(-5.1128\)   | \(-3.68168\)  | \(-1.43112\)  |               |
| 100   | QED      | \(-5.1874\)   | \(-2.17346\)  | \(-0.13159\)  | \(-3.14553\)  |
|       | \( H_{NMS} \) | \(-5.5500\)   | \(-4.12298\)  | \(-1.42707\)  |               |
|       | QED      | \(-5.8824\)   | \(-2.57461\)  | \(-0.17719\)  | \(-3.48500\)  |
|       | \( H_{NMS} \) | \(-6.3170\)   | \(-4.90663\)  | \(-1.41037\)  |               |
| 100   | QED      | \(-7.3895\)   | \(-3.46536\)  | \(-0.28818\)  | \(-4.21237\)  |
|       | \( H_{NMS} \) | \(-7.9851\)   | \(-6.64491\)  | \(-1.34018\)  |               |
TABLE IV. The interelectronic-interaction correction of first order in $1/Z$ to the one-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. (30).

| Z | Approach | $B_{1}(\alpha Z)$ | $B_{1s}(\alpha Z)$ | $B_{1s2}(\alpha Z)$ | $B(\alpha Z)$ |
|---|----------|-------------------|-------------------|-------------------|---------------|
| 5 | QED      | −1.99828          | 0.00266           | 0.00047           | −1.99556      |
|   | H_{NMS}  | −1.99831          | 0.00289           | —                 | −1.99542      |
| 10| QED      | −1.11258          | 0.01017           | 0.00034           | −1.10207      |
|   | H_{NMS}  | −1.11278          | 0.01169           | —                 | −1.10109      |
| 20| QED      | −1.17123          | 0.03906           | 0.00150           | −1.13066      |
|   | H_{NMS}  | −1.17275          | 0.04899           | —                 | −1.12375      |
| 30| QED      | −1.27558          | 0.08863           | 0.00305           | −1.18391      |
|   | H_{NMS}  | −1.28056          | 0.11905           | —                 | −1.16151      |
| 40| QED      | −1.43815          | 0.16579           | 0.00404           | −1.26832      |
|   | H_{NMS}  | −1.45015          | 0.23572           | —                 | −1.21443      |
| 50| QED      | −1.68116          | 0.28397           | 0.00274           | −1.39445      |
|   | H_{NMS}  | −1.70605          | 0.42351           | —                 | −1.28254      |
| 60| QED      | −2.04377          | 0.46749(1)        | −0.00418          | −1.58047      |
|   | H_{NMS}  | −2.09154          | 0.72595           | —                 | −1.36559      |
| 70| QED      | −2.56593          | 0.76112(1)        | −0.02356          | −1.85838(1)   |
|   | H_{NMS}  | −2.68384          | 1.22278           | —                 | −1.56106      |
| 80| QED      | −3.47332          | 1.25346(1)        | −0.07027          | −2.29013      |
|   | H_{NMS}  | −3.63420          | 2.07194           | —                 | −1.56226      |
| 90| QED      | −4.94405          | 2.12768(1)        | −0.17879          | −2.99576(1)   |
|   | H_{NMS}  | −5.24001          | 3.59851           | —                 | −1.64115      |
| 92| QED      | −5.35164          | 2.37701(1)        | −0.21386          | −3.18849(1)   |
|   | H_{NMS}  | −5.68680          | 4.03754           | —                 | −1.64926      |
| 95| QED      | −6.06731          | 2.82181(1)        | −0.27938          | −3.52488(1)   |
|   | H_{NMS}  | −6.47332          | 4.82083           | —                 | −1.65249      |
| 100| QED | −7.62960(1) 3.81396(4) | −0.43661(1) | −4.25225(3) |
|    | H_{NMS}  | −8.19725          | 6.57466           | —                 | −1.62259      |
The one-electron contribution is evaluated in the present work, while the two-electron contribution is taken from Ref. [30]. The interelectronic-interaction correction of first order in \(1/Z\) is given in terms of the function \(B(\alpha Z)/Z\) defined by Eq. [30]. The one-electron contribution is evaluated in the present work, while the two-electron contribution is taken from Ref. [30].

