Test of Many-Electron QED Effects in the Hyperfine Splitting of Heavy High-Z Ions

A. V. Volotka,[1,2] D. A. Glazov,[2] O. V. Andreev,[2] V. M. Shabaev,[2] I. I. Tupitsyn,[2] and G. Plunien[1]

[1]*Institut für Theoretische Physik, Technische Universität Dresden, Mommsenstraße 13, D-01062 Dresden, Germany*

[2]*Department of Physics, St. Petersburg State University, Oulianovskaya 1, Petrodvorets, 198504 St. Petersburg, Russia*

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A rigorous evaluation of the two-photon exchange corrections to the hyperfine structure in lithiumlike heavy ions is presented. As a result, the theoretical accuracy of the specific difference between the hyperfine splitting values of H- and Li-like Bi ions is significantly improved. This opens a possibility for the stringent test of the many-electron QED effects on a few percent level in the strongest electromagnetic field presently available in experiments.

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Accurate measurements of the ground-state hyperfine structure performed in H-like ^{209}Bi, ^{165}Ho, ^{185}Re, ^{187}Re, ^{207}Pb, ^{203}Tl, and ^{205}Tl [1–5] were intended to probe QED in the strong electromagnetic field generated by a heavy nucleus. However, accurate calculations revealed that the uncertainty of the predicted hyperfine splittings, which mainly originates from the nuclear magnetization distribution correction (the Bohr-Weisskopf effect), is comparable in magnitude with the QED correction, see, e.g., Refs. [6]. Accordingly, a direct identification of QED effects on the hyperfine splitting in heavy H-like ions appeared to be unfeasible. It was shown instead, that this uncertainty can be significantly reduced in a specific difference of the hyperfine splitting values of H- and Li-like ions with the same nucleus [7]: $\Delta' E = \Delta E^{(2s)} - \xi \Delta E^{(1s)}$, where $\Delta E^{(1s)}$ and $\Delta E^{(2s)}$ are the hyperfine splittings of H- and Li-like ions, respectively, and the parameter ξ is chosen to cancel the Bohr-Weisskopf correction. The parameter ξ can be calculated to a rather high accuracy independently of the employed nuclear magnetization distribution model. Thereby, the stringent tests of QED in strong fields can be achieved by studying the specific difference of the hyperfine splitting values in H- and Li-like ions.

Till recently there existed only an indirect measurement of the $2s$ hyperfine splitting in lithiumlike Bi ion with an accuracy of about 3% [8]. Direct measurements with high-precision laser spectroscopy are feasible at the current experimental storage ring (ESR) and future HITRAP facilities in GSI [9]. Just recently, after 13 years of various attempts, the hyperfine splitting of the ground-state Li-like Bi ion has been directly observed in GSI [10].

Achievement of the required theoretical accuracy for the specific hyperfine splitting difference for H- and Li-like heavy ions demands the rigorous evaluation of various QED and interelectronic-interaction effects. Since the influence of one-electron QED corrections is considerably reduced in the specific difference, the total value of $\Delta' E$ is essentially determined by the screened radiative and interelectronic-interaction corrections. Recently, the screened self-energy and a dominant part of the screened vacuum-polarization contributions have been calculated rigorously within a systematic QED approach [11,12]. This calculation represents an essential advance beyond the local screening potential approximation employed in the previous works [13–15]. As concerns the interelectronic-interaction contribution, up to now it was evaluated rigorously only up to the first order in $1/Z$, see, e.g., Ref. [16]. The contributions of second- and higher-order in $1/Z$ were calculated within the Breit approximation employing many-body perturbation theory and configuration-interaction methods [13,15,17,18]; however, for high-Z ions such calculations can provide only an approximate estimation of these corrections. In the present Letter we report on the complete evaluation of the second-order interelectronic-interaction corrections within a rigorous QED approach. As the most interesting application of these results we present improved theoretical predictions for the specific difference between the ground-state hyperfine splitting values of H- and Li-like Bi ions.

