Evaluation of the low-lying energy levels of two- and three-electron configurations for multi-charged ions

O. Yu. Andreev*, 1 L. N. Labzowsky, 1 G. Plunien, 2 and G. Soff2

1 Institute of Physics, St. Petersburg State University, Ulyanovskaya ul. 1, 198904, Petershof, St. Petersburg, Russia
2 Institut für Theoretische Physik, Technische Universität Dresden, Mommsenstraße 13, D-01062, Dresden, Germany

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Accurate QED evaluations of the one- and two-photon interelectron interaction for low lying two- and three-electron configurations for ions with nuclear charge numbers 60 ≤ Z ≤ 93 are performed. The three-photon interaction is also partly taken into account. The Coulomb gauge is employed. The results are compared with available experimental data and with different calculations. A detailed investigation of the behaviour of the energy levels of the configurations 1s1/22s1/2 1S0, 1s1/22p1/2 3P0, 1s1/22s1/2 3S1 near the crossing points Z = 64 and Z = 92 is carried out. The crossing points are important for the future experimental search for parity nonconserving (PNC) effects in highly charged ions.

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I. INTRODUCTION

During the most recent years the energy levels of two- and three-electron configurations are under very intensive experimental and theoretical investigation.

Accurate calculations of the energy levels for the two-electron configurations 1s1/22s1/2 1S0, 1s1/22p1/2 3P0, and 1s1/22s1/2 3S1 were already performed in [1,2]. In these papers the interelectron interaction has been considered in various approximations: on the basis of variational Schrödinger-wave functions with inclusion of relativistic corrections [3] and using relativistic many-body perturbation theory (RMBPT) [2]. For a long time these approaches defined the standard concerning the level of accuracy. In recent years due to new developments in experimental and theoretical methods the necessity to improve the accuracy of calculations became urgent. Recently, rigorous QED evaluations of two-photon exchange corrections for low lying configurations [3] have been performed.

First calculations of the energy levels for the three-electron configuration have been presented in [3,4]. As in the early papers on two-electron ions in these calculations the two- and many-photon exchange has been considered approximately. Complete QED calculations of the two-photon exchange for three-electron ions have been performed in [4,5]. Within the framework of RMBPT the three-photon exchange has also been taken into account in [3,4,6].

In this paper we present an extension of previous calculations for two-and three-electron ions [4] for a variety of Z values. Here we include also the evaluations for the 1s1/22p1/2 3P0 level, which have not been performed in [4]. Special attention has been paid to elaborate the behaviour of the 1s1/22s1/2 1S0 and 1s1/22p1/2 3P0 levels near Z = 64 and Z = 92, where they become very close to each other. Accordingly, these system become suitable for monitoring parity-nonconserving (PNC) effects. Experimental investigations of PNC effects in two-electron highly charged ions are under intensive discussion [7,8]. The preparation of such experiments requires a precise knowledge of the exact difference between these energy levels.

II. THEORY

In this article we evaluate corrections to the energy levels due to photon exchange. To calculate these corrections we employ the adiabatic S-matrix approach [4,17] and the line profile approach (LPA) [8]. Both methods are based on the Furry picture [19], which describes the many-electron atom as a set of bound electrons, moving in the external field of the nucleus and interacting with each other via the exchange of photons. With the aid of the Feynman rules for bound-state QED [20,21], the processes giving rise to corrections to the energy levels can be represented in terms of Feynman graphs. The photon-exchange corrections evaluated in this article are depicted in Figs. [1,2].

As it has been shown in Refs. [22,21] the S-matrix approach is best suited for the evaluation of corrections described by the irreducible parts of the diagrams. However, its application to the evaluation of the reducible parts becomes
rather complicated. Accordingly, for calculating the reducible parts we utilized the LPA. For a detailed description and for the application of this method we refer to [20].

The Coulomb gauge will be used throughout this paper. The photon propagators for Coulomb (g = c) and transverse (g = t) photons are given by [21]:

\[
D_{\mu_1 \mu_2}^g(x_1, x_2) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\Omega I_{\mu_1 \mu_2}^g(\Omega, r_{12}) e^{i\Omega(t_1 - t_2)}
\]  

(1)

together with the temporal Fourier transforms

\[
I_{\mu_1 \mu_2}^c(\Omega, r_{12}) = \frac{\delta_{\mu_1 4} \delta_{\mu_2 4}}{r_{12}}
\]  

(2)

and

\[
I_{\mu_1 \mu_2}^k(\Omega, r_{12}) = \left( \frac{\delta_{\mu_1 \mu_2}}{r_{12}} e^{i\Omega r_{12}} + \nabla_{1\mu_1} \nabla_{2\mu_2} \frac{1 - e^{i\Omega r_{12}}}{|\Omega|^2} \right) (1 - \delta_{\mu_1 4})(1 - \delta_{\mu_2 4}).
\]  

(3)

A. The two-electron configurations

At first we consider the photon exchange corrections for two-electron configurations. The wavefunction of a two-electron configurations is represented by

\[
\Psi_{J M_1 J_2 l_1 l_2}(r_1, r_2) = N \sum_{m_1 m_2} C_{J M_1}^{j_1 j_2}(m_1 m_2) [\psi_{j_1 l_1 m_1}(r_1) \psi_{j_2 l_2 m_2}(r_2) - \psi_{j_1 l_1 m_1}(r_2) \psi_{j_2 l_2 m_2}(r_1)],
\]  

(4)

where \( N = 1/2 \) for equivalent electrons and \( N = 1/\sqrt{2} \) for non-equivalent electrons, \( C_{J M_1}^{j_1 j_2}(m_1 m_2) \) is a Clebsch-Gordan symbol. By means of Eq. 1 we can specify the configuration 1s2s\(^3\)S\(_1\) by setting \( a, b = 1s_+, 2s_+ \), where \( \pm \) denote the two different projections of the total electron angular momentum and we can derive the energy corrections according to the formula:

\[
\Delta E(1s2s\(^3\)S\(_1\)) = F_{1s_+2s_+:1s_+2s_+}.
\]  

(5)

\[
F_{ab\cdots} = F_{abcd} - F_{bacd}.
\]  

(6)

Here \( F_{ab\cdots} \) denotes a function of one-electron states which are described by wave functions \( \psi_a, \psi_b, \ldots \). The form of the function \( F \) depends on the type of Feynman graph under consideration (see below). For the electron configurations 1s2s\(^1\)S\(_0\) and 1s2p\(^3\)P\(_0\) the energy corrections are given by

\[
\Delta E(1s2s\(^1\)S\(_0\)) = F_{1s_+2s_+:1s_+2s_+} - F_{1s_+2s_+:1s_+2s_+},
\]  

(7)

and

\[
\Delta E(1s2p\(^3\)P\(_0\)) = F_{1s_+2p_+:1s_+2p_+} - F_{1s_+2p_+:1s_+2p_+},
\]  

(8)

respectively. The corrections due to one-photon exchange are represented by the graph in Fig. 1. This diagram is irreducible so that the \( S \)-matrix approach can be applied leading to

\[
F_{a'b'ab}^{(1)} = \sum_g I_g^{(1)}(\varepsilon_{a'} - \varepsilon_a)_{a'b'ab}.
\]  

(9)

Here we have introduced the following notation (see definitions Eqs. 1 and 3)

\[
I_{a'b'ab}^g(\Omega) = \sum_{\mu_1 \mu_2} \int \bar{\psi}_{a'}(r_1) \bar{\psi}_{b'}(r_2) \gamma_{\mu_1 \mu_2}^{(1)} \psi_{a}(r_1) \psi_{b}(r_2) d^3 r_1 d^3 r_2,
\]  

(10)

where the Dirac matrices \( \gamma_{\mu_1}^{(i)} \) are acting on wave functions depending on spatial variables \( r_i \), respectively. For \( g = c \) Eq. 1 determines the first-order Coulomb correction while for \( g = t \) we obtain the first-order Breit correction.
The two-photon exchange corrections are represented by the graphs in Fig. [2]. The “box” diagram is reducible. Its reducible part is defined by the condition \( \varepsilon_{n_1} + \varepsilon_{n_3} = \varepsilon_a + \varepsilon_b \). The “cross” diagram is irreducible. However, it is most convenient to extract the contribution with \( n_1, n_2 \) equal to \( a \) or \( b \) and to treat it like a reducible part of the “cross” diagram. Contributions due to states \( n_1, n_2 \) included in the reducible parts are called reference state contributions. Application of the S-matrix approach for calculating the irreducible part and of the LPA for the reducible part of the “box” and “cross” diagrams, respectively, results in the explicit formulas:

\[
F^{(2)}_{a'b'ab}(\text{box, irr}) = \sum_{gg'} \sum' \left\{ \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{F^{g'}(\Omega)_{a'b'n_{1}n_{2}}F^{g}(\Omega - \varepsilon_{a'} + \varepsilon_a)_{n_{3}n_{2}ab}}{\varepsilon_a + \varepsilon_b - \varepsilon_{n_1} - \varepsilon_{n_2}} d\Omega \right\} ,
\]

\[
F^{(2)}_{a'b'ab}(\text{box, red}) = \frac{1}{2} \sum_{gg'} \sum' \left\{ \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{F^{g'}(\Omega)_{b'n_{1}n_{2}}F^{g}(\Omega - \varepsilon_{a'} + \varepsilon_a)_{n_{3}n_{2}ab}}{\varepsilon_a + \varepsilon_b - \varepsilon_{n_1} - \varepsilon_{n_2}} d\Omega \right\} ,
\]

\[
F^{(2)}_{a'b'ab}(\text{cross, irr}) = \sum_{gg'} \sum' \left\{ \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{F^{g'}(\Omega)_{n_{1}n_{2}a}F^{g}(\Omega - \varepsilon_{a'} + \varepsilon_a)_{n_{3}n_{2}b}}{\varepsilon_a + \varepsilon_b - \varepsilon_{n_1} - \varepsilon_{n_2}} d\Omega \right\} ,
\]

\[
F^{(2)}_{a'b'ab}(\text{cross, red}) = \sum_{gg'} \sum' \left\{ \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{F^{g'}(\Omega)_{n_{1}n_{2}a}F^{g}(\Omega - \varepsilon_{a'} + \varepsilon_a)_{n_{3}n_{2}b}}{\varepsilon_a + \varepsilon_b - \varepsilon_{n_1} - \varepsilon_{n_2}} d\Omega \right\} .
\]

The prime at the summation symbols indicates that only the reference state members are ejected. The double prime indicates that only the reference state members are retained. In order to avoid division by zero in Eq. (13) in the case \( a = b' \) and \( n_1 = n_2 \) one has to take the limit \( \varepsilon_{n_1} \rightarrow \varepsilon_{n_2} \) in both terms on the right-hand side. Thus the singularities cancel. It should be stressed that Eqs. (12) and (14) it follows automatically, that the corrections vanish for \( g = g' = c \). The case \( g = g' = c \) corresponds to the Coulomb-Breit correction, the case \( g = g' = t \) determines the Breit-Breit and the case \( g = c, g' = t \) or \( g = t, g' = c \) refers to the Coulomb-Breit interaction.