| Z  | Approach | One-electron | Two-electron | Total   |
|----|----------|--------------|--------------|---------|
|    |          | \(A\)        | \(B/Z\)      | \(A + B/Z\) |
| 5  | QED      | 1.000 133    | -0.125 270   | 0.00 267 35 | 0.901 597 |
|    | H\_MS   | 0.999 999    | -0.125 244   | 0.00 267 31 | 0.901 486 |
| 10 | QED      | 1.000 937    | -0.063 080   | 0.00 134 86 | 0.951 343 |
|    | H\_MS   | 0.999 990    | -0.062 987   | 0.00 134 73 | 0.950 476 |
| 20 | QED      | 1.006 497    | -0.032 542   | 0.00 069 88 | 0.980 943 |
|    | H\_MS   | 0.999 907    | -0.032 220   | 0.00 069 44 | 0.974 631 |
| 30 | QED      | 1.020 211    | -0.022 964   | 0.00 049 46 | 1.002 193 |
|    | H\_MS   | 0.999 597    | -0.022 777   | 0.00 048 44 | 0.982 163 |
| 40 | QED      | 1.045 879    | -0.018 751   | 0.00 040 31 | 1.031 159 |
|    | H\_MS   | 0.998 745    | -0.017 532   | 0.00 038 83 | 0.985 051 |
| 50 | QED      | 1.088 554    | -0.016 842   | 0.00 035 87 | 1.075 299 |
|    | H\_MS   | 0.996 618    | -0.014 853   | 0.00 032 56 | 0.985 021 |
| 60 | QED      | 1.155 941    | -0.016 308   | 0.00 034 03 | 1.143 036 |
|    | H\_MS   | 0.991 803    | -0.013 186   | 0.00 028 74 | 0.981 491 |
| 70 | QED      | 1.260 160    | -0.016 889   | 0.00 034 01 | 1.246 672 |
|    | H\_MS   | 0.980 589    | -0.012 044   | 0.00 025 90 | 0.971 134 |
| 80 | QED      | 1.423 296    | -0.018 713   | 0.00 035 59 | 1.408 143 |
|    | H\_MS   | 0.956 496    | -0.011 133   | 0.00 023 46 | 0.947 709 |
| 90 | QED      | 1.681 978    | -0.022 263   | 0.00 038 96 | 1.663 612 |
|    | H\_MS   | 0.900 953    | -0.010 088   | 0.00 020 93 | 0.892 958 |
| 92 | QED      | 1.750 397    | -0.023 262   | 0.00 039 00 | 1.731 125 |
|    | H\_MS   | 0.883 145    | -0.009 816   | 0.00 020 36 | 0.875 365 |
| 95 | QED      | 1.867 993    | -0.025 016   | 0.00 041 49 | 1.847 127 |
|    | H\_MS   | 0.850 865    | -0.009 346   | 0.00 019 43 | 0.843 462 |
| 100| QED      | 2.114 564    | -0.028 806   | 0.00 047 46 | 2.090 235 |

The nuclear recoil contribution to the binding energy of the \(1s^2\) state. The values obtained within the independent-electron approximation (to zeroth order in \(1/Z\)) are given in terms of the function \(A(\alpha Z)\) defined by Eq. [38]. The results obtained as the difference of the values presented in Tables VII and VI in Figs. 8 and 9 correspond to the calculations within the Breit approximation, \(A(\alpha Z)\), and give the indication of how different terms relate to each other.

We stress that the interelectronic-interaction correction under consideration becomes particularly impor-
TABLE VI. The nuclear recoil contribution to the binding energy of the $1s^22s$ state. The values obtained within the independent-electron approximation (to zeroth order in $1/Z$) are given in terms of the function $A(\alpha Z)$ defined by Eq. (38). The interelectronic-interaction correction of first order in $1/Z$ are given in terms of the function $B(\alpha Z)/Z$ defined by Eq. (39). The one-electron contribution is evaluated in the present work, while the two-electron contribution is taken from Ref. [30].

