A QED Calculation of Electron Interaction for He-Like and Li-Like Highly Charged Ions

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Abstract. A rigorous quantum electrodynamic (QED) calculation of the corrections to electron interaction for configurations $1s_{1/2}2s_{1/2}\,{}^1S_0$, $1s_{1/2}2p_{1/2}\,{}^3P_0$, $1s_{1/2}2s_{1/2}\,{}^3S_1$ of He-like ions and for configurations $(1s_{1/2})^2 2s_{1/2}$ and $(1s_{1/2})^2 2p_{1/2}$ of Li-like ions for the all nuclear charges $10 \leq Z \leq 92$ is performed. The calculation is carried out in the Coulomb gauge. Coulomb-Coulomb and Coulomb-Breit parts are calculated exactly, Breit-Breit part of the correction is calculated within disregard of retardation.

1 Introduction

The available experimental data of the splitting of levels $(1s_{1/2})^2 2s_{1/2}$ and $(1s_{1/2})^2 2p_{1/2}$ for Li-like uranium [1] are still record in precision. In this connection it is of a great interest to the theory in the sense of verification of quantum electrodynamics in the strong field of nucleus. A considerable number of theoretical works was devoted to the calculations of the various QED corrections for the ground $(1s_{1/2})^2 2s_{1/2}$ and excited $(1s_{1/2})^2 2p_{1/2}$ configurations of a ion $^{238}U^{89+}$. The results of these calculations are presented in Table 1. As it is seen from the table, the main contribution to level splitting $2p_{1/2} - 2s_{1/2}$ in $^{238}U^{89+}$ comes from the electron interaction. Up to now this interaction gave the primary error to the evaluation of the level splitting, as long as evaluations within RMBPT (see the explanation of the abbreviation in Table 1) sets aside a number of effects: 1) negative-frequency states, 2) interaction with cross photons, 3) retardation for exchange of transverse photons.

The present calculation takes into account all these effects for Coulomb-Coulomb and Coulomb-Breit interaction and omits effects 1)–3) for Breit-Breit interaction. On the other hand we, in contrast to [2], carry out all the calculations in the point nucleus approximation. The corrections to the finite size of nucleus for the bound energy as well as the corrections to the finite size of nucleus for electron interaction are considered separately (see Table 1).

To calculate corrections within the bounds of QED we apply the S-matrix approach in Furry representation and Feynman diagram technique. This approach is based on the adiabatic S-matrix Gell-Mann and Low [15] and Sucher formula [16] (see the details in [17,18,19]). At that it is essentially to differ the contributions of so called “reducible” and “irreducible” diagrams. The diagrams are called “irreducible” if while summing up over intermediate states there is no initial (or “reference”) state of atom. The contribution of “reference” states is represented by “reducible” diagrams. These diagrams are singular and so it is

Table 1. The level splitting $2p_{1/2} - 2s_{1/2}$ in U^{89+}

Correction	Numerical results (eV)	Reference
Electron interaction: relativistic		
many body perturbation theory (RMBPT)	322.33(15)	[2]
Electron interaction: QED-INT:		
1st order	367.67	This work
2nd order	−13.40	This work
The correction to the finite size of nucleus (NS):		
to bound energy	−33.35	[3]
to electron interaction (1st order)	1.16	This work
Self energy of electron (SE)	−55.87	[4]
Vacuum polarization (VP)	12.94	[5]
Screening:		
SE	1.52	[4,6]
VP	−0.36	[5,7]
The second order radiative corrections:		
SESE (not complete)	0.09	[8]
VPVP	0.13	[5,9]
SEVP	−0.21	[10,11,12]
Nuclear recoil	−0.07	[13]
Nuclear polarization	0.03	[14]
Theory:		
with using of RMBPT	280.48(15)	
with using of QED-INT	280.27	This work
Experiment	280.59(9)	[1]

Notice: The correction to the finite size of nucleus is included in corrections RMBPT, SE, VP and others but is not included in QED-INT. A correction NS in Table 1 is derived as the difference between corrections NS for $2p_{1/2}$ and $2s_{1/2}$ states of U^{91+}.

necessary to carry out a special procedure [17,18,19] to regularize them. In the case of two-electron exchange the contribution of "reference" states does exist only for energy-dependent (containing retardation) interaction, therefore it is absent for Coulomb-Coulomb interaction [17]. The corrections to reference state (CRS) for two-electron atom take different form for the case of equal energies

(the ground state) and different ones (excited states). The explicit expression CRS in the Coulomb gauge for Coulomb-Breit interaction was derived in [20] (equal energies) and for different energies in [21,22,23]. The expressions for CRS in the Feynman gauge were carried out in [24] for the ground state and in [25] for excited states. The numerical computation of CRS for the ground state He-like ions were performed in [26,27] in the Feynman gauge. The numerical computation of CRS in the Coulomb gauge for two-electron and partially for three-electron configurations were carried out in [22,23]. The results of the latter calculations will be used in the present work. As a matter of fact the contribution of reducible part (CRS) takes place only in "box" diagrams. In the "cross" diagrams the contribution of "reference" states is not singular and there is no need to single it out. Nevertheless it is usually convenient to do so. For example in the case of a configuration $(1s_{1/2})^2$ the contributions of CRS for "box" and "cross" diagrams cancel each other.