For high-\( Z \) ions considered in this work the third-order contribution turns out to be small and it is sufficient to take into account its dominant part only. Accordingly, we consider only the third-order Coulomb and unretarded Breit “box” corrections. The corresponding Feynman graph is displayed in Fig. [3]. The formula for the irreducible part of the third-order “box” correction can be derived in the same manner as for the corrections given by Eqs. (11, 13). It takes the form

\[
F^{(3)}_{a'b'ab}(\text{box, irr}) = \sum_{gg'} \sum' \sum'' \left\{ \frac{F^{g'}(\Omega)_{a'b'n_{1}n_{2}n_{3}n_{4}n_{5}}F^{g}(\Omega - \varepsilon_{a'} + \varepsilon_a)_{n_{1}n_{2}n_{3}n_{4}n_{5}}}{\varepsilon_{n_3} + \varepsilon_{n_4} - \varepsilon_{a'} - \varepsilon_b} d\Omega \right\} ,
\]

where the prime indicates that the reference state contributions are excluded from the summation. Here the reference states are defined by the conditions \( \varepsilon_{n_1} + \varepsilon_{n_3} = \varepsilon_a + \varepsilon_b \) or \( \varepsilon_{n_3} + \varepsilon_{n_4} = \varepsilon_a + \varepsilon_b \). Applying the LPA to the graph in Fig. [3] we derive the following expression for the reducible part

\[
F^{(3)}_{a'b'ab}(\text{box, red}) = \sum_{gg'} \sum' \sum'' \left\{ \frac{F^{g'}(\Omega)_{a'b'n_{1}n_{2}n_{3}n_{4}n_{5}}F^{g}(\Omega - \varepsilon_{a'} + \varepsilon_a)_{n_{1}n_{2}n_{3}n_{4}}}{\varepsilon_{n_3} + \varepsilon_{n_4} - \varepsilon_{a'} - \varepsilon_b} d\Omega \right\} \times \left\{ \frac{(-1)}{2(\varepsilon_{n_3} + \varepsilon_{n_4} - \varepsilon_{a'} - \varepsilon_b)^2} + \frac{(-1)}{2(\varepsilon_{n_1} + \varepsilon_{n_2} - \varepsilon_a - \varepsilon_b)^2} \right\} ,
\]
where the double prime indicates that the summation is running only over the reference states. The terms leading to vanishing denominators in Eq. (16) should be omitted.

B. The three-electron configurations

Now we turn to three-electron ions. Here we consider three-electron configurations with a closed (1s)² shell, which can be described by the wave function

\[ \Psi(r_1, r_2, r_3) = \frac{1}{\sqrt{3!}} \sum_{i,j,k=1,2,3} \epsilon_{ijk} \psi_i(r_1)\psi_j(r_2)\psi_k(r_3). \]  

(17)

\( \epsilon_{ijk} \) denotes the Levi-Civita symbol and \( \psi_i(r) \), \( \psi_j(r) \), \( \psi_k(r) \) denote one-electron wave functions.

As in the two-electron case we have to consider representations corresponding to the two-electron Feynman graphs depicted in Figs. 4 and 5. Their contribution to the energy shift is given by

\[ \Delta E(\{abc\}) = F_{ab,ab} + F_{bc,bc} + F_{ca,ca}, \]  

(18)

where \( F_{ab,cd} \) is given by Eqs. 10 and 12. The set \( \{abc\} \) is equal to the set \( \{1s_+,1s_-,2s_1/2\} \) for the configuration \((1s)^22s_1/2\) and to the set \( \{1s_+,1s_-,2p_{1/2}\} \) for the configuration \((1s)^22p_{1/2}\), respectively. The symbol ± refers to the different angular momentum projections.

Besides the two-electron diagrams, in three-electron problem we have to take into account the additional three-electron Feynman graphs depicted in Figs. 4 and 5. The contribution of the three-electron graphs can be calculated according to

\[ \Delta E(\{abc\}) = \sum_{i,j,k=1,2,3} \epsilon_{ij,k} \epsilon_{ijk} F_{ij,k}^{(3)}(ijk), \]  

(19)

where the indices 1, 2, 3 at F symbol must be replaced by \( a, b, c \) respectively, i.e. \( F_{abc,abc} \equiv F_{123123} \), etc. Eq. (19) includes the contribution of the “direct” and all possible “exchange” diagrams which occur in the three-electron case.

Expressions for \( F_{a'b'c';abc} \) corresponding to the graph in Fig. 4 are

\[ F_{a'b'c';abc}^{(2)(\text{step, irr})} = \sum_{gg'} \sum_{n} \sum_{n'} \frac{I_F^{(a_n - a_{n'})} n a b a'}{\epsilon_a + \epsilon_b - \epsilon_{a'} - \epsilon_n} I_F^{(c_{c'} - c_n)} n b c c', \]  

(20)

\[ F_{a'b'c';abc}^{(2)(\text{step, red})} = \sum_{gg'} \sum_{n} \sum_{n'} \frac{\partial}{\partial \omega} \left[ I_F^{(a_n - a_{n'}) + \omega} n a b a' I_F^{(c_{c'} - c_n + \omega)} n b c c' \right] |_{\omega = 0}, \]  

(21)

where the prime at the summation symbol indicates that the summation runs over all \( n \) except for the case when the set of one-electron states \( \{a', n, c\} \) is equivalent to the set \( \{a, b, c\} \). The latter refers to reference states. The double prime implies that the summation runs over the reference states only. For the two-electron contributions we have here \( g, g' = c, t \). No reducible contribution arises for \( g = g' = c \).

As it has been mentioned above, for the three-photon corrections we take into account only their dominant parts, i.e., the third-order Coulomb and unretarded Breit “box” contributions. The corresponding tree-electron Feynman graphs are displayed in Fig. 6. The formulas for the irreducible and the reducible parts of the third-order “box” correction are derived in the same manner as in Eqs. (15-16). The irreducible part can be expressed as

\[ F_{a'b'c';abc}^{(3)(\text{step-box, irr})} = \sum_{gg'} \sum_{n_1 n_2 n_3} \sum_{n_1 n_2 n_3'} \frac{I_F^{(a_{n_1} - a_{n_1'}) n_2 c c'} I_F^{(a_{n_2} - a_{n_2'}) n_3 c c'} I_F^{(a_{n_3} - a_{n_3'}) n_1 c c'}}{(\epsilon_{n_1} + \epsilon_{n_1'} - \epsilon_{a'} - \epsilon_{a'} - \epsilon_{a} - \epsilon_{b}) (\epsilon_{n_2} + \epsilon_{n_2'} - \epsilon_{a} - \epsilon_{b}) (\epsilon_{n_3} + \epsilon_{n_3'} - \epsilon_{a} - \epsilon_{b})} + 2 \sum_{gg'} \sum_{n_1 n_2 n_3} \sum_{n_1 n_2 n_3'} \frac{I_F^{(a_{n_1} - a_{n_1'}) n_2 c c'} I_F^{(a_{n_2} - a_{n_2'}) n_3 c c'} I_F^{(a_{n_3} - a_{n_3'}) n_1 c c'}}{(\epsilon_{n_1} + \epsilon_{n_1'} - \epsilon_{a'} - \epsilon_{a'} - \epsilon_{a} - \epsilon_{b}) (\epsilon_{n_2} + \epsilon_{n_2'} - \epsilon_{a} - \epsilon_{b}) (\epsilon_{n_3} + \epsilon_{n_3'} - \epsilon_{a} - \epsilon_{b})} + \sum_{gg'} \sum_{n_1 n_2 n_3} \sum_{n_1 n_2 n_3'} \frac{I_F^{(a_{n_1} - a_{n_1'}) n_2 c c'} I_F^{(a_{n_2} - a_{n_2'}) n_3 c c'} I_F^{(a_{n_3} - a_{n_3'}) n_1 c c'}}{(\epsilon_{n_1} + \epsilon_{n_1'} - \epsilon_{a'} - \epsilon_{a'} - \epsilon_{a} - \epsilon_{b}) (\epsilon_{n_2} + \epsilon_{n_2'} - \epsilon_{a} - \epsilon_{b}) (\epsilon_{n_3} + \epsilon_{n_3'} - \epsilon_{a} - \epsilon_{b})}, \]  

(22)
where the prime at the summation symbols indicates that the first summation does not run over states for which either the set \( \{ n_1, n_2, c \} \) or the set \( \{ n_1, n_3, c' \} \) are equivalent to the set \( \{ a, b, c \} \); the second summation does not run over the states for which the sets \( \{ n_1, n_2, c \} \) or \( \{ a', n_3, c' \} \) are equivalent to the set \( \{ a, b, c \} \) and the third summation does not run over the states for which the sets \( \{ n_1, n_2, b' \} \) or \( \{ n_1, n_3, b' \} \) are equivalent to the set \( \{ a, b, c \} \) (the cases of reference states). The reducible part of the third-order “step-box” corrections (see Fig. 5) can be cast into the form

\[
F^{(3)\text{(step-box, red)}}_{a'b'c'a'c'b} = \sum_{g'g''} \sum_{n_1n_2n_3} I^g_{a'b'c'1} I^{g'}_{b'n_3} I^{g''}_{c'n_2} I^{g''}_{1n_2ab} \\
\times \left\{ \frac{(-1)}{2(\varepsilon_{n_1} + \varepsilon_{n_3} - \varepsilon_{a'} - \varepsilon_{b'})^2} + \frac{(-1)}{2(\varepsilon_{n_1} + \varepsilon_{n_2} - \varepsilon_{a} - \varepsilon_{b})^2} \right\} \\
+ 2 \sum_{n_1n_2n_3} I^{g''}_{b'c'n_3} I^{g''}_{a'n_3} I^{g''}_{n_2} I^{g''}_{n_1n_2ab} \\
\times \left\{ \frac{(-1)}{2(\varepsilon_{n_1} + \varepsilon_{n_2} - \varepsilon_{a} - \varepsilon_{b})^2} + \frac{(-1)}{2(\varepsilon_{n_3} + \varepsilon_{a'} - \varepsilon_{a} - \varepsilon_{c'})^2} \right\} ,
\]

where the double prime at the summation symbols indicates that the summations run over the corresponding reference states only (see the explanations for Eq. (22)). It becomes evident that the contributions due to the graphs Fig. 5b, c are equal. Therefore, we account for them by taking twice the contribution of the graph Fig. 5b.

### III. NUMERICAL RESULTS AND DISCUSSION

The major result of the present work consists in the calculation of the two- and three-photon exchange corrections to the energy levels of two-electron configurations \(^2S_0\), \(^2P_0\), \(^2S_1\) and three-electron configurations \((1s)^22s_{1/2}\), \((1s)^22p_{1/2}\). The two-photon exchange correction represents the leading part of the perturbation theory in second order. Accordingly, the main uncertainty of the theoretical values calculated earlier has been due to this correction.