| $Z$ | Approach | One-electron | Two-electron | Total |
|-----|----------|--------------|--------------|-------|
|     |          | $A$           | $B/Z$        | $A+B/Z$ |
| 5   | QED      | 1.125 184   | $-0.204 919$ | 0.0    | 0.031 254 | 0.951 519 |
|     | $H_{MS}$ | 1.125 041   | $-0.204 885$ | 0.0    | 0.031 250 | 0.951 406 |
| 10  | QED      | 1.126 174   | $-0.103 049$ | 0.0    | 0.015 782 | 1.038 907 |
|     | $H_{MS}$ | 1.125 157   | $-0.102 927$ | 0.0    | 0.015 768 | 1.037 998 |
| 20  | QED      | 1.132 673   | $-0.052 858$ | 0.0    | 0.008 209 | 1.088 024 |
|     | $H_{MS}$ | 1.125 574   | $-0.052 430$ | 0.0    | 0.008 162 | 1.081 306 |
| 30  | QED      | 1.148 368   | $-0.036 940$ | 0.0    | 0.005 841 | 1.117 269 |
|     | $H_{MS}$ | 1.126 105   | $-0.036 022$ | 0.0    | 0.005 732 | 1.095 815 |
| 40  | QED      | 1.177 480   | $-0.029 770$ | 0.0    | 0.004 792 | 1.152 501 |
|     | $H_{MS}$ | 1.126 443   | $-0.028 132$ | 0.0    | 0.004 581 | 1.102 892 |
| 50  | QED      | 1.225 681   | $-0.026 328$ | 0.0    | 0.004 295 | 1.203 648 |
|     | $H_{MS}$ | 1.125 841   | $-0.023 641$ | 0.0    | 0.003 927 | 1.106 127 |
| 60  | QED      | 1.301 675   | $-0.025 069$ | 0.0    | 0.004 103 | 1.280 709 |
|     | $H_{MS}$ | 1.122 836   | $-0.020 832$ | 0.0    | 0.003 505 | 1.105 510 |
| 70  | QED      | 1.419 249   | $-0.025 535$ | 0.0    | 0.004 129 | 1.397 843 |
|     | $H_{MS}$ | 1.113 475   | $-0.018 924$ | 0.0    | 0.003 199 | 1.097 750 |
| 80  | QED      | 1.603 600   | $-0.027 874$ | 0.0    | 0.004 350 | 1.580 076 |
|     | $H_{MS}$ | 1.090 736   | $-0.017 458$ | 0.0    | 0.002 940 | 1.076 217 |
| 90  | QED      | 1.897 002   | $-0.032 780$ | 0.0    | 0.004 793 | 1.869 014 |
|     | $H_{MS}$ | 1.034 184   | $-0.015 901$ | 0.0    | 0.002 666 | 1.020 949 |
| 92  | QED      | 1.974 823   | $-0.034 191$ | 0.0    | 0.004 914 | 1.945 547 |
|     | $H_{MS}$ | 1.015 556   | $-0.015 512$ | 0.0    | 0.002 603 | 1.002 647 |
| 95  | QED      | 2.108 737   | $-0.036 684$ | 0.0    | 0.005 120 | 2.077 172 |
|     | $H_{MS}$ | 0.981 468   | $-0.014 846$ | 0.0    | 0.002 500 | 0.969 122 |
| 100 | QED      | 2.390 112   | $-0.042 124$ | 0.0    | 0.005 542 | 2.353 531 |
|     | $H_{MS}$ | 0.902 234   | $-0.013 402$ | 0.0    | 0.002 294 | 0.891 126 |

 tant when a cancellation of the zeroth-order contributions occurs. For instance, the one-electron contribution for the $1s^2$ core cancels in the $2p_{1/2}-2s$ transition in Li-like ions within the independent-electron approximation. As a result, the nontrivial QED contributions of zeroth and first orders in $1/Z$ are of comparable magnitude for low- and middle-$Z$ ions for this transition. In this regard, one can expect even stronger cancellation of the leading-order contributions in the case of the $2p_{1/2}-2p_{1/2}$ transition in B-like ions; see the related discussion for the QED contribution to the field shift in Ref. [13]. In addition, the $ab$ initio treatment of the electron-electron interaction correction to all orders in $\alpha Z$ may even change the sign of the correction. Indeed, one can see that the solid lines in Fig. 4 do not cross each other in contrast to the dashed ones. All this leads to the conclusion that the high-precision calculations of the nuclear recoil effect need to take into account the QED contribution beyond the independent-electron approximation.