For numerical evaluation (to sum over the entire spectrum of Dirac equation) B-splines are used [28], in particular the version developed by I.A. Goidenko [29]. Earlier the full QED calculations were carried out only for the ground $(1s_{1/2})^2$ state He-like ions for the various nuclear charges Z. At that ones used either B-splines or the technique of discretization of radial Dirac equations [27]. As well as in [27] we used the Coulomb gauge. For control we reproduced the results of the calculation of $(1s_{1/2})^2$ state and compared them with ones of [27]. Coulomb-Coulomb interaction is reproduced for every Z with the accuracy, on average, 0.01 %, Coulomb-Breit is with the accuracy 0.05 % and Breit-Breit (with disregarding retardation) is with the accuracy 0.1 %. The small discrepancy is explained by the difference in the numerical procedures applied in [27] and in this work.

2 Electron Interaction in He-like Ions

In the case of two-electron configuration the electron interaction in second order (in the fine structure constant α) is expressed by the Feynman diagrams in Fig.1. In the case of configuration $1s2s\,{}^1S_0$, $A, B = 1s_-, 2s_+$, where $\pm$ designates different projections of angular momentum. In the case of configuration $1s2p_{1/2}\,{}^3P_0$, $A, B = 1s_-, 2p_{1/2+}$, for configuration $1s2s\,{}^3S_1$, $A, B = 1s_+, 2s_+$. The contributions of the "direct" and "exchange" diagrams are considered in the following way:

$$\Delta E_{\rm AB}^{\rm box/cross} = a(\Delta E_{\rm ABAB}^{\rm box/cross} - \Delta E_{\rm BAAB}^{\rm box/cross}) \,, \tag{1}$$

where in the case of Coulomb-Coulomb and Breit-Breit interaction $a = 1$ and in the case of Coulomb-Breit interaction $a = 2$ (the contributions of the diagrams Fig.1c, f and the diagrams Fig.1d, e are equal, so it is convenient to consider them as doubled contribution of the diagrams Fig.c, f).

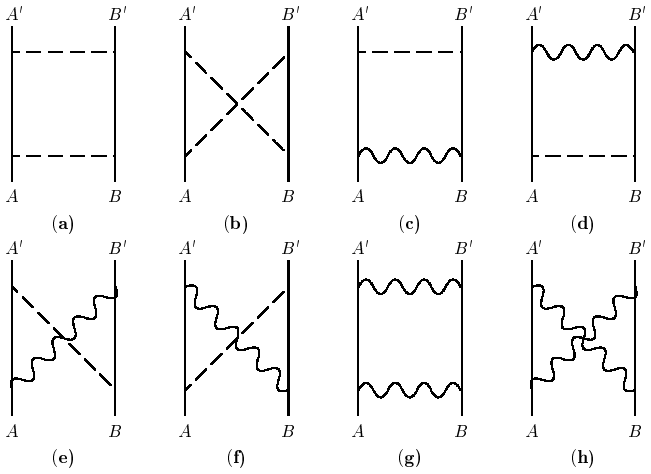

Fig. 1. Two-electron Feynman diagrams representing electron interaction in the second order. Solid line corresponds to electrons, dotted line corresponds to the Coulomb photons, wavy line corresponds to transverse photons (Breit interaction). If $A' = A$ and $B' = B$ then the diagram is called "direct", otherwise, if $A' = B$ and $B' = A$ the diagram is called "exchange". Letters A, B denote one-electron state

2.1 Coulomb-Coulomb Interaction in the Case of Two-Electron Configurations

Coulomb-Coulomb interaction for two-electron atom is represented by the Feynman diagrams Fig.1a, b.