In order to represent the Coulomb potential of the nucleus we employ a Fermi model for the nuclear density distribution

\[
\rho(r) = \frac{N}{1 + \exp[(r - c)/a]},
\]

where \( N \) is a normalization constant, \( a = 0.5350 \text{ fm} \) and \( c \) is deduced via the equation

\[
4\pi \int_0^\infty \rho(r)r^4 \, dr = \langle r^2 \rangle ,
\]

where \( \langle r^2 \rangle^{1/2} \) is the root-mean-square nuclear radius. In Table 1 we also display the values for the nuclear root-mean-square radii employed in this work. They have been taken from [23]. For nuclei with charge numbers \( Z \) not presented in [23] we utilize the empirical formula [23]

\[
\langle r^2 \rangle^{1/2} = (0.836 A^{1/3} + 0.570) \text{ fm},
\]

where \( A \) is the atomic mass number.

The results of our calculation of the two-photon exchange correction are presented in Tables I, II, VI, VII for two-electron configurations and in Tables VI, IX, XI, XIX for three-electron configurations, respectively. Our calculation is performed rigorously within the framework of QED. For reasons of clarity the corresponding corrections referring to contributions of the Feynman graphs in Figs. 2 and 3 are also listed separately in these tables. For details concerning the numerical procedure we refer to [4]. The accuracy of the present calculations is on the level of about 0.0001 a.u.

We also have taken into account the dominant part of the three-photon exchange correction. Details of the approximation made were given in Sec. I. The results of the calculation for the three-photon exchange correction
are presented in Tables XII, XIII, XIV, XV, XVI, XVII for two-electron configurations and in Tables XVIII, XIX, XX, XXI for three-electron configurations, respectively. Again, the contribution due to the exchange of the various photons are compiled separately in the tables. The correction caused by the exchange of three Breit photons is not included since it was found to be less than 0.001 eV. In view of the approximation used to evaluate the three-photon exchange correction these values are given within an inaccuracy of about 10%.\[4\]

In Tables XXII, XXIII, XXIV, XXV, XXXI, XXXII, XXXIV, XXXV provide the most accurate theoretical predictions for the energy levels at present.

From the results presented in Table XXXVI one can conclude that the configurations $2^1S_0$ and $2^3P_0$ cross within the interval $60 < Z < 70$. Experimental investigation of PNC effects in heliumlike ions requires a precise knowledge of the energy difference between these levels at $Z = 63$.\[13\] UT theory\[1\] predicts a value for this difference of about 0.168 eV, while the calculation presented in this paper gives a larger value of 0.593 eV. However, our calculations predict that the crossing of these levels takes place near $Z = 66$ with an energy difference of about $-0.016$ eV. Nevertheless, the He-like Eu ion ($Z = 63$) seems most suitable for the search of PNC effects\[13\]. We also investigated the splitting $E(2^1S_0) - E(2^3P_0)$ for two isotopes $^{151}$Eu and $^{153}$Eu and obtained an energy difference 0.001 eV, which does not change the conclusions made in\[13\]. The present calculation also indicates that the other crossing point can be expected to be close to $Z = 89, 90$.

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TABLE I. The values of nuclear root-mean-square radii employed in this work.

|        | $^{142}$Nd | $^{152}$Sm | $^{153}$Eu | $^{155}$Gd | $^{159}$Tb | $^{165}$Dy | $^{166}$Er | $^{173}$Yb | $^{202}$Hg | $^{231}$Ta | $^{238}$U | $^{237}$Np |
|--------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| $(r^2)^{1/2}$ (fm) | 4.914      | 5.032      | 5.041      | 5.090      | 5.099      | 5.224      | 5.165      | 5.317      | 5.467      | 5.700      | 5.860      | 5.744      |

TABLE II. Different contributions to the second-order interelectron interaction for the two-electron configuration $1s_{1/2}2s_{1/2}$ (eV). The numbers in the Table present the ionization energy of the $2s_{1/2}$ electron with the opposite sign.

| Contribution       | $Z = 60$ | 62 | 63 | 64 | 65 | 66 | 68 | 70 |
|--------------------|----------|----|----|----|----|----|----|----|
| Coulomb-Coulomb    |          |    |    |    |    |    |    |    |
| $\Delta E_{\text{box,irr}}$ | -3.929   | -3.996 | -4.032 | -4.069 | -4.107 | -4.146 | -4.230 | -4.314 |
| $\Delta E_{\text{cross,irr}}$ | 0.019    | 0.021  | 0.022  | 0.023  | 0.024  | 0.025  | 0.028  | 0.030 |
| $\Delta E_{\text{total}}$    | -3.909   | -3.975 | -4.010 | -4.046 | -4.083 | -4.120 | -4.203 | -4.284 |
| Coulomb-Breit      |          |    |    |    |    |    |    |    |
| $\Delta E_{\text{box,irr}}$ | -1.195   | -1.287 | -1.335 | -1.384 | -1.435 | -1.487 | -1.595 | -1.709 |
| $\Delta E_{\text{box,red}}$ | 0.492    | 0.534  | 0.555  | 0.577  | 0.600  | 0.624  | 0.673  | 0.726 |
| $\Delta E_{\text{cross,irr}}$ | -0.064   | -0.066 | -0.066 | -0.067 | -0.068 | -0.071 | -0.075 | -0.079 |
| $\Delta E_{\text{cross,red}}$ | -0.055   | -0.062 | -0.065 | -0.069 | -0.072 | -0.076 | -0.084 | -0.093 |
| $\Delta E_{\text{total}}$    | -0.822   | -0.881 | -0.911 | -0.943 | -0.976 | -1.010 | -1.080 | -1.155 |
| Breit-Breit        |          |    |    |    |    |    |    |    |
| $\Delta E_{\text{box,irr}}$ | -0.105   | -0.119 | -0.126 | -0.133 | -0.141 | -0.148 | -0.164 | -0.183 |
| $\Delta E_{\text{box,red}}$ | 0.037    | 0.042  | 0.045  | 0.048  | 0.052  | 0.055  | 0.063  | 0.071 |
| $\Delta E_{\text{cross,irr}}$ | 0.017    | 0.018  | 0.020  | 0.022  | 0.025  | 0.027  | 0.030  | 0.033 |
| $\Delta E_{\text{cross,red}}$ | 0.001    | 0.002  | 0.002  | 0.002  | 0.002  | 0.003  | 0.003  | 0.003 |
| $\Delta E_{\text{total}}$    | -0.050   | -0.057 | -0.059 | -0.061 | -0.062 | -0.064 | -0.068 | -0.076 |
| Total              | -4.781   | -4.913 | -4.980 | -5.049 | -5.120 | -5.194 | -5.350 | -5.515 |

TABLE III. Different contributions to the second-order interelectron interaction for the two-electron configuration $1s_{1/2}2s_{1/2}$ (eV). The numbers in the Table present the ionization energy of the $2s_{1/2}$ electron with the opposite sign.

| Contribution       | $Z = 80$ | 91 | 92 | 93 |
|--------------------|----------|----|----|----|
| Coulomb-Coulomb    |          |    |    |    |
| $\Delta E_{\text{box,irr}}$ | -4.845   | -5.676 | -5.768 | -5.867 |
| $\Delta E_{\text{cross,irr}}$ | 0.046    | 0.071  | 0.074  | 0.077 |
| $\Delta E_{\text{total}}$    | -4.799   | -5.605 | -5.695 | -5.790 |
| Coulomb-Breit      |          |    |    |    |
| $\Delta E_{\text{box,irr}}$ | -2.375   | -3.391 | -3.499 | -3.618 |
| $\Delta E_{\text{box,red}}$ | 1.037    | 1.516  | 1.569  | 1.624 |
| $\Delta E_{\text{cross,irr}}$ | -0.108   | -0.138 | -0.140 | -0.145 |
| $\Delta E_{\text{cross,red}}$ | -0.146   | -0.232 | -0.242 | -0.252 |
| $\Delta E_{\text{total}}$    | -1.592   | -2.245 | -2.312 | -2.391 |
| Breit-Breit        |          |    |    |    |
| $\Delta E_{\text{box,irr}}$ | -0.302   | -0.508 | -0.528 | -0.554 |
| $\Delta E_{\text{box,red}}$ | 0.127    | 0.228  | 0.239  | 0.251 |
| $\Delta E_{\text{cross,irr}}$ | 0.055    | 0.087  | 0.093  | 0.098 |
| $\Delta E_{\text{cross,red}}$ | 0.007    | 0.013  | 0.014  | 0.014 |
| $\Delta E_{\text{total}}$    | -0.113   | -0.181 | -0.185 | -0.190 |
| Total              | -6.504   | -8.032 | -8.184 | -8.371 |
TABLE IV. Different contributions to the second-order interelectron interaction for the two-electron configuration $1s_{1/2}2p_{1/2}^3P_0$ (eV). The numbers in the Table present the ionization energy of the $2p_{1/2}$ electron with the opposite sign.

| Contribution          | $Z = 60$ | 62 | 63 | 64 | 65 | 66 | 68 | 70 |
|-----------------------|----------|----|----|----|----|----|----|----|
| **Coulomb-Coulomb**   |          |    |    |    |    |    |    |    |
| $\Delta E_{\text{box, irr}}$ | -2.748  | -2.813 | -2.847 | -2.882 | -2.918 | -2.956 | -3.035 | -3.118 |
| $\Delta E_{\text{cross, irr}}$ | 0.006  | 0.007 | 0.007 | 0.007 | 0.008 | 0.009 | 0.010 | 0.012 |
| $\Delta E_{\text{total}}$ | -2.743  | -2.806 | -2.840 | -2.875 | -2.910 | -2.947 | -3.024 | -3.107 |
| **Coulomb-Breit**     |          |    |    |    |    |    |    |    |
| $\Delta E_{\text{box, irr}}$ | -1.162  | -1.259 | -1.310 | -1.363 | -1.417 | -1.473 | -1.587 | -1.708 |
| $\Delta E_{\text{box, red}}$ | 0.048  | 0.053 | 0.056 | 0.059 | 0.062 | 0.065 | 0.071 | 0.079 |
| $\Delta E_{\text{cross, irr}}$ | -0.024  | -0.027 | -0.029 | -0.031 | -0.033 | -0.035 | -0.037 | -0.039 |
| $\Delta E_{\text{cross, red}}$ | -0.077  | -0.084 | -0.088 | -0.093 | -0.097 | -0.102 | -0.111 | -0.122 |
| $\Delta E_{\text{total}}$ | -1.214  | -1.317 | -1.372 | -1.428 | -1.486 | -1.545 | -1.664 | -1.789 |
| **Breit-Breit**       |          |    |    |    |    |    |    |    |
| $\Delta E_{\text{box, irr}}$ | -0.102  | -0.123 | -0.134 | -0.145 | -0.156 | -0.167 | -0.188 | -0.209 |
| $\Delta E_{\text{box, red}}$ | 0.002  | 0.003 | 0.003 | 0.003 | 0.004 | 0.004 | 0.005 | 0.005 |
| $\Delta E_{\text{cross, irr}}$ | -0.013  | -0.014 | -0.015 | -0.015 | -0.016 | -0.018 | -0.020 | -0.022 |
| $\Delta E_{\text{cross, red}}$ | 0.002  | 0.002 | 0.003 | 0.003 | 0.003 | 0.003 | 0.004 | 0.004 |
| $\Delta E_{\text{total}}$ | -0.111  | -0.132 | -0.143 | -0.154 | -0.165 | -0.177 | -0.199 | -0.222 |
| **Total**             |          |    |    |    |    |    |    |    |
| $\Delta E$            | -4.068  | -4.256 | -4.354 | -4.456 | -4.561 | -4.670 | -4.888 | -5.117 |