C. Mass shift of binding and transition energies

As noted above, in order to obtain accurate theoretical predictions for the mass shift of binding and transition energies one has to account for the second- and higher-order electron-electron interaction corrections to the nuclear recoil effect as well. In the present work, we evaluate these contributions within the lowest-order relativistic approximation by employing the MS operator (4) and the Dirac-Coulomb-Breit Hamiltonian. The calculations are performed by means of two independent methods. First, we have calculated the expectation value of the MS operator with the many-electron wave function obtained by the configuration-interaction
TABLE VII. The nuclear recoil contribution to the binding energy of the 1s^2 2p_{1/2} state. The values obtained within the independent-electron approximation (to zeroth order in 1/Z) are given in terms of the function A(αZ) defined by Eq. (38). The interelectronic-interaction correction of first order in 1/Z is given in terms of the function B(αZ)/Z defined by Eq. (39). The one-electron contribution is evaluated in the present work, while the two-electron contribution is taken from Ref. [30].

| Z   | Approach | One-electron | Two-electron | Total |
|-----|----------|--------------|--------------|-------|
|     |          | A          | B/Z          |       |
| 5   | QED      | 1.125 174  | −0.219 111  | −0.077 986 | 0.088 710 | 0.916 786 |
|     | MS       | 1.125 041  | −0.219 084  | −0.077 986 | 0.088 706 | 0.916 676 |
| 10  | QED      | 1.126 100  | −0.110 207  | −0.077 835 | 0.044 519 | 0.982 578 |
|     | MS       | 1.125 157  | −0.110 109  | −0.077 833 | 0.044 505 | 0.981 720 |
| 20  | QED      | 1.132 153  | −0.056 533  | −0.077 225 | 0.022 595 | 1.020 990 |
|     | MS       | 1.125 580  | −0.056 188  | −0.077 196 | 0.022 542 | 1.014 739 |
| 30  | QED      | 1.146 728  | −0.039 464  | −0.076 199 | 0.015 449 | 1.046 514 |
|     | MS       | 1.126 131  | −0.038 717  | −0.076 046 | 0.015 315 | 1.026 684 |
| 40  | QED      | 1.173 729  | −0.031 708  | −0.074 741 | 0.012 011 | 1.079 291 |
|     | MS       | 1.126 526  | −0.030 361  | −0.074 234 | 0.011 734 | 1.033 666 |
| 50  | QED      | 1.218 400  | −0.027 889  | −0.072 820 | 0.010 076 | 1.127 767 |
|     | MS       | 1.126 073  | −0.025 651  | −0.071 506 | 0.009 563 | 1.038 480 |
| 60  | QED      | 1.288 793  | −0.026 341  | −0.070 388 | 0.008 916 | 1.200 980 |
|     | MS       | 1.123 422  | −0.022 760  | −0.067 442 | 0.008 034 | 1.041 254 |
| 70  | QED      | 1.397 653  | −0.026 548  | −0.067 367 | 0.008 234 | 1.311 973 |
|     | MS       | 1.114 927  | −0.020 872  | −0.061 327 | 0.006 777 | 1.039 506 |
| 80  | QED      | 1.568 287  | −0.028 627  | −0.063 632 | 0.007 903 | 1.483 931 |
|     | MS       | 1.094 163  | −0.019 528  | −0.051 886 | 0.005 537 | 1.028 286 |
| 90  | QED      | 1.839 863  | −0.033 286  | −0.058 988 | 0.007 886 | 1.755 474 |
|     | MS       | 1.042 421  | −0.018 239  | −0.036 694 | 0.004 028 | 0.991 517 |
| 92  | QED      | 1.911 923  | −0.034 657  | −0.057 926 | 0.007 923 | 1.827 262 |
|     | MS       | 1.025 379  | −0.017 927  | −0.032 597 | 0.003 658 | 0.978 513 |
| 95  | QED      | 2.035 959  | −0.037 104  | −0.056 235 | 0.008 007 | 1.950 628 |
|     | MS       | 0.994 205  | −0.017 395  | −0.025 536 | 0.003 036 | 0.954 310 |
| 100 | QED      | 2.296 765  | −0.042 522  | −0.053 123 | 0.008 235 | 2.209 355 |
|     | MS       | 0.921 775  | −0.016 226  | −0.010 645 | 0.001 757 | 0.896 661 |

The one- and two-electron parts of the corresponding contribution are evaluated with the use of the NMS (1) and SMS (2) operators, respectively, and given explicitly. The uncertainties specified in Table VIII correspond to the numerical errors only. They are obtained by analyzing the convergence of the results with respect to the number of the radial and angular basis-set functions. We note that the two-electron part is more sensitive to the correlation effects than the one-electron part. As a result, the corresponding uncertainty is generally bigger for low- and middle-Z ions. On the other hand, there is a cancellation between the one- and two-electron contributions which allows us to obtain more accurate data for the total values.
TABLE VIII. The interelectronic-interaction correction of second and higher orders in $1/Z$ to binding energies of the $1s^2$, $1s^22s$, and $1s^22p_{1/2}$ states within the Breit approximation expressed in terms of the dimensionless function $C(\alpha Z, Z)$ defined by Eq. (40).