The contribution of irreducible part of "box" and "cross" diagrams is expressed by

$$\Delta E^{\mathrm{box,irr}}_{\mathrm{A'B'AB}} = e^4 \sum_{\mathrm{n_1,n_2 \neq AB}} \frac{\Lambda_1^{(+)}\Lambda_2^{(+)} - \Lambda_1^{(-)}\Lambda_2^{(-)}}{E_{\mathrm{A}} + E_{\mathrm{B}} - E_{\mathrm{n_1}} - E_{\mathrm{n_2}}} \left(\frac{1}{r_{12}}\right)_{\mathrm{A'B'n_1n_2}} \left(\frac{1}{r_{34}}\right)_{\mathrm{n_1n_2AB}}, \quad (2)$$

$$\Delta E^{\mathrm{cross,irr}}_{\mathrm{A'B'AB}} = e^4 \sum_{\mathrm{n_1,n_2 \neq AB}} \frac{\Lambda_1^{(+)}\Lambda_2^{(-)} - \Lambda_1^{(-)}\Lambda_2^{(+)}}{E_{\mathrm{A}} - E_{\mathrm{B'}} + E_{\mathrm{n_1}} - E_{\mathrm{n_2}}} \left(\frac{1}{r_{14}}\right)_{\mathrm{B'n_2n_1A}} \left(\frac{1}{r_{23}}\right)_{\mathrm{n_1A'Bn_2}}, \quad (3)$$

where $\Lambda_i^{(\pm)}$ are projectors on the states with positive (negative) energies $E_{\mathrm{n_i}}$. Summation over intermediate states is taken over both positive and negative energies. Here we remind that the reducible corrections $\Delta E^{\mathrm{box,red}}_{\mathrm{AB}}$ and $\Delta E^{\mathrm{cross,red}}_{\mathrm{AB}}$ to Coulomb-Coulomb interaction are absent [17].

Table 2. Various contributions to electron interaction in second order for a two-electron configuration $1s_{1/2}2s_{1/2}\,{}^1S_0$ (eV)

Contribution	$Z = 10$	30	70	80	92
Coulomb-Coulomb					
$\Delta E^{\rm box,irr}$	−2.2151	−2.3175	−2.9816	−3.3191	−3.9079
$\Delta E^{\rm cross,irr}$	0.0001	0.0015	0.0163	0.0250	0.0413
ΔE	−2.2150	−2.3160	−2.9653	−3.2941	−3.8666
Coulomb-Breit					
$\Delta E^{\rm box,irr}$	−0.0107	−0.0905	−0.5111	−0.7093	−1.0358
$\Delta E^{\rm box,red}$	0.0001	0.0023	0.0377	0.0595	0.0981
$\Delta E^{\rm cross,irr}$	−0.0003	−0.0077	−0.0819	−0.1191	−0.1775
$\Delta E^{\rm cross,red}$	−0.0001	−0.0018	−0.0240	−0.0384	−0.0648
ΔE	−0.0111	−0.0977	−0.5794	−0.8072	−1.0503
Breit-Breit					
ΔE	−0.0001	−0.0054	−0.1005	−0.1625	−0.2760
Total					
ΔE	−2.2262	−2.4192	−3.6452	−4.2638	−5.1929

2.2 Coulomb-Breit Interaction in the Case of Two-Electron Configurations

Coulomb-Breit interaction for two-electron atom is represented by the Feynman diagrams Fig.1c, d, e, f. In this case the corrections to energy are given by

$$\Delta E^{\rm box,irr}_{\rm A'B'AB} = e^4 \sum_{\rm n_1,n_2\neq AB} \frac{1}{E_{\rm A}+E_{\rm B}-E_{\rm n_1}-E_{\rm n_2}} \left(\frac{1}{r_{12}}\right)_{\rm A'B'n_1n_2} \times \Big(V_1(E_{\rm A}-E_{\rm n_1},E_{\rm n_1},r_{34}) + V_1(E_{\rm B}-E_{\rm n_2},E_{\rm n_2},r_{34})\Big)_{\rm n_1n_2AB}, \quad (4)$$

$$\Delta E^{\rm cross,irr}_{\rm A'B'AB} = e^4 \sum_{\rm n_1,n_2\neq AB} \frac{1}{E_{\rm A}-E_{\rm B'}+E_{\rm n_1}-E_{\rm n_2}} \left(\frac{1}{r_{14}}\right)_{\rm B'n_2n_1A} \times \Big(V_1(E_{\rm B}-E_{\rm n_1},E_{\rm n_1},r_{23}) - V_1(E_{\rm A'}-E_{\rm n_2},E_{\rm n_2},r_{23})\Big)_{\rm n_1A'Bn_2}, \quad (5)$$

where

$$V_1(\beta,E_{\rm n},r) = (-1)\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2\frac{\beta}{|\beta|r}\left[\Theta(E_{\rm n})\Theta(\beta)\cos(|\beta|r) - \frac{1}{\pi}\Phi(|\beta|r)\right]$$

Table 3. Various contributions to electron interaction in second order for a two-electron configuration $1s_{1/2}2p_{1/2}\,{}^3P_0$ (eV)