The second-order interelectronic-interaction corrections in the presence of an external potential correspond to the third-order perturbation theory terms. Nowadays, several approaches are used for derivation of the formal expressions for perturbation serial terms from the first principles of QED: the two-time Green-function method [19], the covariant-evolution-operator method [20], and the line profile approach [21]. Here, we employ the two-time Green-function method. To simplify the derivation we specify the formalism regarding the closed-shell electrons as belonging to a redefined vacuum. In this way we have to consider all two-loop diagrams for the valence electron in the presence of magnetic perturbation, i.e., 30 nonequivalent diagrams. These diagrams encompass the second-order interelectronic-interaction corrections, the one-electron two-loop, and the screened one-loop radiative corrections. In our recent works [11,12] we have evaluated the screened radiative corrections. The generic types of the second-order interelectronic-interaction diagrams, where we now focus on, are depicted in Figs. 1 and 2. The interelectronic-interaction corrections to the hyperfine splitting were

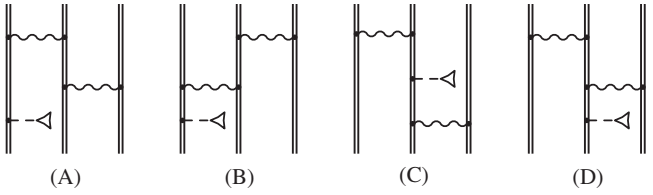

FIG. 1. Feynman diagrams representing the three-electron part of the two-photon-exchange corrections to the hyperfine splitting. The wavy line indicates the photon propagator and the double line indicates the electron propagators in the Coulomb field. The dashed line terminated with the triangle denotes the hyperfine interaction.

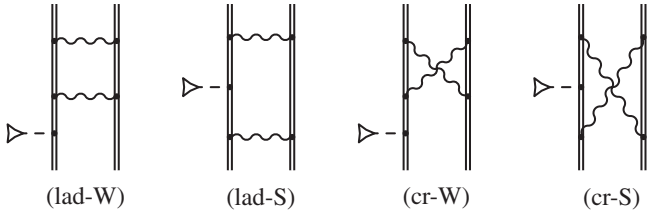

FIG. 2. Feynman diagrams representing the two-electron part of the two-photon-exchange corrections to the hyperfine splitting. Notations are the same as in Fig. 1.

usually denoted by the terms $B(\alpha Z)/Z$ and $C(Z,\alpha Z)/Z^2$, see, e.g., Ref. [15]. The term $B(\alpha Z)/Z$ determines the interelectronic-interaction correction of the first order in $1/Z$, while the interelectronic-interaction corrections of second- and higher-orders are denoted by the term $C(Z,\alpha Z)/Z^2$. Here, we isolate the terms of the second- and higher-orders: $C(Z,\alpha Z)/Z^2 = C(\alpha Z)/Z^2 + D(Z,\alpha Z)/Z^3$, where $C(\alpha Z)/Z^2$ corresponds to the interelectronic-interaction corrections of the second-order in $1/Z$ only (Figs. 1 and 2), and the term $D(Z,\alpha Z)/Z^3$ represents the third- and higher-order corrections in $1/Z$. As in Ref. [19], we call the parts of diagrams *reducible* when an intermediate-state energy coincides with the reference-state energy and *irreducible* otherwise. The irreducible parts of the three-electron diagrams depicted in Fig. 1 yield the following contributions

$$C^{\mathrm{3el,A}} = 2Z^2 G_a \sum_{b_1,b_2}\sum_{P,Q}(-1)^{P+Q}{\sum_n}'\Bigg\{\frac{\langle PaPb_2|I(\Delta_{Paa})|\xi_a n\rangle\langle nb_1|I(\Delta_{b_1Qb_1})|Qb_2Qb_1\rangle}{\varepsilon_{b_2}-\varepsilon_n} + \frac{\langle Pb_2Pa|I(\Delta_{Pb_2b_2})|\xi_{b_2} n\rangle\langle nb_1|I(\Delta_{b_1Qb_1})|QaQb_1\rangle}{\varepsilon_a-\varepsilon_n} + \frac{\langle Pb_2Pb_1|I(\Delta_{Pb_2b_2})|\xi_{b_2} n\rangle\langle na|I(\Delta_{aQa})|Qb_1Qa\rangle}{\varepsilon_{b_1}-\varepsilon_n} + \frac{\langle PaPb_1|I(\Delta_{Pab_2})|\xi_{b_2} n\rangle\langle nb_2|I(\Delta_{b_2Qb_1})|QaQb_1\rangle}{\varepsilon_a+\varepsilon_{b_1}-\varepsilon_{b_2}-\varepsilon_n} + \frac{1}{2}\frac{\langle Pb_2Pb_1|I(\Delta_{Pb_2a})|\xi_a n\rangle\langle na|I(\Delta_{aQb_1})|Qb_2Qb_1\rangle}{\varepsilon_{b_1}+\varepsilon_{b_2}-\varepsilon_a-\varepsilon_n}\Bigg\}, \quad (1)$$