TABLE V. Different contributions to the second-order interelectron interaction for the two-electron configuration $1s_{1/2}2p_{1/2}^3P_0$ (eV). The numbers in the Table present the ionization energy of the $2p_{1/2}$ electron with the opposite sign.

| Contribution          | $Z = 80$ | 91 | 92 | 93 |
|-----------------------|----------|----|----|----|
| **Coulomb-Coulomb**   |          |    |    |    |
| $\Delta E_{\text{box, irr}}$ | -3.636  | -4.472 | -4.567 | -4.667 |
| $\Delta E_{\text{cross, irr}}$ | 0.022  | 0.042 | 0.044 | 0.047 |
| $\Delta E_{\text{total}}$ | -3.614  | -4.430 | -4.523 | -4.620 |
| **Coulomb-Breit**     |          |    |    |    |
| $\Delta E_{\text{box, irr}}$ | -2.475  | -3.670 | -3.810 | -3.949 |
| $\Delta E_{\text{box, red}}$ | 0.124  | 0.199 | 0.208 | 0.216 |
| $\Delta E_{\text{cross, irr}}$ | -0.053  | -0.070 | -0.072 | -0.073 |
| $\Delta E_{\text{cross, red}}$ | -0.187  | -0.302 | -0.310 | -0.323 |
| $\Delta E_{\text{total}}$ | -2.590  | -3.842 | -3.985 | -4.128 |
| **Breit-Breit**       |          |    |    |    |
| $\Delta E_{\text{box, irr}}$ | -0.377  | -0.695 | -0.743 | -0.790 |
| $\Delta E_{\text{box, red}}$ | 0.011  | 0.023 | 0.025 | 0.026 |
| $\Delta E_{\text{cross, irr}}$ | -0.036  | -0.064 | -0.066 | -0.068 |
| $\Delta E_{\text{cross, red}}$ | 0.008  | 0.017 | 0.018 | 0.020 |
| $\Delta E_{\text{total}}$ | -0.394  | -0.718 | -0.766 | -0.811 |
| **Total**             |          |    |    |    |
| $\Delta E$            | -6.598  | -8.991 | -9.274 | -9.560 |
TABLE VI. Different contributions to the second-order interelectron interaction for the two-electron configuration \(1s_{1/2}2s_{1/2}\) \(^3S_1\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution | \(Z = 60\) | \(Z = 62\) | \(Z = 63\) | \(Z = 64\) | \(Z = 65\) | \(Z = 66\) | \(Z = 68\) | \(Z = 70\) |
|--------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| \(\Delta E_{\text{box,irr}}\) | -1.535 | -1.555 | -1.565 | -1.575 | -1.586 | -1.597 | -1.620 | -1.643 |
| \(\Delta E_{\text{cross,irr}}\) | 0.001 | 0.002 | 0.002 | 0.002 | 0.002 | 0.002 | 0.002 | 0.003 |
| \(\Delta E_{\text{total}}\) | -1.534 | -1.553 | -1.563 | -1.574 | -1.584 | -1.595 | -1.617 | -1.641 |
| Coulomb-Breit | | | | | | | | |
| \(\Delta E_{\text{box,irr}}\) | -0.006 | -0.007 | -0.007 | -0.007 | -0.008 | -0.008 | -0.008 | -0.008 |
| \(\Delta E_{\text{cross,irr}}\) | -0.005 | -0.006 | -0.007 | -0.007 | -0.008 | -0.008 | -0.008 | -0.008 |
| \(\Delta E_{\text{total}}\) | -0.013 | -0.015 | -0.016 | -0.016 | -0.018 | -0.018 | -0.019 | -0.019 |
| Breit-Breit | | | | | | | | |
| \(\Delta E_{\text{box,irr}}\) | 0.001 | 0.001 | 0.001 | 0.002 | 0.003 | 0.003 | 0.003 | 0.004 |
| \(\Delta E_{\text{cross,irr}}\) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| \(\Delta E_{\text{total}}\) | 0.005 | 0.006 | 0.007 | 0.008 | 0.008 | 0.009 | 0.010 | 0.012 |
| Total | \(\Delta E\) | -1.542 | -1.562 | -1.572 | -1.582 | -1.593 | -1.605 | -1.626 | -1.648 |

TABLE VII. Different contributions to the second-order interelectron interaction for the two-electron configuration \(1s_{1/2}2s_{1/2}\) \(^3S_1\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution | \(Z = 80\) | \(Z = 91\) | \(Z = 92\) | \(Z = 93\) |
|--------------|-------------|-------------|-------------|-------------|
| Coulomb-Coulomb | | | | |
| \(\Delta E_{\text{box,irr}}\) | -1.785 | -1.995 | -2.017 | -2.041 |
| \(\Delta E_{\text{cross,irr}}\) | 0.005 | 0.008 | 0.009 | 0.009 |
| \(\Delta E_{\text{total}}\) | -1.780 | -1.986 | -2.009 | -2.032 |
| Coulomb-Breit | | | | |
| \(\Delta E_{\text{box,irr}}\) | -0.010 | -0.011 | -0.012 | -0.012 |
| \(\Delta E_{\text{cross,irr}}\) | -0.009 | -0.015 | -0.015 | -0.016 |
| \(\Delta E_{\text{total}}\) | -0.024 | -0.032 | -0.032 | -0.033 |
| Breit-Breit | | | | |
| \(\Delta E_{\text{box,irr}}\) | 0.004 | 0.005 | 0.005 | 0.006 |
| \(\Delta E_{\text{cross,irr}}\) | 0.011 | 0.017 | 0.018 | 0.017 |
| \(\Delta E_{\text{total}}\) | 0.015 | 0.024 | 0.024 | 0.025 |
| Total | \(\Delta E\) | -1.789 | -1.995 | -2.018 | -2.040 |
TABLE VIII. Different contributions to the second-order interelectron interaction for the three-electron configuration \((1s)^22s_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution | \(Z = 60\) | 62 | 63 | 64 | 65 | 66 | 68 | 70 |
|--------------|-----------|----|----|----|----|----|----|----|
| Coulomb-Coulomb | \(\Delta E_{\text{box},\text{irr}}\) | -4.267 | -4.330 | -4.363 | -4.397 | -4.432 | -4.468 | -4.546 | -4.622 |
| | \(\Delta E_{\text{cross},\text{irr}}\) | 0.012 | 0.013 | 0.013 | 0.014 | 0.015 | 0.016 | 0.017 | 0.019 |
| | \(\Delta E_{\text{step},\text{irr}}\) | -4.046 | -4.104 | -4.134 | -4.165 | -4.197 | -4.229 | -4.298 | -4.370 |
| | \(\Delta E_{\text{total}}\) | -8.302 | -8.421 | -8.484 | -8.548 | -8.614 | -8.682 | -8.826 | -8.974 |
| Coulomb-Breit | \(\Delta E_{\text{box},\text{red}}\) | -0.806 | -0.653 | -0.678 | -0.703 | -0.729 | -0.755 | -0.809 | -0.866 |
| | \(\Delta E_{\text{cross},\text{irr}}\) | 0.243 | 0.263 | 0.274 | 0.285 | 0.296 | 0.308 | 0.332 | 0.357 |
| | \(\Delta E_{\text{cross},\text{red}}\) | -0.033 | -0.041 | -0.042 | -0.044 | -0.045 | -0.046 | -0.049 | -0.051 |
| | \(\Delta E_{\text{step},\text{irr}}\) | -0.027 | -0.030 | -0.032 | -0.033 | -0.035 | -0.037 | -0.041 | -0.045 |
| | \(\Delta E_{\text{step},\text{red}}\) | -0.171 | -0.184 | -0.191 | -0.197 | -0.204 | -0.212 | -0.226 | -0.242 |
| | \(\Delta E_{\text{total}}\) | -0.640 | -0.690 | -0.715 | -0.742 | -0.768 | -0.795 | -0.851 | -0.909 |
| Breit-Breit | \(\Delta E_{\text{box},\text{irr}}\) | -0.051 | -0.057 | -0.061 | -0.064 | -0.067 | -0.071 | -0.078 | -0.088 |
| | \(\Delta E_{\text{box},\text{red}}\) | 0.018 | 0.021 | 0.023 | 0.025 | 0.026 | 0.028 | 0.031 | 0.035 |
| | \(\Delta E_{\text{cross},\text{irr}}\) | 0.015 | 0.016 | 0.017 | 0.018 | 0.018 | 0.020 | 0.022 | 0.024 |
| | \(\Delta E_{\text{cross},\text{red}}\) | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.002 | 0.002 |
| | \(\Delta E_{\text{step},\text{irr}}\) | 0.008 | 0.009 | 0.009 | 0.010 | 0.011 | 0.012 | 0.013 | 0.015 |
| | \(\Delta E_{\text{step},\text{red}}\) | -0.003 | -0.003 | -0.003 | -0.004 | -0.004 | -0.004 | -0.005 | -0.006 |
| | \(\Delta E_{\text{total}}\) | -0.012 | -0.013 | -0.013 | -0.013 | -0.013 | -0.013 | -0.013 | -0.014 |
| Total | \(\Delta E\) | -8.954 | -9.124 | -9.213 | -9.303 | -9.395 | -9.490 | -9.690 | -9.898 |

TABLE IX. Different contributions to the second-order interelectron interaction for the three-electron configuration \((1s)^22s_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution | \(Z = 80\) | 91 | 92 | 93 |
|--------------|-----------|----|----|----|
| Coulomb-Coulomb | \(\Delta E_{\text{box},\text{irr}}\) | -5.100 | -5.830 | -5.910 | -5.995 |
| | \(\Delta E_{\text{cross},\text{irr}}\) | 0.030 | 0.048 | 0.050 | 0.052 |
| | \(\Delta E_{\text{step},\text{irr}}\) | -4.802 | -5.455 | -5.526 | -5.601 |
| | \(\Delta E_{\text{total}}\) | -9.872 | -11.238 | -11.386 | -11.543 |
| Coulomb-Breit | \(\Delta E_{\text{box},\text{irr}}\) | -1.202 | -1.712 | -1.771 | -1.825 |
| | \(\Delta E_{\text{box},\text{red}}\) | 0.509 | 0.743 | 0.768 | 0.795 |
| | \(\Delta E_{\text{cross},\text{irr}}\) | -0.089 | -0.092 | -0.092 | -0.095 |
| | \(\Delta E_{\text{cross},\text{red}}\) | -0.071 | -0.111 | -0.115 | -0.120 |
| | \(\Delta E_{\text{step},\text{irr}}\) | -0.330 | -0.453 | -0.465 | -0.478 |
| | \(\Delta E_{\text{step},\text{red}}\) | -0.094 | -0.144 | -0.149 | -0.155 |
| | \(\Delta E_{\text{total}}\) | -1.256 | -1.768 | -1.824 | -1.879 |
| Breit-Breit | \(\Delta E_{\text{box},\text{irr}}\) | -0.143 | -0.245 | -0.253 | -0.267 |
| | \(\Delta E_{\text{box},\text{red}}\) | 0.064 | 0.114 | 0.120 | 0.126 |
| | \(\Delta E_{\text{cross},\text{irr}}\) | 0.044 | 0.071 | 0.075 | 0.078 |
| | \(\Delta E_{\text{cross},\text{red}}\) | 0.004 | 0.009 | 0.009 | 0.010 |
| | \(\Delta E_{\text{step},\text{irr}}\) | 0.027 | 0.049 | 0.052 | 0.054 |
| | \(\Delta E_{\text{step},\text{red}}\) | -0.010 | -0.019 | -0.020 | -0.021 |
| | \(\Delta E_{\text{total}}\) | -0.015 | -0.021 | -0.017 | -0.019 |
| Total | \(\Delta E\) | -11.143 | -13.028 | -13.228 | -13.441 |
### Table X