Contribution	$Z = 10$	30	70	80	92
Coulomb-Coulomb					
$\Delta E^{\mathrm{box,irr}}$	−23.4767	−4.8112	−3.8906	−4.3179	−5.1877
$\Delta E^{\mathrm{cross,irr}}$	0.0000	0.0004	0.0118	0.0214	0.0421
ΔE	−23.4767	−4.8108	−3.8788	−4.2965	−5.1456
Coulomb-Breit					
$\Delta E^{\mathrm{box,irr}}$	0.3393	0.2087	−0.6197	−1.0412	−1.7758
$\Delta E^{\mathrm{box,red}}$	0.0000	0.0009	0.0146	0.0106	0.0062
$\Delta E^{\mathrm{cross,irr}}$	−0.0004	−0.0088	−0.0772	−0.1113	−0.1710
$\Delta E^{\mathrm{cross,red}}$	0.0000	−0.0003	−0.0029	−0.0027	−0.0016
ΔE	0.3389	0.2007	−0.6851	−1.1447	−1.9421
Breit-Breit					
ΔE	−0.0016	−0.0191	−0.2419	−0.3935	−0.6831
Total					
ΔE	−23.1393	−4.6291	−4.8058	−5.8347	−7.7708

$$+(-1)(\boldsymbol{\nabla}_1\boldsymbol{\alpha}_1)(\boldsymbol{\nabla}_2\boldsymbol{\alpha}_2)\frac{1}{\beta|\beta|r}\left[\Theta(E_{\mathrm{n}})\Theta(\beta)\left(1-\cos(|\beta|r)\right)\right.$$
$$\left.+\frac{1}{\pi}\left(\Phi(|\beta|r)-\frac{\pi}{2}-|\beta|r\ln(|\beta|r)\right)\right]\,, \tag{6}$$

$$\Phi(x) = \mathrm{ci}(x)\sin(x) - \mathrm{si}(x)\cos(x)\,, \tag{7}$$

$\mathrm{ci}(x)$, $\mathrm{ci}(x)$ are integral sine and cosine.

The expressions for $\Delta E^{\mathrm{box,red}}$ and $\Delta E^{\mathrm{cross,red}}$ are carried out in [21,22,23]. The results of calculations by the formulas (4), (5) are presented in Tables 2, 3 and 4. In the tables there are also included the values of $\Delta E^{\mathrm{box,red}}_{\mathrm{AB}}$ and $\Delta E^{\mathrm{cross,red}}_{\mathrm{AB}}$ taken from [22,23].

2.3 Breit-Breit Interaction in the Case of Two-Electron Configurations

Breit-Breit interaction is calculated within disregard of negative frequency states, interaction with crossed photons (Fig.1h) and retardation. Thus Breit-Breit interaction is expressed by Feynman diagram Fig.1g. The formulas for “box” dia-

Table 4. Various contributions to electron interaction in second order for a two-electron configuration $1s_{1/2}2s_{1/2}\,{}^3S_1$ (eV)

Contribution	$Z=10$	30	70	80	92
Coulomb-Coulomb					
$\Delta E^{\rm box,irr}$	−1.2960	−1.3452	−1.6440	−1.7864	−2.0220
$\Delta E^{\rm cross,irr}$	0.0000	0.0001	0.0025	0.0045	0.0088
ΔE	−1.2960	−1.3451	−1.6415	−1.7819	−2.0133
Coulomb-Breit					
$\Delta E^{\rm box,irr}$	−0.0002	−0.0019	−0.0085	−0.0105	−0.0127
$\Delta E^{\rm box,red}$	0.0000	0.0001	0.0002	0.0002	0.0001
$\Delta E^{\rm cross,irr}$	−0.0002	−0.0037	−0.0331	−0.0460	−0.0635
$\Delta E^{\rm cross,red}$	0.0000	0.0004	0.0073	0.0118	0.0200
ΔE	−0.0004	−0.0050	−0.0341	−0.0446	−0.0560
Breit-Breit					
ΔE	0.0000	−0.0003	−0.0078	−0.0134	−0.0243
Total					
ΔE	−1.2964	−1.3504	−1.6834	−1.8398	−2.0936

gram are

$$\Delta E^{\rm box,irr}_{\rm A'B'AB} = e^4 \sum_{\rm n_1n_2\neq AB} \frac{\Lambda_1^{(+)}\Lambda_2^{(+)}(V_2(r_{12}))_{\rm A'B'n_1n_2}(V_2(r_{34}))_{\rm n_1n_2AB}}{E_{\rm A}+E_{\rm B}-E_{\rm n_1}-E_{\rm n_2}}\,, \qquad (8)$$

$$V_2(r) = (-1)\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2\frac{1}{r} + (-1)(\boldsymbol{\nabla}_1\boldsymbol{\alpha}_1)(\boldsymbol{\nabla}_2\boldsymbol{\alpha}_2)\frac{r}{2}\,. \qquad (9)$$

Because of disregarding retardation there is not the correction $\Delta E^{\rm box,red}_{\rm AB}$. The results of calculations by formula (8) are presented in Tables 2, 3 and 4. In these tables there are also given the total results for the all calculated two-electron configurations.