| $Z$ | $1s^2$ | | | $1s^22s$ | | | $1s^22p_{1/2}$ | | |
|-----|-------|---|---|-------|---|---|-------|---|
|     | $C_{vel}$ | $C_{pol}$ | $C_{tot}$ | $C_{vel}$ | $C_{pol}$ | $C_{tot}$ | $C_{vel}$ | $C_{pol}$ | $C_{tot}$ |
| 5   | 0.1580(2) | -0.1145(3) | 0.0434(2) | 0.4167(2) | -0.1741(3) | 0.2426(2) | 0.5513(2) | -0.3497(6) | 0.2015(4) |
| 10  | 0.1656(2) | -0.1196(5) | 0.0460(3) | 0.4233(2) | -0.1834(5) | 0.2399(3) | 0.5546(2) | -0.3445(8) | 0.2101(5) |
| 20  | 0.1930(5) | -0.1328(10) | 0.0601(5) | 0.4624(5) | -0.2039(11) | 0.2584(6) | 0.6070(6) | -0.3688(15) | 0.2382(9) |
| 30  | 0.2396(7) | -0.1534(13) | 0.0862(6) | 0.5322(8) | -0.2351(14) | 0.2971(6) | 0.7050(9) | -0.4144(18) | 0.2906(9) |
| 40  | 0.3045(11) | -0.1813(17) | 0.1232(7) | 0.6315(13) | -0.2772(18) | 0.3543(7) | 0.8482(14) | -0.4768(23) | 0.3713(10) |
| 50  | 0.3900(17) | -0.2163(21) | 0.1737(10) | 0.7650(19) | -0.3306(23) | 0.4344(11) | 1.0439(20) | -0.5532(29) | 0.4906(13) |
| 60  | 0.4985(27) | -0.2582(27) | 0.2403(17) | 0.9376(31) | -0.3945(30) | 0.5430(20) | 1.3022(31) | -0.6372(36) | 0.6650(20) |
| 70  | 0.6322(42) | -0.3055(35) | 0.3267(30) | 1.1546(49) | -0.4674(38) | 0.6872(35) | 1.6362(47) | -0.7142(45) | 0.9221(32) |
| 80  | 0.7902(66) | -0.3549(44) | 0.4353(50) | 1.4169(77) | -0.5444(49) | 0.8725(60) | 2.0582(72) | -0.7509(56) | 1.3073(53) |
| 90  | 0.954(10) | -0.3966(57) | 0.5509(80) | 1.696(12) | -0.6116(64) | 1.084(95) | 2.552(11) | -0.6657(71) | 1.8861(83) |
| 100 | 1.018(12) | -0.4080(64) | 0.610(10) | 1.890(14) | -0.6316(73) | 1.177(12) | 2.793(13) | -0.5202(80) | 2.272(10) |

TABLE IX. The mass shifts of the binding energies of the $1s^2$, $1s^22s$, and $1s^22p_{1/2}$ states and the mass shift of the $2p_{1/2}^2$ state in Li-like ions in terms of the dimensionless function $P(\alpha Z, Z)$ defined by Eq. (41) and the $K$ factor (in eV·amu) defined by Eq. (42).