Different contributions to the second-order interelectron interaction for the three-electron configuration \((1s)^22p_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2p_{1/2}\) electron with the opposite sign.

| Contribution          | Z = 60 | 62 | 63 | 64 | 65 | 66 | 68 | 70 |
|-----------------------|--------|----|----|----|----|----|----|----|
| Coulomb-Coulomb       |        |    |    |    |    |    |    |    |
| \(\Delta E_{\text{box,irr}}\) | -8.253 | -8.276 | -8.294 | -8.317 | -8.345 | -8.378 | -8.456 | -8.552 |
| \(\Delta E_{\text{cross,irr}}\) | 0.013  | 0.015 | 0.016 | 0.017 | 0.018 | 0.019 | 0.021 | 0.024 |
| \(\Delta E_{\text{step,irr}}\) | -5.202 | -5.462 | -5.591 | -5.721 | -5.851 | -5.981 | -6.244 | -6.512 |
| \(\Delta E_{\text{total}}\) | -13.443 | -13.723 | -13.870 | -14.022 | -14.178 | -14.340 | -14.679 | -15.040 |
| Coulomb-Breit         |        |    |    |    |    |    |    |    |
| \(\Delta E_{\text{box,irr}}\) | 0.226  | 0.170 | 0.137 | 0.102 | 0.066 | 0.029 | -0.047 | -0.131 |
| \(\Delta E_{\text{box,red}}\) | 0.023  | 0.024 | 0.026 | 0.027 | 0.028 | 0.029 | 0.032 | 0.034 |
| \(\Delta E_{\text{cross,irr}}\) | -0.026 | -0.029 | -0.031 | -0.033 | -0.035 | -0.037 | -0.040 | -0.042 |
| \(\Delta E_{\text{cross,red}}\) | -0.048 | -0.052 | -0.054 | -0.057 | -0.059 | -0.061 | -0.066 | -0.072 |
| \(\Delta E_{\text{step,irr}}\) | -1.766 | -1.823 | -1.853 | -1.883 | -1.915 | -1.948 | -2.016 | -2.088 |
| \(\Delta E_{\text{step,red}}\) | -0.075 | -0.082 | -0.086 | -0.089 | -0.093 | -0.097 | -0.105 | -0.114 |
| \(\Delta E_{\text{total}}\) | -1.666 | -1.792 | -1.862 | -1.934 | -2.008 | -2.085 | -2.242 | -2.413 |
| Breit-Breit           |        |    |    |    |    |    |    |    |
| \(\Delta E_{\text{box,irr}}\) | -0.112 | -0.130 | -0.138 | -0.145 | -0.152 | -0.158 | -0.170 | -0.184 |
| \(\Delta E_{\text{box,red}}\) | 0.001  | 0.001 | 0.002 | 0.002 | 0.002 | 0.002 | 0.002 | 0.003 |
| \(\Delta E_{\text{cross,irr}}\) | 0.004  | 0.007 | 0.009 | 0.011 | 0.013 | 0.016 | 0.023 | 0.030 |
| \(\Delta E_{\text{cross,red}}\) | 0.002  | 0.003 | 0.003 | 0.003 | 0.003 | 0.003 | 0.004 | 0.004 |
| \(\Delta E_{\text{step,irr}}\) | 0.119  | 0.125 | 0.127 | 0.130 | 0.132 | 0.135 | 0.140 | 0.145 |
| \(\Delta E_{\text{step,red}}\) | 0.003  | 0.003 | 0.003 | 0.003 | 0.004 | 0.004 | 0.004 | 0.005 |
| \(\Delta E_{\text{total}}\) | 0.017  | 0.009 | 0.006 | 0.005 | 0.004 | 0.003 | 0.003 | 0.003 |
| Total                 |        |    |    |    |    |    |    |    |
| \(\Delta E\)          | -15.092 | -15.506 | -15.726 | -15.951 | -16.182 | -16.422 | -16.919 | -17.450 |

### Table XI

Different contributions to the second-order interelectron interaction for the three-electron configuration \((1s)^22p_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2p_{1/2}\) electron with the opposite sign.

| Contribution          | Z = 80 | 91 | 92 | 93 |
|-----------------------|--------|----|----|----|
| Coulomb-Coulomb       |        |    |    |    |
| \(\Delta E_{\text{box,irr}}\) | -9.313 | -10.792 | -10.968 | -11.155 |
| \(\Delta E_{\text{cross,irr}}\) | 0.043  | 0.078 | 0.082 | 0.087 |
| \(\Delta E_{\text{step,irr}}\) | -7.984 | -10.080 | -10.309 | -10.548 |
| \(\Delta E_{\text{total}}\) | -17.254 | -20.794 | -21.195 | -21.616 |
| Coulomb-Breit         |        |    |    |    |
| \(\Delta E_{\text{box,irr}}\) | -0.619 | -1.366 | -1.446 | -1.532 |
| \(\Delta E_{\text{box,red}}\) | 0.051  | 0.078 | 0.081 | 0.084 |
| \(\Delta E_{\text{cross,irr}}\) | -0.060 | -0.082 | -0.078 | -0.084 |
| \(\Delta E_{\text{cross,red}}\) | -0.105 | -0.166 | -0.166 | -0.174 |
| \(\Delta E_{\text{step,irr}}\) | -2.524 | -3.195 | -3.269 | -3.346 |
| \(\Delta E_{\text{step,red}}\) | -0.173 | -0.278 | -0.291 | -0.304 |
| \(\Delta E_{\text{total}}\) | -3.430 | -5.009 | -5.170 | -5.357 |
| Breit-Breit           |        |    |    |    |
| \(\Delta E_{\text{box,irr}}\) | -0.389 | -0.567 | -0.585 | -0.622 |
| \(\Delta E_{\text{box,red}}\) | 0.005  | 0.011 | 0.012 | 0.013 |
| \(\Delta E_{\text{cross,irr}}\) | 0.056  | 0.113 | 0.118 | 0.123 |
| \(\Delta E_{\text{cross,red}}\) | 0.009  | 0.017 | 0.018 | 0.019 |
| \(\Delta E_{\text{step,irr}}\) | 0.168  | 0.189 | 0.191 | 0.193 |
| \(\Delta E_{\text{step,red}}\) | 0.009  | 0.014 | 0.014 | 0.015 |
| \(\Delta E_{\text{total}}\) | -0.143 | -0.223 | -0.232 | -0.259 |
| Total                 |        |    |    |    |
| \(\Delta E\)          | -20.827 | -26.027 | -26.597 | -27.232 |
TABLE XII. Different contributions to the third-order interelectron interaction for the two-electron configuration \(1s_{1/2}2s_{1/2}^1S_0\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution              | \(Z = 60\) | 62  | 63  | 64  | 65  | 66  | 68  | 70  |
|---------------------------|------------|-----|-----|-----|-----|-----|-----|-----|
| Coulomb-Coulomb-Coulomb   | 0.010      | 0.010 | 0.010 | 0.010 | 0.010 | 0.010 | 0.010 | 0.010 |
| Coulomb-Coulomb-Breit     | 0.011      | 0.011 | 0.011 | 0.012 | 0.012 | 0.012 | 0.013 | 0.013 |
| Coulomb-Breit-Breit       | 0.005      | 0.005 | 0.005 | 0.005 | 0.006 | 0.006 | 0.006 | 0.006 |
| Total                     | 0.026      | 0.026 | 0.026 | 0.027 | 0.027 | 0.028 | 0.029 | 0.029 |

TABLE XIII. Different contributions to the third-order interelectron interaction for the two-electron configuration \(1s_{1/2}2s_{1/2}^1S_0\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution              | \(Z = 80\) | 91  | 92  | 93  |
|---------------------------|------------|-----|-----|-----|
| Coulomb-Coulomb-Coulomb   | 0.012      | 0.016 | 0.016 | 0.017 |
| Coulomb-Coulomb-Breit     | 0.016      | 0.022 | 0.022 | 0.023 |
| Coulomb-Breit-Breit       | 0.008      | 0.011 | 0.012 | 0.012 |
| Total                     | 0.036      | 0.049 | 0.050 | 0.052 |

TABLE XIV. Different contributions to the third-order interelectron interaction for the two-electron configuration \(1s_{1/2}2p_{1/2}^3P_0\) (eV). The numbers in the Table present the ionization energy of the \(2p_{1/2}\) electron with the opposite sign.

| Contribution              | \(Z = 60\) | 62  | 63  | 64  | 65  | 66  | 68  | 70  |
|---------------------------|------------|-----|-----|-----|-----|-----|-----|-----|
| Coulomb-Coulomb-Coulomb   | -0.005     | -0.004 | -0.004 | -0.004 | -0.004 | -0.003 | -0.003 | -0.003 |
| Coulomb-Coulomb-Breit     | 0.011      | 0.012 | 0.012 | 0.013 | 0.014 | 0.014 | 0.015 | 0.015 |
| Coulomb-Breit-Breit       | 0.006      | 0.005 | 0.005 | 0.006 | 0.006 | 0.006 | 0.007 | 0.008 |
| Total                     | 0.013      | 0.013 | 0.014 | 0.015 | 0.016 | 0.017 | 0.019 | 0.020 |

TABLE XV. Different contributions to the third-order interelectron interaction for the two-electron configuration \(1s_{1/2}2p_{1/2}^3P_0\) (eV). The numbers in the Table present the ionization energy of the \(2p_{1/2}\) electron with the opposite sign.

| Contribution              | \(Z = 80\) | 91  | 92  | 93  |
|---------------------------|------------|-----|-----|-----|
| Coulomb-Coulomb-Coulomb   | 0.000      | 0.004 | 0.004 | 0.005 |
| Coulomb-Coulomb-Breit     | 0.021      | 0.032 | 0.033 | 0.034 |
| Coulomb-Breit-Breit       | 0.013      | 0.020 | 0.021 | 0.022 |
| Total                     | 0.034      | 0.056 | 0.058 | 0.061 |