3 Electron Interaction in Li-like Ions

In the case of three-electron configuration the electron interaction in second order is expressed as before by the diagrams Fig.1. Here in the case of configuration $(1s_{1/2})^2 2s_{1/2}$ symbols A, B vary over $A, B = 1s_+, 1s_-, 2s_+$ and in the case of configuration $(1s_{1/2})^2 2p_{1/2}$ the symbols vary over $A, B = 1s_+, 1s_-, 2p_{1/2+}$. Then it is necessary to take into account three-electron diagrams represented by Fig.2.

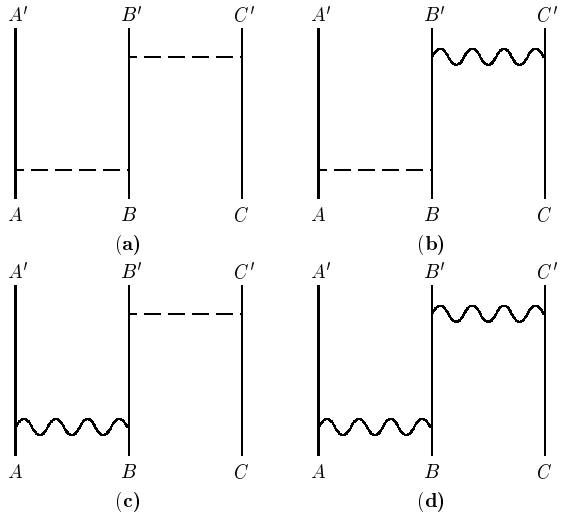

Fig. 2. Three-electron Feynman diagrams representing electron interaction in three-electron atoms in the second order. The designations are the same as in Fig.1

Here in the case of configuration $(1s)^2 2s_{1/2}$ symbols A, B, C vary over $A, B, C = 1s_+, 1s_-, 2s_+$ and in the case of configuration $(1s)^2 2p_{1/2}$ the symbols vary over $A, B, C = 1s_+, 1s_-, 2p_{1/2+}$.

The contributions of "box" and "cross" diagrams for three-electron configurations are given by the following formulas

$$\Delta E^{\rm box/cross}_{\rm ABC} = \Delta E^{\rm box/cross}_{\rm AB} + \Delta E^{\rm box/cross}_{\rm AC} + \Delta E^{\rm box/cross}_{\rm BC} \,, \tag{10}$$

where $\Delta E^{\rm box}_{\rm AB}$ and $\Delta E^{\rm cross}_{\rm AB}$ are defined above.

The contributions of "step" diagrams are determined by

$$\Delta E^{\rm step}_{\rm ABC} = a \sum_{\rm i'j'k'i\ j\ k\ =1,2,3} \varepsilon_{\rm i'j'k'} \varepsilon_{\rm i\ j\ k}\ \Delta E^{\rm step}_{\rm i'j'k'i\ j\ k} \,, \tag{11}$$

where states A, B, C are denoted by $1, 2, 3$ respectively. In the case of Coulomb-Coulomb and Breit-Breit interaction $a = 1$. In the case of Coulomb-Breit interaction $a = 2$ (because of the contributions of the diagrams Fig.2b and Fig.2c are equal this interaction is considered as doubled contribution of the diagram Fig.2b). $\varepsilon_{\rm i\ j\ k}$ is an antisymmetric unit tensor.

3.1 Coulomb-Coulomb Interaction in the Case of Three-Electron Configurations

Coulomb-Coulomb interaction for three-electron atom is represented by two-electron Feynman diagrams Fig.1a, b and three-electron diagrams Fig.2a.

The formulas for irreducible part of the diagram Fig.2a are

$$\Delta E^{\mathrm{step,irr}}_{\mathrm{A'B'C'ABC}} = e^4 \sum_{(\mathrm{E_A}-\mathrm{E_{A'}}+\mathrm{E_B}-\mathrm{E_n}\neq 0)} \frac{1}{E_\mathrm{A}-E_{\mathrm{A'}}+E_\mathrm{B}-E_\mathrm{n}} \times \left(\frac{1}{r_{12}}\right)_{\mathrm{nA'BA}} \left(\frac{1}{r_{34}}\right)_{\mathrm{B'C'nC}} . \tag{12}$$

The contribution of reducible part of the diagram Fig.2a in the case of Coulomb-Coulomb interaction vanishes. The contributions of different diagrams and their separate parts in the case of Coulomb-Coulomb interaction for the configurations $(1s_{1/2})^2 2s_{1/2}$ and $(1s_{1/2})^2 2p_{1/2}$ are presented in Tables 5 and 6.