| $Z$ | $1s^2$ | | | $1s^22s$ | | | $1s^22p_{1/2}$ | | |
|-----|-------|---|---|-------|---|---|-------|---|
|     | $P$ | $K$ | | | $P$ | $K$ | | | $P$ | $K$ | |
| 5   | 0.90334(1) | 0.337116(3) | 0.96122(1) | 0.357819(3) | 0.92485(2) | 0.35415(1) | -0.036376(19) | -0.013575(7) |
| 10  | 0.95180(1) | 1.42082(2) | 1.04131(2) | 1.55442(2) | 0.98468(1) | 1.46089(2) | -0.056628(6) | -0.08453(1) |
| 20  | 0.98110(10) | 5.85817(57) | 1.08867(10) | 6.50051(62) | 1.02159(10) | 6.09994(58) | -0.067085(8) | -0.40057(5) |
| 30  | 1.00230(30) | 13.4658(40) | 1.11761(32) | 15.0150(44) | 1.04685(30) | 14.0643(40) | -0.070762(24) | -0.95068(32) |
| 40  | 1.03130(69) | 24.632(16) | 1.15279(74) | 27.533(18) | 1.07958(69) | 25.785(16) | -0.073203(57) | -1.7184(14) |
| 50  | 1.0756(13) | 40.140(50) | 1.2041(15) | 44.935(54) | 1.1282(13) | 42.103(50) | -0.07587(12) | -2.8316(43) |
| 60  | 1.1438(24) | 61.47(13) | 1.2817(26) | 68.88(14) | 1.2019(24) | 64.59(13) | -0.07975(22) | -4.286(12) |
| 70  | 1.249(41) | 91.36(30) | 1.4004(45) | 102.43(33) | 1.3144(42) | 96.14(31) | -0.08599(39) | -6.309(28) |
| 80  | 1.4142(74) | 135.11(71) | 1.5868(81) | 151.60(77) | 1.4902(75) | 142.37(72) | -0.09656(70) | -9.225(67) |
| 90  | 1.680(18) | 203.1(22) | 1.887(20) | 228.2(24) | 1.772(18) | 214.3(22) | -0.1148(15) | -13.88(19) |
| 100 | 1.751(23) | 221.2(29) | 1.967(25) | 248.6(32) | 1.847(23) | 233.4(29) | -0.1198(19) | -15.14(24) |

Finally, in Table IX we compile the total theoretical predictions for the mass shifts of the following quantities: (i) the ground-state binding energy of He-like ions; (ii) the binding energy of the $1s^22s$ state; (iii) the binding energy of the $1s^22p_{1/2}$ state; (iv) the $2p_{1/2}^2$ transition energy in Li-like ions. The results are expressed in terms of the dimensionless function $P(\alpha Z, Z)$ defined according to

$$\Delta E_{\text{rec}} = \frac{m}{M}(\alpha Z)^2 P(\alpha Z, Z) mc^2$$ (41)
FIG. 7. 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.

and the $K$ factor (in units of eV·amu) defined by

$$\Delta E_{\text{rec}} = \frac{K}{M}.$$  \hfil (42)

The total theoretical predictions comprise the QED results for the zeroth-order, $A(\alpha Z)$, and first-order, $B(\alpha Z)/Z$, contributions from Tables I and II–IV respectively, as well as the higher-order correlation correction within the Breit approximation, $C(\alpha Z, Z)/Z^2$, from Table VIII. In addition, within the independent-electron approximation we account for the correction $\delta A_{\text{Breit}}^\text{ins,1el}(\alpha Z)$, which determines the difference between the exact treatment of the nuclear size correction to the low-order one-electron nuclear recoil effect and its evaluation by the formula (22) with the wave functions for the extended nucleus; see Ref. [47] and the discussion above. Therefore, the function $P(\alpha Z, Z)$ in Eq. (41) can be represented as follows

$$P(\alpha Z, Z) = A(\alpha Z) + \delta A_{\text{Breit}}^\text{ins,1el}(\alpha Z) + \frac{B(\alpha Z)}{Z} + \frac{C(\alpha Z, Z)}{Z^2}.$$  \hfil (43)

We note that the reduced-mass dependence in the Lamb shift also contributes to the nuclear recoil effect; see, e.g., the discussion in Ref. [48] and references therein. This contribution and the uncertainty related with it are out of the scope of the present work. They have to be taken into account separately.

Besides the numerical uncertainties discussed above, there are several sources for the theoretical uncertainties shown in parentheses in Table VIII. First of all, we take into account the uncertainty due to uncalculated radiative nuclear recoil correction. To this end, we multiply the nontrivial one-electron QED contribution (28) obtained within the independent-electron approximation by the factor of 2$\alpha$. Second, we estimate the uncertainty due to the approximate treatment of the nuclear

FIG. 8. The nuclear recoil effect on the binding energy of the 1s$^2$ state to first order in 1/Z. The solid lines stand for the results of the QED calculations to all orders in $\alpha Z$ while the dashed lines correspond to the calculations based on the mass shift (MS) operator given by Eq. (3). The contributions of zeroth order in 1/Z, $P_{[0]}(\alpha Z) = A(\alpha Z)$, and the sums of zeroth and first orders in 1/Z, $P_{[0,1]}(\alpha Z, Z) = A(\alpha Z) + B(\alpha Z)/Z$, are shown with blue (circles) and red (squares) lines, respectively.