TABLE XVI. Different contributions to the third-order interelectron interaction for the two-electron configuration \(1s_{1/2}2s_{1/2}^3S_1\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution              | \(Z = 60\) | 62  | 63  | 64  | 65  | 66  | 68  | 70  |
|---------------------------|------------|-----|-----|-----|-----|-----|-----|-----|
| Coulomb-Coulomb-Coulomb   | -0.001     | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 |
| Coulomb-Coulomb-Breit     | 0.001      | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| Coulomb-Breit-Breit       | 0.000      | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| Total                     | -0.001     | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 |
TABLE XVII. Different contributions to the third-order interelectron interaction for the two-electron configuration $1s_{1/2}2s_{1/2}^3S_1$ (eV). The numbers in the Table present the ionization energy of the $2s_{1/2}$ electron with the opposite sign.

| Contribution | Z = 80 | 91 | 92 | 93 |
|--------------|--------|----|----|----|
| Coulomb-Coulomb-Coulomb | -0.001 | 0.000 | 0.000 | 0.000 |
| Coulomb-Coulomb-Breit | 0.001 | 0.001 | 0.001 | 0.001 |
| Coulomb-Breit-Breit | 0.000 | 0.000 | 0.000 | 0.000 |
| Total | 0.000 | 0.001 | 0.001 | 0.001 |

TABLE XVIII. Different contributions to the third-order interelectron interaction for the three-electron configuration $(1s)^22s_{1/2}$ (eV). The numbers in the Table present the ionization energy of the $2s_{1/2}$ electron with the opposite sign.

| Contribution | Z = 60 | 62 | 63 | 64 | 65 | 66 | 68 | 70 |
|--------------|--------|----|----|----|----|----|----|----|
| Coulomb-Coulomb-Coulomb | 0.003 | 0.004 | 0.004 | 0.005 | 0.006 | 0.006 | 0.007 | 0.008 |
| Coulomb-Coulomb-Breit | 0.014 | 0.014 | 0.015 | 0.016 | 0.016 | 0.016 | 0.016 | 0.017 |
| Coulomb-Breit-Breit | 0.002 | 0.003 | 0.004 | 0.005 | 0.006 | 0.006 | 0.006 | 0.006 |
| Total | 0.018 | 0.021 | 0.023 | 0.025 | 0.027 | 0.028 | 0.029 | 0.031 |

TABLE XIX. Different contributions to the third-order interelectron interaction for the three-electron configuration $(1s)^22s_{1/2}$ (eV). The numbers in the Table present the ionization energy of the $2s_{1/2}$ electron with the opposite sign.

| Contribution | Z = 80 | 91 | 92 | 93 |
|--------------|--------|----|----|----|
| Coulomb-Coulomb-Coulomb | 0.015 | 0.025 | 0.026 | 0.027 |
| Coulomb-Coulomb-Breit | 0.021 | 0.028 | 0.029 | 0.030 |
| Coulomb-Breit-Breit | 0.007 | 0.011 | 0.011 | 0.012 |
| Total | 0.043 | 0.064 | 0.066 | 0.069 |

TABLE XX. Different contributions to the third-order interelectron interaction for the three-electron configuration $(1s)^22p_{1/2}$ (eV). The numbers in the Table present the ionization energy of the $2p_{1/2}$ electron with the opposite sign.

| Contribution | Z = 60 | 62 | 63 | 64 | 65 | 66 | 68 | 70 |
|--------------|--------|----|----|----|----|----|----|----|
| Coulomb-Coulomb-Coulomb | 0.002 | 0.005 | 0.007 | 0.009 | 0.011 | 0.013 | 0.016 | 0.019 |
| Coulomb-Coulomb-Breit | 0.049 | 0.051 | 0.053 | 0.054 | 0.055 | 0.056 | 0.058 | 0.059 |
| Coulomb-Breit-Breit | 0.010 | 0.011 | 0.011 | 0.011 | 0.011 | 0.012 | 0.012 | 0.012 |
| Total | 0.061 | 0.067 | 0.071 | 0.074 | 0.077 | 0.080 | 0.085 | 0.090 |

TABLE XXI. Different contributions to the third-order interelectron interaction for the three-electron configuration $(1s)^22p_{1/2}$ (eV). The numbers in the Table present the ionization energy of the $2p_{1/2}$ electron with the opposite sign.

| Contribution | Z = 80 | 91 | 92 | 93 |
|--------------|--------|----|----|----|
| Coulomb-Coulomb-Coulomb | 0.041 | 0.079 | 0.083 | 0.088 |
| Coulomb-Coulomb-Breit | 0.084 | 0.116 | 0.119 | 0.124 |
| Coulomb-Breit-Breit | 0.017 | 0.030 | 0.031 | 0.033 |
| Total | 0.142 | 0.225 | 0.233 | 0.245 |
TABLE XXII. Different contributions to the total energy of the two-electron configuration 1s\(^1/2\)2s\(^1/2\)\(^1\)S\(_0\) (eV). The numbers in the Table present the ionization energy of the 2s\(^1/2\) electron with the opposite sign.

| Contribution          | Z = 60       | 62       | 63       | 64       | Ref. |
|-----------------------|--------------|----------|----------|----------|------|
| Zero-order            | −13063.004   | −14015.106 | −14506.589 | −15008.567 | TW   |
| Nuclear size (NS)     | 0.928        | 1.201    | 1.342    | 1.519    | TW   |
| First-order interelectron interaction | 438.812 | 458.300 | 468.260 | 478.371 | TW   |
| Second-order interelectron interaction | −4.781 | −4.913 | −4.980 | −5.049 | TW   |
| Third-order interelectron interaction | 0.026 | 0.026 | 0.026 | 0.027 | TW   |
| SE with NS            | 11.409       | 12.896   | 13.700   | 14.544   |       |
| VP with NS            | −1.621       | −1.893   | −2.042   | −2.201   |       |
| SE screening          | −0.257       | −0.289   | −0.304   | −0.320   |       |
| VP screening          | 0.100        | 0.113    | 0.120    | 0.126    |       |
| Recoil                | 0.055        | 0.057    | 0.058    | 0.059    |       |
| Total                 | −12618.333   | −13549.608 | −14030.409 | −14521.491 | TW   |

TABLE XXIII. Different contributions to the total energy of the two-electron configuration 1s\(^1/2\)2s\(^1/2\)\(^1\)S\(_0\) (eV). The numbers in the Table present the ionization energy of the 2s\(^1/2\) electron with the opposite sign.

| Contribution          | Z = 65       | 66       | 68       | 70       | Ref. |
|-----------------------|--------------|----------|----------|----------|------|
| Zero-order            | −15521.201   | −16044.661 | −17124.764 | −18250.361 | TW   |
| Nuclear size (NS)     | 1.696        | 1.968    | 2.386    | 3.099    | TW   |
| First-order interelectron interaction | 488.637 | 499.061 | 520.422 | 542.484 | TW   |
| Second-order interelectron interaction | −5.120 | −5.194 | −5.350 | −5.515 | TW   |
| Third-order interelectron interaction | 0.027 | 0.028 | 0.029 | 0.029 | TW   |
| SE with NS            | 15.427       | 16.358   | 18.363   | 20.589   |       |
| VP with NS            | −2.374       | −2.557   | −2.962   | −3.419   |       |
| SE screening          | −0.335       | −0.351   | −0.382   | −0.413   |       |
| VP screening          | 0.133        | 0.139    | 0.164    | 0.188    |       |
| Recoil                | 0.060        | 0.061    | 0.064    | 0.067    |       |
| Total                 | −15023.050   | −15535.148 | −16592.030 | −17693.252 | TW   |
TABLE XXIV. Different contributions to the total energy of the two-electron configuration 1s_{1/2}2s_{1/2} 1S_0 (eV). The numbers in the Table present the ionization energy of the 2s_{1/2} electron with the opposite sign.

| Contribution          | Z = 80  | 91    | 92    | 93    | Ref. |
|-----------------------|---------|-------|-------|-------|------|
| Zero-order            | −24622.160 | −33320.132 | −34215.481 | −35130.460 | TW   |
| Nuclear size (NS)     | 9.34    | 32.50 | 37.76 | 40.94 | TW   |
| First-order           |         |       |       |       |      |
| interelectron         | 665.38  | 832.758 | 850.116 | 868.029 | TW   |
| interaction           |         |       |       |       |      |
| Second-order          |         |       |       |       |      |
| interelectron         | −6.504  | −8.032 | −8.184 | −8.371 | TW   |
| interaction           |         |       | −8.2131 |       |      |
| Third-order           |         |       |       |       |      |
| interelectron         | 0.038   | 0.049 | 0.052 | 0.052 | TW   |
| interaction           |         |       |       |       |      |
| SE with NS            | 35.3911 | 62.226 | 65.4183 | 68.739 | TW   |
| VP with NS            | −6.900  | −14.632 | −15.658 | −16.770 | TW   |
| SE screening          | −0.651  | −1.087 | −1.127 | −1.167 | TW   |
| VP screening          | 0.354   | 0.729 | 0.777 | 0.825 | TW   |
| Recoil                | 0.086   | 0.122 | 0.127 | 0.132 | TW   |
| Total                 | −23925.626 | −32415.499 | −33286.200 | −34178.051 | TW   |

TABLE XXV. Different contributions to the total energy of the two-electron configuration 1s_{1/2}2p_{1/2} 3P_0 (eV). The numbers in the Table present the ionization energy of the 2p_{1/2} electron with the opposite sign.

| Contribution          | Z = 60  | 62    | 63    | 64    | Ref. |
|-----------------------|---------|-------|-------|-------|------|
| Zero-order            | −13063.004 | −14015.106 | −14506.589 | −15008.567 | TW   |
| Nuclear size (NS)     | 0.038   | 0.052 | 0.061 | 0.071 | TW   |
| First-order           |         |       |       |       |      |
| interelectron         | 447.329 | 468.642 | 479.586 | 490.731 | TW   |
| interaction           |         |       |       |       |      |
| Second-order          |         |       |       |       |      |
| interelectron         | −4.068  | −4.256 | −4.354 | −4.456 | TW   |
| interaction           | −4.0645 |       |       |       |      |
| Third-order           |         |       |       |       |      |
| interelectron         | 0.013   | 0.013 | 0.014 | 0.015 | TW   |
| interaction           |         |       |       |       |      |
| SE with NS            | 0.298   | 0.406 | 0.469 | 0.539 | TW   |
| VP with NS            | −0.098  | −0.124 | −0.139 | −0.155 | TW   |
| SE screening          | −0.112  | −0.133 | −0.144 | −0.155 | TW   |
| VP screening          | 0.035   | 0.039 | 0.042 | 0.044 | TW   |
| Recoil                | 0.050   | 0.051 | 0.052 | 0.052 | TW   |
| Total                 | −12619.519 | −13550.416 | −14031.002 | −14521.881 | TW   |
TABLE XXVI. Different contributions to the total energy of the two-electron configuration $1s_{1/2}2p_{1/2}^3P_0$ (eV). The numbers in the Table present the ionization energy of the $2p_{1/2}$ electron with the opposite sign.