3.2 Coulomb-Breit Interaction in the Case of Three-Electron Configurations

Besides taking into account the two-electron diagrams Fig.1c, d, e, f, Coulomb-Breit interaction for three-electron atom represented by the three-electron diagrams Fig.2b, c (as it is mentioned above the contribution of the diagrams Fig.2b, c is considered as doubled contribution of the diagram Fig.2b). The formulas for irreducible part of the diagram Fig.2b is (see the Appendix)

$$\Delta E^{\mathrm{step,irr}}_{\mathrm{A'B'C'ABC}} = e^4 \sum_{(\mathrm{E_A}-\mathrm{E_{A'}}+\mathrm{E_B}-\mathrm{E_n}\neq 0)} \frac{1}{E_\mathrm{A}-E_{\mathrm{A'}}+E_\mathrm{B}-E_\mathrm{n}} \times \left(\frac{1}{r_{12}}\right)_{\mathrm{nA'BA}} \Big(V_3(E_{\mathrm{C'}}-E_\mathrm{C}, r_{34})\Big)_{\mathrm{B'C'nC}} . \tag{13}$$

In the case of Coulomb-Breit three-electron diagrams there is nonvanishing contribution of the reducible part. This contribution is not considered in [21,22,23]. In order to calculate it we used adiabatic S-matrix in the way it was done for reducible part of two-electron diagram in [20]. The details of the calculation are presented in Appendix. The result of it is

$$\Delta E^{\mathrm{step,red}}_{\mathrm{A'B'C'ABC}} = e^4 \sum_{(\mathrm{E_A}-\mathrm{E_{A'}}+\mathrm{E_B}-\mathrm{E_n}=0)} \left(\frac{1}{r_{12}}\right)_{\mathrm{nA'BA}} \times \left(\frac{\mathrm{d}}{\mathrm{d}\beta} V_3(\beta, r_{34}) \Big|_{\beta=\mathrm{E_{C'}}-\mathrm{E_C}}\right)_{\mathrm{B'C'nC}} . \tag{14}$$

The contributions of different diagrams and their separate parts in the case of Coulomb-Breit interaction for configuration $(1s_{1/2})^2 2s_{1/2}$ and $(1s_{1/2})^2 2p_{1/2}$ are presented in Tables 5 and 6.

3.3 Breit-Breit Interaction in the Case of Three-Electron Configurations

Breit-Breit interaction for three-electron atom is represented by both the two-electron diagrams Fig.1g, h and the three-electron diagram Fig.2d. The formula

Table 5. Contributions of various diagrams and their separate parts for a three-electron configuration $(1s_{1/2})^2 2p_{1/2}$ (eV)

Contribution	$Z = 10$	30	70	80	92
Coulomb-Coulomb					
$\Delta E^{\mathrm{box,irr}}$	−72.7258	−16.6997	−13.8695	−15.1334	−17.7170
$\Delta E^{\mathrm{cross,irr}}$	0.0006	0.0158	0.1721	0.2603	0.4175
$\Delta E^{\mathrm{step,irr}}$	58.2577	1.4736	−6.5155	−7.9919	−10.3374
ΔE	−14.4675	−15.2103	−20.2128	−22.8650	−27.6369
Coulomb-Breit					
$\Delta E^{\mathrm{box,irr}}$	0.9712	0.2837	−3.0778	−4.4969	−6.7486
$\Delta E^{\mathrm{box,red}}$	0.0014	0.0388	0.5666	0.8556	1.3198
$\Delta E^{\mathrm{cross,irr}}$	−0.0033	−0.0642	−0.4759	−0.6382	−0.8645
$\Delta E^{\mathrm{cross,red}}$	−0.0013	−0.0370	−0.5166	−0.7945	−1.2549
$\Delta E^{\mathrm{step,irr}}$	−1.0840	−1.2350	−2.2092	−2.7055	−3.5686
$\Delta E^{\mathrm{step,red}}$	0.0000	−0.0004	−0.0069	−0.0087	−0.0058
ΔE	−0.1160	−1.0139	−5.7197	−7.7883	−11.1227
Breit-Breit					
ΔE^{box}	−0.0029	−0.0898	−1.0941	−1.6830	−2.7023
ΔE^{step}	0.0045	0.0421	0.2801	0.3969	0.5928
ΔE	0.0016	−0.0477	−0.8141	−1.2861	−2.1094
Total					
ΔE	−14.5820	−16.2720	−26.7466	−31.9394	−40.8690

for irreducible contribution to energy in approximation of disregarding negative frequency states and retardation is

$$\Delta E^{\mathrm{step,irr}}_{\mathrm{A'B'C'ABC}} = e^4 \sum_{(\mathrm{E_A}-\mathrm{E_{A'}}+\mathrm{E_B}-\mathrm{E_n}\neq 0)} \frac{\Lambda^{(+)}_{\mathrm{n}}(V_2)_{\mathrm{nA'BA}}(V_2)_{\mathrm{B'C'nC}}}{E_{\mathrm{A}} - E_{\mathrm{A'}} + E_{\mathrm{B}} - E_{\mathrm{n}}} \,. \qquad (15)$$

It should be remembered that in disregarding retardation the contribution of the reducible part vanishes. The results of calculations of separate diagrams in the case of Breit-Breit interaction for the configuration $(1s_{1/2})^2 2s_{1/2}$ and $(1s_{1/2})^2 2p_{1/2}$ are presented in Tables 5 and 6. In these tables there are also given the total results for all calculated three-electron configuration.