$$C^{\mathrm{3el,B}} = 2Z^2 G_a \sum_{b_1,b_2}\sum_{P,Q}(-1)^{P+Q}{\sum_n}'\Bigg\{\frac{\langle \xi_{Pa}Pb_2|I(\Delta_{Paa})|an\rangle\langle nb_1|I(\Delta_{b_1Qb_1})|Qb_2Qb_1\rangle}{\varepsilon_{b_2}-\varepsilon_n} + \frac{\langle \xi_{Pb_2}Pa|I(\Delta_{Pb_2b_2})|b_2 n\rangle\langle nb_1|I(\Delta_{b_1Qb_1})|QaQb_1\rangle}{\varepsilon_a-\varepsilon_n} + \frac{\langle \xi_{Pb_2}Pb_1|I(\Delta_{Pb_2b_2})|b_2 n\rangle\langle na|I(\Delta_{aQa})|Qb_1Qa\rangle}{\varepsilon_{b_1}-\varepsilon_n} + \frac{\langle \xi_{Pa}Pb_1|I(\Delta_{Pab_2})|b_2 n\rangle\langle nb_2|I(\Delta_{b_2Qb_1})|QaQb_1\rangle}{\varepsilon_a+\varepsilon_{b_1}-\varepsilon_{b_2}-\varepsilon_n} + \frac{1}{2}\frac{\langle \xi_{Pb_2}Pb_1|I(\Delta_{Pb_2a})|an\rangle\langle na|I(\Delta_{aQb_1})|Qb_2Qb_1\rangle}{\varepsilon_{b_1}+\varepsilon_{b_2}-\varepsilon_a-\varepsilon_n}\Bigg\}, \quad (2)$$

$$C^{\mathrm{3el,C}} = Z^2 G_a \sum_{b_1,b_2}\sum_{P,Q}(-1)^{P+Q}{\sum_{n_1,n_2}}'\Bigg\{\frac{\langle Pb_2Pa|I(\Delta_{Pb_2b_2})|b_2n_1\rangle\langle n_1|T_0|n_2\rangle\langle n_2b_1|I(\Delta_{b_1Qb_1})|QaQb_1\rangle}{(\varepsilon_a-\varepsilon_{n_1})(\varepsilon_a-\varepsilon_{n_2})} + 2\frac{\langle Pb_2Pb_1|I(\Delta_{Pb_2b_2})|b_2n_1\rangle\langle n_1|T_0|n_2\rangle\langle n_2a|I(\Delta_{aQa})|Qb_1Qa\rangle}{(\varepsilon_{b_1}-\varepsilon_{n_1})(\varepsilon_{b_1}-\varepsilon_{n_2})} + \frac{\langle PaPb_1|I(\Delta_{Pab_2})|b_2n_1\rangle\langle n_1|T_0|n_2\rangle\langle n_2b_2|I(\Delta_{b_2Qb_1})|QaQb_1\rangle}{(\varepsilon_a+\varepsilon_{b_1}-\varepsilon_{b_2}-\varepsilon_{n_1})(\varepsilon_a+\varepsilon_{b_1}-\varepsilon_{b_2}-\varepsilon_{n_2})} + \frac{1}{2}\frac{\langle Pb_2Pb_1|I(\Delta_{Pb_2a})|an_1\rangle\langle n_1|T_0|n_2\rangle\langle n_2a|I(\Delta_{aQb_1})|Qb_2Qb_1\rangle}{(\varepsilon_{b_1}+\varepsilon_{b_2}-\varepsilon_a-\varepsilon_{n_1})(\varepsilon_{b_1}+\varepsilon_{b_2}-\varepsilon_a-\varepsilon_{n_2})}\Bigg\}, \quad (3)$$