| Contribution                      | $Z = 65$       | 66   | 68   | 70   | Ref. |
|-----------------------------------|----------------|------|------|------|------|
| Zero-order                        | $-15521.201$   |      |      |      |      |
| Nuclear size (NS)                 | 0.083          | 0.099| 0.129| 0.180| TW   |
| First-order interelectron         | 502.083        | 513.649| 537.458| 562.218| TW   |
| Interaction                       |                |      |      |      |      |
| Second-order interelectron        |                |      |      |      |      |
| Interaction                       |                |      |      |      |      |
| Third-order interelectron         |                |      |      |      |      |
| Interaction                       |                |      |      |      |      |
| SE with NS                        | 0.016          | 0.017| 0.019| 0.020| TW   |
| VP with NS                        |                |      |      |      |      |
| SE screening                      |                |      |      |      |      |
| VP screening                      |                |      |      |      |      |
| Recoil                            |                |      |      |      |      |
| Total                             | $-15023.203$   | $-15535.132$| $-16591.468$| $-17692.311$| TW   |

TABLE XXVII. Different contributions to the total energy of the two-electron configuration $1s_{1/2}2p_{1/2}^3P_0$ (eV). The numbers in the Table present the ionization energy of the $2p_{1/2}$ electron with the opposite sign.

| Contribution                      | $Z = 80$       | 91   | 92   | 93   | Ref. |
|-----------------------------------|----------------|------|------|------|------|
| Zero-order                        | $-24622.160$   |      |      |      |      |
| Nuclear size (NS)                 | 0.75           | 3.68 | 4.41 | 4.93 | TW   |
| First-order interelectron         | 702.993        | 902.031| 923.176| 944.984| TW   |
| Interaction                       |                |      |      |      |      |
| Second-order interelectron        |                |      |      |      |      |
| Interaction                       |                |      |      |      |      |
| Third-order interelectron         |                |      |      |      |      |
| Interaction                       |                |      |      |      |      |
| SE with NS                        | 0.034          | 0.056| 0.058| 0.061| TW   |
| VP with NS                        |                |      |      |      |      |
| SE screening                      |                |      |      |      |      |
| VP screening                      |                |      |      |      |      |
| Recoil                            |                |      |      |      |      |
| Total                             | $-23922.785$   | $-32417.470$| $-33290.711$| $-34183.109$| TW   |
TABLE XXVIII. Different contributions to the total energy of the two-electron configuration 1s_{1/2}2s_{1/2}^{3}S_{1} (eV). The numbers in the Table present the ionization energy of the 2s_{1/2} electron with the opposite sign.

| Contribution          | Z = 60  | 62     | 63     | 64     | Ref. |
|-----------------------|---------|--------|--------|--------|------|
| Zero-order            | −13063.004 | −14015.106 | −14506.589 | −15008.567 | TW   |
| Nuclear size (NS)     | 0.928   | 1.201  | 1.342  | 1.519  | TW   |
| First-order           |         |        |        |        |      |
| interelectront        | 333.849 | 347.123 | 353.854 | 360.649 | TW   |
| interaction           |         |        |        |        |      |
| Second-order          |         |        |        |        |      |
| interelectront        | −1.542  | −1.562  | −1.572  | −1.582  | TW   |
| interaction           | −1.5455 |        |        |        |      |
| Third-order           |         |        |        |        |      |
| interelectront        | −0.001  | −0.001  | −0.001  | −0.001  | TW   |
| interaction           |         |        |        |        |      |
| SE with NS            | 11.409  | 12.896  | 13.700  | 14.544  |       |
| VP with NS            | −1.621  | −1.893  | −2.042  | −2.201  |       |
| SE screening          | −0.196  | −0.218  | −0.229  | −0.240  |       |
| VP screening          | 0.052   | 0.058   | 0.061   | 0.064   |       |
| Recoil                | 0.055   | 0.057   | 0.058   | 0.059   |       |
| Total                 | −12710.071 | −13657.445 | −14141.418 | −14635.756 | TW   |

TABLE XXIX. Different contributions to the total energy of the two-electron configuration 1s_{1/2}2s_{1/2}^{3}S_{1} (eV). The numbers in the Table present the ionization energy of the 2s_{1/2} electron with the opposite sign.

| Contribution          | Z = 65  | 66     | 68     | 70     | Ref. |
|-----------------------|---------|--------|--------|--------|------|
| Zero-order            | −15521.201 | −16044.661 | −17124.764 | −18250.361 | TW   |
| Nuclear size (NS)     | 1.696   | 1.968  | 2.386  | 3.099  | TW   |
| First-order           |         |        |        |        |      |
| interelectront        | 367.512 | 374.442 | 388.524 | 402.904 | TW   |
| interaction           |         |        |        |        |      |
| Second-order          |         |        |        |        |      |
| interelectront        | −1.593  | −1.605  | −1.626  | −1.648  | TW   |
| interaction           |         |        |        | −1.6548 |      |
| Third-order           |         |        |        |        |      |
| interelectront        | 0.000   | 0.000   | 0.000   | 0.000   | TW   |
| interaction           |         |        |        |        |      |
| SE with NS            | 15.427  | 16.358  | 18.363  | 20.589  |       |
| VP with NS            | −2.374  | −2.557  | −2.962  | −3.419  |       |
| SE screening          | −0.251  | −0.263  | −0.285  | −0.307  |       |
| VP screening          | 0.067   | 0.070   | 0.081   | 0.092   |       |
| Recoil                | 0.060   | 0.061   | 0.064   | 0.067   |       |
| Total                 | −15140.657 | −15656.187 | −16720.219 | −17828.984 | TW   |
TABLE XXX. Different contributions to the total energy of the two-electron configuration \(1s_{1/2}2s_{1/2}^2S_1\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution | \(Z = 80\) | 91 | 92 | 93 | Ref. |
|--------------|-------------|----|----|----|------|
| Zero-order   | −24622.160  | −33220.132 | −34215.481 | −35130.460 | TW |
| Nuclear size (NS) | 9.34 | 32.50 | 37.76 | 40.94 | TW |
| First-order interelectron interaction | 480.13 | 578.374 | 588.169 | 598.188 | TW |
| Second-order interelectron interaction | −1.789 | −1.995 | −2.018 | −2.040 | TW |
| Third-order interelectron interaction | 0.000 | 0.000 | 0.000 | 0.000 | TW |
| SE with NS | 35.391 | 62.226 | 65.418 | 68.739 | 27,28 |
| VP with NS | −6.914 | −14.632 | −15.658 | −16.770 | 29,30 |
| SE screening | −0.470 | −0.754 | −0.780 | −0.806 | 29 |
| VP screening | 0.162 | 0.310 | 0.329 | 0.347 | 30 |
| Recoil | 0.086 | 0.122 | 0.127 | 0.132 | 31 |
| Total | −24106.224 | −32663.981 | −33542.134 | −34441.730 | TW |

TABLE XXXI. Different contributions to the total energy of the three-electron configuration \((1s)^22s_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution | \(Z = 60\) | 62 | 63 | 64 | Ref. |
|--------------|-------------|----|----|----|------|
| Zero-order   | −13063.004  | −14015.106 | −14506.589 | −15008.567 | TW |
| Nuclear size (NS) | 0.928 | 1.201 | 1.342 | 1.519 | TW |
| First-order interelectron interaction | 720.180 | 749.835 | 764.911 | 780.160 | TW |
| Second-order interelectron interaction | −8.954 | −9.124 | −9.213 | −9.303 | TW |
| Third-order interelectron interaction | 0.018 | 0.021 | 0.023 | 0.025 | TW |
| SE with NS | 11.409 | 12.896 | 13.700 | 14.544 | 27,28 |
| VP with NS | −1.621 | −1.893 | −2.042 | −2.201 | 29,30 |
| SE screening | −0.820 | −0.911 | −0.957 | −1.002 | 29 |
| VP screening | 0.119 | 0.138 | 0.147 | 0.156 | 30 |
| Recoil | 0.055 | 0.057 | 0.058 | 0.059 | 31 |
| Total | −12341.690 | −13262.886 | −13738.620 | −14224.610 | TW |
TABLE XXXII. Different contributions to the total energy of the three-electron configuration \((1s)^22s_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution               | \(Z = 65\)  | 66  | 68  | 70  | Ref. |
|----------------------------|--------------|-----|-----|-----|------|
| Zero-order                 | -15521.201  |     |     |     | TW   |
| Nuclear size (NS)          | 1.696        | 1.968 | 2.386 | 3.099 | TW   |
| First-order                |              |     |     |     |      |
| interelectron              | 795.587      | 811.194 | 842.996 | 875.598 | TW   |
| interaction                | -9.395       | -9.490 | -9.690 | -9.898 | TW   |
| Second-order               |              |     |     |     |      |
| interelectron              | 0.027        | 0.028 | 0.029 | 0.031 | TW   |
| interaction                |              |     |     |     |      |
| Third-order                |              |     |     |     |      |
| interelectron              | 15.427       | 16.358 | 18.363 | 20.589 | TW   |
| interaction                | -2.374       | -2.557 | -2.962 | -3.419 | TW   |
| SE with NS                 | -1.048       | -1.093 | -1.205 | -1.316 | TW   |
| interaction                | 0.166        | 0.175 | 0.200 | 0.225 | TW   |
| VP with NS                 | 0.060        | 0.061 | 0.064 | 0.067 | TW   |
| VP screening               | -11.143      | -13.028 | -13.228 | -13.441 | TW   |
| SE screening               | -11.147      | -13.226 |              |          |      |
| Third-order                |              |     |     |     |      |
| interelectron              | 0.943        | 0.064 | 0.066 | 0.069 | TW   |
| interaction                | 0.055        | 0.078 |          |          |      |
| Nuclear polarization       | -2.537       | -2.843 | -3.151 | -3.467 |       |
| Total                      | -14721.055   | -15228.017 | -16274.583 | -17365.385 | TW   |

TABLE XXXIII. Different contributions to the total energy of the three-electron configuration \((1s)^22s_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2s_{1/2}\) electron with the opposite sign.

| Contribution               | \(Z = 80\)  | 91  | 92  | 93  | Ref. |
|----------------------------|--------------|-----|-----|-----|------|
| Zero-order                 | -24622.160  | -3320.132 | -34215.481 | -35130.460 | TW   |
| Nuclear size (NS)          | 9.34         | 32.50 | 37.76 | 40.94 | TW   |
| First-order                |              |     |     |     |      |
| interelectron              | 795.587      | 811.194 | 842.996 | 875.598 | TW   |
| interaction                | -11.143      | -13.028 | -13.228 | -13.441 | TW   |
| Second-order               |              |     |     |     |      |
| interelectron              | -11.147      | -13.226 |              |          |      |
| Third-order                |              |     |     |     |      |
| interelectron              | 0.943        | 0.064 | 0.066 | 0.069 | TW   |
| interaction                | 0.055        | 0.078 |          |          |      |
| SE with NS                 | 35.391       | 62.226 | 65.418 | 68.739 | TW   |
| VP with NS                 | -6.914       | -14.632 | -15.658 | -16.770 | TW   |
| SE screening               | -2.063       | -3.354 | -3.502 | -3.650 | TW   |
| VP screening               | 0.418        | 0.830 | 0.882 | 0.934 | TW   |
| Recoil                     | 0.086        | 0.122 | 0.127 | 0.132 | TW   |
| Nuclear polarization       |              |     |     |     |      |
| Total                      | -23801.415   | -3244.210 | -33300.658 | -34177.909 | TW   |
TABLE XXXIV. Different contributions to the total energy of the three-electron configuration \((1s)^22p_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2p_{1/2}\) electron with the opposite sign.