Table 6. Contributions of various diagrams and their separate parts for a three-electron configuration $(1s_{1/2})^2 2s_{1/2}$ (eV)

Contribution	$Z = 10$	30	70	80	92
Coulomb-Coulomb					
$\Delta E^{\mathrm{box,irr}}$	−7.8104	−8.0766	−9.9428	−10.9240	−12.6621
$\Delta E^{\mathrm{cross,irr}}$	0.0007	0.0163	0.1669	0.2473	0.3857
$\Delta E^{\mathrm{step,irr}}$	−3.3405	−3.4837	−4.3718	−4.8063	−5.5418
ΔE	−11.1503	−11.5440	−14.1477	−15.4830	−17.8181
Coulomb-Breit					
$\Delta E^{\mathrm{box,irr}}$	−0.0844	−0.6825	−3.4496	−4.5753	−6.3238
$\Delta E^{\mathrm{box,red}}$	0.0013	0.0368	0.5042	0.7778	1.2449
$\Delta E^{\mathrm{cross,irr}}$	−0.0031	−0.0619	−0.4704	−0.6297	−0.8413
$\Delta E^{\mathrm{cross,red}}$	−0.0013	−0.0361	−0.4908	−0.7566	−1.2104
$\Delta E^{\mathrm{step,irr}}$	−0.0051	−0.0470	−0.2916	−0.4030	−0.5816
$\Delta E^{\mathrm{step,red}}$	0.0000	0.0002	0.0131	0.0218	0.0358
ΔE	−0.0926	−0.7905	−4.1850	−5.5650	−7.6764
Breit-Breit					
ΔE^{box}	−0.0012	−0.0488	−0.7976	−1.2469	−2.0191
ΔE^{step}	0.0000	0.0004	0.0134	0.0243	0.0465
ΔE	−0.0012	−0.0484	−0.7842	−1.2226	−1.9725
Total					
ΔE	−11.2441	−12.3829	−19.1169	−22.2706	−27.4670

4 Analysis

For calculations of the first order corrections for uranium ions we took into account the effect of finite size of nucleus. To perform it the Dirac equation for the states $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$ was solved with the potential that corresponds to a Fermi distribution for the nuclear charge

$$\rho(r) = N/(1 + \exp[(r - c)/a]) \,, \tag{16}$$

where normalization constant N if defined by condition

$$4\pi \int_0^\infty \rho(r) r^2 \mathrm{d}r = eZ \,. \tag{17}$$

The parameters for the Fermi distribution are taken from [30] and are $a = 0.5350\,\mathrm{fm}$, $c = 7.167\,\mathrm{fm}$. The results of the calculations are presented in Table 1. There is

given a difference between calculation with the Fermi distribution and one with a point nucleus.

The corrections to finite size of nucleus for the energy of configuration $(1s_{1/2})^2$ in the second order, according [27], yields 0.07 eV. For the difference of the energies of the configurations $(1s_{1/2})^2 2s_{1/2}$ and $(1s_{1/2})^2 2p_{1/2}$ this correction must be considerably less. Thus the nuclear finite size error of our calculation is significantly less, than the total error 0.15 eV given by RMBPT. The main contributions not taken into account in our work are the exact Breit-Breit interaction in the second order and, probably, third order Coulomb-Coulomb interaction.

This work was supported by the Russian Foundation for Basic Research no 99-02-18526.

The authors are grateful to I.A. Goidenko for giving his program of solution of Dirac equation using B-splines.

Appendix

The correction of second order in the fine structure constant (α) (or fourth order in the charge of electron) is given by formula [16]

$$\Delta E_{\rm a}^{(4)} = \lim_{\lambda\to 0} \frac{1}{2}{\rm i}\lambda \left[4 \left\langle \Phi_{\rm a} | S_\lambda^{(4)} | \Phi_{\rm a} \right\rangle - 2 \left\langle \Phi_{\rm a} | S_\lambda^{(2)} | \Phi_{\rm a} \right\rangle^2 \right] . \tag{18}$$