FIG. 9. The nuclear recoil effect on the 2p$_{1/2}$–2s transition energy in Li-like ions to first order in 1/Z. Notations are the same as in Fig. 8.
FIG. 10. (a) The nuclear recoil effect on the $2p_{1/2} - 2s$ transition energy in Li-like ions in terms of the function $P(\alpha Z, Z)$ defined by Eq. (41). The blue dashed line corresponds to the calculation performed by means of the mass shift operator (3) to all order in $1/Z$. The green dashed-dotted line includes the nontrivial QED contribution within the independent-electron approximation (QED[0]). The violet dotted line accounts for the QED correction to first-order in $1/Z$ (QED[0,1]). The red solid line takes into account additionally the finite nuclear size (fns) correction $\delta A_{\text{Breit}}^{\text{fns,1el}}(\alpha Z)$. The corresponding data from Ref. [11] are shown with magenta circles and black diamonds. The error bars are not indicated. (b) The zoomed region for $Z = 68–94$. The uncertainties of the present calculation and Ref. [11] are shown.

In Table IX, we compare our total values for the mass shift of the $2p_{1/2} - 2s$ transition energy in Li-like ions with the theoretical predictions from Ref. [11]. One can see that the data from Ref. [11] lie systematically lower. The more detailed comparison is performed in Figs. 10(a) and 10(b). (Fig. 10(b) provides the zoomed version of Fig. 10(a) which corresponds to the high-Z region ($Z = 68–94$)). The four lines labeled with TW in Fig. 10 represent our data obtained by successive accounting for the different contributions. The blue dashed line displays the results calculated by employing the MS operator (3) and treating the correlation effects to all orders in $1/Z$ within the Breit approximation. The green dashed-dotted line differs from the first one by taking into account the nontrivial QED contribution in zeroth order in $1/Z$. The violet dotted line is obtained by adding the higher-order (in $\alpha Z$) contribution in first order in $1/Z$. Finally, the red solid line includes also the finite nuclear size correction $\delta A_{\text{Breit}}^{\text{fns,1el}}(\alpha Z)$ and corresponds to the total data presented in Table IX. We note that the last two corrections have a different sign and partly cancel each other in the sum. These corrections have not been taken into account in Ref. [11]. The Breit-approximation values and the results with the QED contribution evaluated within the independent-electron approximation from Ref. [11] are shown in Fig. 10 with the magenta circles and black diamonds, respectively. In order not to overload the plot, we omit the error bars in Fig. 10(a). The uncertainties are indicated only in Fig. 10(b). One can see that there is a reasonable agreement between the data from Ref. [11] and the results of the present study. The difference between the final theoretical predictions is explained by the fact that the more subtle effects are taken into account now. As a result, the uncertainty of the nuclear recoil effect is reduced, especially for middle-$Z$ ions, where the contribution of the mass shift to the isotope shifts is more significant. The results obtained are in demand in view of the existing and forthcoming experimental investigations of the relativistic and QED nuclear recoil effect [6, 57–59].
V. SUMMARY

To summarize, we have developed the rigorous QED formalism which allows us to calculate the electron-electron interaction correction to the one-electron part of the nuclear recoil effect on binding energies in atoms and ions nonperturbatively in the parameter αZ. The method derived was employed for the ab initio calculations of the one-electron nuclear recoil contribution to the binding energies of the 1s2 state in He-like ions and 1s22s and 1s22p1/2 states in Li-like ions in the wide range Z = 5–100. The corresponding contribution to the 2p1/2–2s transition energy in Li-like ions was studied as well. The one-electron part of the nuclear recoil effect was combined with the two-electron part considered recently in Ref. [30]. The all-order (in αZ) results to zeroth and first orders in 1/Z were compared with the values obtained by applying the mass shift operator within the (m/M)(αZ)4mc2 approximation only. Finally, the QED calculations to first order in 1/Z were supplemented with the higher-order correlation corrections evaluated within the Breit approximation. As a result, the most accurate theoretical predictions for the mass shifts of the binding and transition energies in He- and Li-like ions have been obtained.

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