| Contribution          | \(Z = 60\)     | 62  | 63  | 64  | Ref. |
|-----------------------|-----------------|-----|-----|-----|------|
| Zero-order            | -13063.004      |     |     |     | TW   |
| Nuclear size (NS)     | 0.038           | 0.052| 0.061| 0.071|TW   |
| First-order           |                 |     |     |     |      |
| interelectron interaction | 875.619      | 913.798| 933.291| 953.066|TW   |
| Second-order          |                 |     |     |     |      |
| interelectron interaction | -15.092      | -15.506| -15.726| -15.951|TW   |
| Third-order           |                 |     |     |     |      |
| interelectron interaction | 0.061        | 0.067| 0.071| 0.074|TW   |
| SE with NS            | 0.298           | 0.406| 0.469| 0.539|      |
| VP with NS            | -0.098          | -0.124| -0.139| -0.155|      |
| SE screening          | -0.262          | -0.303| -0.324| -0.345|      |
| VP screening          | 0.044           | 0.053| 0.057| 0.061|      |
| Recoil                | 0.023           | 0.024| 0.025| 0.025|      |
| Total                 | -12202.373      | -13116.639| -13588.804| -14071.182|TW   |

TABLE XXXV. Different contributions to the total energy of the three-electron configuration \((1s)^22p_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2p_{1/2}\) electron with the opposite sign.

| Contribution          | \(Z = 65\)     | 66  | 68  | 70  | Ref. |
|-----------------------|-----------------|-----|-----|-----|------|
| Zero-order            | -15521.201      |     |     |     | TW   |
| Nuclear size (NS)     | 0.083           | 0.099| 0.129| 0.180|TW   |
| First-order           |                 |     |     |     |      |
| interelectron interaction | 973.133      | 993.500| 1035.185| 1078.206|TW   |
| Second-order          |                 |     |     |     |      |
| interelectron interaction | -16.182      | -16.422| -16.919| -17.450|TW   |
| Third-order           |                 |     |     |     |      |
| interelectron interaction | 0.077        | 0.080| 0.085| 0.090|TW   |
| SE with NS            | 0.615           | 0.700| 0.899| 1.137|      |
| VP with NS            | -0.173          | -0.193| -0.239| -0.297|      |
| SE screening          | -0.365          | -0.386| -0.442| -0.498|      |
| VP screening          | 0.066           | 0.070| 0.083| 0.095|      |
| Recoil                | 0.026           | 0.027| 0.028| 0.029|      |
| Total                 | -14563.921      | -15067.186| -16105.955| -17188.869|TW   |
TABLE XXXVI. Different contributions to the total energy of the three-electron configuration \((1s)^22p_{1/2}\) (eV). The numbers in the Table present the ionization energy of the \(2p_{1/2}\) electron with the opposite sign.

| Contribution | \(Z = 80\) | 91 | 92 | 93 | Ref. |
|--------------|-------------|----|----|----|------|
| Zero-order   | -24622.160  | -33320.132 | -34215.481 | -35130.460 | TW |
| Nuclear size (NS) | 0.75 | 3.68 | 4.41 | 4.93 | TW |
| First-order interaction | 1317.19 | 1642.274 | 1676.142 | 1710.926 | TW |
| Second-order interaction | -20.827 | -26.027 | -26.597 | -27.232 | TW |
| Third-order interaction | 0.142 | 0.225 | 0.233 | 0.245 | TW |
| SE with NS | 3.234 | 8.772 | 9.550 | 10.376 | TW |
| VP with NS | -0.834 | -2.451 | -2.704 | -2.982 | TW |
| SE screening | -0.931 | -1.860 | -1.977 | -2.095 | TW |
| VP screening | 0.203 | 0.483 | 0.522 | 0.560 | TW |
| Recoil | 0.038 | 0.054 | 0.056 | 0.057 | TW |
| Nuclear polarization | | | -0.0039 | | |
| Total | -23323.195 | -31694.982 | -32555.850 | -33435.675 | TW |

TABLE XXXVII. Different theoretical data for the energy levels of two-electron configurations. The numbers in the Table present the ionization energy of the \(2s_{1/2}\) or \(2p_{1/2}\) electron with the opposite sign, respectively.

| Contribution | \(Z = 60\) | 62 | 63 | 64 | 65 | 66 | 68 | 70 |
|--------------|-------------|----|----|----|----|----|----|----|
| \(E(2^2S_0)\) This work | -12618.333 | -1349.608 | -14030.409 | -14521.491 | -15023.050 | -15535.148 | -16592.030 | -17693.252 |
| Drake | -12618.188 | -1354.412 | -14030.191 | -14521.251 | -15022.780 | -15534.938 | -16591.716 | -17692.948 |
| Plante et al | -12618.629 | -1354.909 | -14521.817 | -15535.580 | -16592.446 | -17693.778 |
| \(E(2^2P_0)\) This work | -12619.519 | -1355.416 | -14031.002 | -14521.881 | -15023.203 | -15535.132 | -16591.468 | -17692.311 |
| Drake | -12619.024 | -1354.822 | -14030.359 | -14521.184 | -15022.452 | -15534.324 | -16590.550 | -17691.276 |
| Plante et al | -12619.639 | -1355.526 | -14521.987 | -15535.239 | -16591.592 | -17692.458 |
| \(E(2^2S_1)\) This work | -12720.071 | -13657.445 | -14141.418 | -14635.756 | -15140.657 | -15656.187 | -16720.219 | -17828.984 |
| Drake | -12720.166 | -13657.533 | -14141.506 | -14635.845 | -15140.741 | -15656.359 | -16720.343 | -17829.187 |
| Plante et al | -12720.253 | -13657.628 | -14635.951 | | | | | |
| \(E(2^2P_0) - E(2^2P_0)\) This work | 1.186 | 0.808 | 0.593 | 0.390 | 0.153 | -0.016 | -0.562 | -0.941 |
| Drake | 0.835 | 0.411 | 0.168 | -0.067 | -0.328 | -0.614 | -1.166 | -1.672 |
| Plante et al | 1.010 | 0.617 | 0.170 | | | -0.341 | -0.855 | -1.320 |
| \(E(2^2S_0) - E(2^2S_1)\) This work | 101.738 | 107.837 | 111.009 | 114.265 | 117.607 | 121.039 | 128.189 | 135.732 |
| Drake | 101.978 | 108.121 | 111.315 | 114.594 | 117.961 | 121.421 | 128.626 | 136.240 |
| Plante et al | 101.624 | 107.719 | 114.134 | | | 120.895 | 128.027 | 135.556 |
| \(E(2^2P_0) - E(2^2S_1)\) This work | 100.552 | 107.029 | 110.416 | 113.875 | 117.454 | 121.055 | 128.751 | 136.673 |
| Drake | 101.143 | 107.710 | 111.147 | 114.661 | 118.290 | 122.035 | 129.793 | 137.911 |
| Plante et al | 100.614 | 107.102 | 113.963 | | | 121.236 | 128.882 | 136.876 |
TABLE XXXVIII. Different theoretical data for the energy levels of two-electron configurations. The numbers in the Table present the ionization energy of the 2s\(_{1/2}\) or 2p\(_{1/2}\) electron with the opposite sign, respectively.

| Contribution | Z = 80     | 91            | 92            | 93            |
|--------------|------------|---------------|---------------|---------------|
| \(E(2^2S_0)\) |            |               |               |               |
| This work    | -23925.626 | -32415.499    | -33286.200    | -34178.051    |
| Drake \[1\]  | -23924.725 | -32413.255    | -33284.719    | -34175.303    |
| Plante et al \[2\] | -23926.313 | -13549.909    | -33288.445    |            |
| \(E(2^2P_0)\) |            |               |               |               |
| This work    | -23922.785 | -32417.470    | -33290.711    | -34183.109    |
| Drake \[1\]  | -23920.774 | -32413.464    | -33286.535    | -34178.540    |
| Plante et al \[2\] | -23922.959 | -13550.526    | -33291.084    |            |
| \(E(2^2S_1)\) |            |               |               |               |
| This work    | -24106.224 | -32663.981    | -33542.134    | -34441.730    |
| Drake \[1\]  | -24106.335 | -32664.052    | -33543.167    | -34441.681    |
| Plante et al \[2\] | -24106.610 | -33543.870    |            |            |
| \(E(2^2S_0) - E(2^2P_0)\) |            |               |               |               |
| This work    | -2.841     | 1.971         | 4.511         | 5.058         |
| Drake \[1\]  | -3.951     | 0.209         | 1.816         | 3.237         |
| Plante et al \[2\] | -3.354     |            | 2.640         |            |
| \(E(2^2S_0) - E(2^2S_1)\) |            |               |               |               |
| This work    | 180.598    | 248.482       | 255.934       | 263.679       |
| Drake \[1\]  | 181.610    | 250.796       | 258.448       | 266.378       |
| Plante et al \[2\] | 180.297    |            | 255.425       |            |
| \(E(2^2P_0) - E(2^2S_1)\) |            |               |               |               |
| This work    | 183.439    | 246.511       | 251.423       | 258.621       |
| Drake \[1\]  | 185.561    | 250.587       | 256.632       | 263.141       |
| Plante et al \[2\] | 183.651    |            | 252.786       |            |
FIG. 1. Feynman graph, describing the first-order interelectron interaction. The double solid lines correspond to bound electrons in the field of the nucleus, the wavy line corresponds to the sum of the Coulomb and Breit (transverse) photons. If \( a' = a \) and \( b' = b \) the graph is called “direct”, in case \( a' = b, \ b' = a \) we call it “exchange” graph. The latter name should be understood in connection with respect to permutation symmetry.

FIG. 2. Feynman graphs describing the second-order interelectron interaction. The graph a) is called “box” and the graph b) is called “cross”. Notations are the same as in Fig. 1. By \( n_1, n_2 \) the summation over intermediate states is indicated.

FIG. 3. The third-order “box” Feynman graph. The notations are the same as in Figs. 1, 2. Here the wavy lines with the cross denote the sum of the Coulomb and unretarded Breit interaction.

FIG. 4. The second-order “step” graph for three-electron ions. The notations are the same as in Figs. 1, 2.
FIG. 5. The third-order “step-box” graphs. The wavy line with the cross denotes the sum of the Coulomb and unretarded Breit interactions. Otherwise, the notations are the same as in Figs. 1, 2, 3.