The contribution of "step" diagram Fig.2b is expressed by formula ($x = (\boldsymbol{r}, {\rm i}t)$):

$$\begin{aligned} \left\langle \Phi_{\rm a'} | S_\lambda^{(4)} | \Phi_{\rm a} \right\rangle = (-{\rm i}e)^4 \int {\rm d}x_1 {\rm d}x_2 {\rm d}x_3 {\rm d}x_4 \exp[-\lambda(|t_1| + |t_2| + |t_3| + |t_4|)] \\ \times \overline{\psi}_{\rm A'}(x_1)\gamma_{\mu_1}\psi_{\rm A}(x_1)\overline{\psi}_{\rm B'}(x_4)\gamma_{\mu_4} S(x_4 x_2)\gamma_{\mu_2}\psi_{\rm B}(x_2) \\ \times \overline{\psi}_{\rm C'}(x_3)\gamma_{\mu_3}\psi_{\rm C}(x_3) D^{\rm c}_{\mu_1\mu_2}(x_1 x_2) D^{\rm t}_{\mu_3\mu_4}(x_3 x_4) , \end{aligned} \tag{19}$$

where $S(x_1 x_2)$ is the electron propagator

$$S(x_1 x_2) = \frac{1}{2\pi{\rm i}} \int_{-\infty}^{+\infty} {\rm d}\omega {\rm e}^{{\rm i}\omega(t_1 - t_2)} \sum_{\rm n} \frac{\psi_{\rm n}(\boldsymbol{r}_1)\overline{\psi}_{\rm n}(\boldsymbol{r}_2)}{E_{\rm n}(1 - {\rm i}0) + \omega} , \tag{20}$$

$D^{\rm c/t}_{\mu\nu}(x_1 x_2)$ is the photon propagator of Coulomb (c) and transverse (t) photons

$$D^{\rm c}_{\mu\nu}(x_1 x_2) = -\frac{\rm i}{r_{12}} \delta(t_1 - t_2)\delta_{\mu 4}\delta_{\nu 4} , \tag{21}$$

$$\begin{aligned} D^{\rm t}_{\mu\nu}(x_1 x_2) = \frac{(1 - \delta_{\mu 4})(1 - \delta_{\nu 4})}{2\pi{\rm i}} \left\{ \frac{\delta_{\mu\nu}}{r_{12}} \int_{-\infty}^{+\infty} \exp\left[{\rm i}\Omega(t_1 - t_2)\right] \exp\left[{\rm i}|\Omega| r_{12}\right] {\rm d}\Omega \right. \\ \left. + \nabla_{1\mu}\nabla_{2\nu} \frac{1}{r_{12}} \int_{-\infty}^{+\infty} \exp\left[{\rm i}\Omega(t_1 - t_2)\right] \frac{1 - \exp\left[{\rm i}|\Omega| r_{12}\right]}{\Omega^2} {\rm d}\Omega \right\} . \end{aligned} \tag{22}$$

Having performed in (19) the integration over times, ω, Ω and taking into account that we are interested in the real part of $\Delta E_{\rm a}^{(4)}$ we get:

$$\begin{aligned}\left\langle \Phi_{\rm a'}|S_\lambda^{(4)}|\Phi_{\rm a}\right\rangle = e^4 \sum_{({\rm E_A}-{\rm E_{A'}}+{\rm E_B}-{\rm E_n}\neq 0)} \left(\frac{-{\rm i}}{2\lambda}\right)\left(\frac{1}{r_{12}}\right)_{\rm nA'BA} \frac{\Big(V_3(E_{\rm C'}-E_{\rm C},r_{34})\Big)_{\rm B'C'nC}}{E_{\rm A}-E_{\rm A'}+E_{\rm B}-E_{\rm n}} \\ +e^4 \sum_{({\rm E_A}-{\rm E_{A'}}+{\rm E_B}-{\rm E_n}=0)} \\ \left[\left(\frac{-{\rm i}}{2\lambda}\right)\left(\frac{1}{r_{12}}\right)_{\rm nA'BA}\left(\frac{\rm d}{{\rm d}\beta}V_3(\beta,r_{34})\,\Big|_{\beta={\rm E_{C'}}-{\rm E_C}}\right)_{\rm B'C'nC}\right. \\ \left.+\left(\frac{-1}{2\lambda^2}\right)\left(\frac{1}{r_{12}}\right)_{\rm nA'BA}\Big(V_3(E_{\rm C'}-E_{\rm C},r_{34})\Big)_{\rm B'C'nC}\right] \\ +O(\lambda^0)\,, \end{aligned} \tag{23}$$

$$V_3(\beta,r)=(-1)\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2\frac{\cos(|\beta|r)}{r}+(-1)(\boldsymbol{\nabla}_1\boldsymbol{\alpha}_1)(\boldsymbol{\nabla}_2\boldsymbol{\alpha}_2)\frac{1-\cos(|\beta|r)}{r|\beta|^2}\,. \tag{24}$$

The first member in (23) gives the irreducible part of "step" diagram Fig.2a, the second determines its reducible part. The third member and the quadratic member in (18) cancel each other.

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