$$C^{3\mathrm{el,D}} = 2Z^2 G_a \sum_{b_1,b_2}\sum_{P,Q}(-1)^{P+Q}\sum_n{}'\Bigg\{\frac{\langle Pa\xi_{Pb_2}|I(\Delta_{Paa})|an\rangle\langle nb_1|I(\Delta_{b_1Qb_1})|Qb_2Qb_1\rangle}{\varepsilon_{b_2}-\varepsilon_n} + \frac{\langle Pb_2\xi_{Pa}|I(\Delta_{Pb_2b_2})|b_2n\rangle\langle nb_1|I(\Delta_{b_1Qb_1})|QaQb_1\rangle}{\varepsilon_a-\varepsilon_n} + \frac{\langle Pb_2\xi_{Pb_1}|I(\Delta_{Pb_2b_2})|b_2n\rangle\langle na|I(\Delta_{aQa})|Qb_1Qa\rangle}{\varepsilon_{b_1}-\varepsilon_n} + \frac{\langle Pa\xi_{Pb_1}|I(\Delta_{Pab_2})|b_2n\rangle\langle nb_2|I(\Delta_{b_2Qb_1})|QaQb_1\rangle}{\varepsilon_a+\varepsilon_{b_1}-\varepsilon_{b_2}-\varepsilon_n} + \frac{1}{2}\frac{\langle Pb_2\xi_{Pb_1}|I(\Delta_{Pb_2a})|an\rangle\langle na|I(\Delta_{aQb_1})|Qb_2Qb_1\rangle}{\varepsilon_{b_1}+\varepsilon_{b_2}-\varepsilon_a-\varepsilon_n}\Bigg\}, \quad (4)$$

where the prime on the sums over intermediate states indicates that terms with vanishing denominators should be omitted in the summation. The irreducible parts of the two-electron diagrams depicted in Fig. 2 yield

$$C^{2\mathrm{el,lad-W}} = Z^2 G_a \sum_b\sum_{P,Q}(-1)^{P+Q}\frac{i}{\pi}\int_{-\infty}^{\infty}d\omega\sum_{n_1,n_2}{}'\frac{\langle PaPb|I(\omega)|n_1n_2\rangle\langle n_1n_2|I(\omega+\Delta_{PaQa})|\xi_{Qa}Qb\rangle}{(\varepsilon_{Pa}+\omega-u\varepsilon_{n_1})(\varepsilon_{Qb}-\omega-\Delta_{PaQa}-u\varepsilon_{n_2})}, \quad (5)$$

$$C^{2\mathrm{el,cr-W}} = Z^2 G_a \sum_b\sum_{P,Q}(-1)^{P+Q}\frac{i}{\pi}\int_{-\infty}^{\infty}d\omega\sum_{n_1,n_2}{}'\frac{\langle Pan_2|I(\omega)|n_1Qb\rangle\langle\xi_{Pb}n_1|I(\omega-\Delta_{PaQa})|n_2Qa\rangle}{(\varepsilon_{Pa}-\omega-u\varepsilon_{n_1})(\varepsilon_{Qb}-\omega-u\varepsilon_{n_2})}, \quad (6)$$

$$C^{2\mathrm{el,lad-S}} = Z^2 G_a \sum_b\sum_{P,Q}(-1)^{P+Q}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\sum_{n_1,n_2,n_3}{}'\frac{\langle PaPb|I(\omega)|n_1n_2\rangle\langle n_2|T_0|n_3\rangle\langle n_1n_3|I(\omega+\Delta_{PaQa})|QaQb\rangle}{(\varepsilon_{Pa}+\omega-u\varepsilon_{n_1})(\varepsilon_{Qb}-\omega-\Delta_{PaQa}-u\varepsilon_{n_2})(\varepsilon_{Qb}-\omega-\Delta_{PaQa}-u\varepsilon_{n_3})}, \quad (7)$$

$$C^{2\mathrm{el,cr-S}} = Z^2 G_a \sum_b\sum_{P,Q}(-1)^{P+Q}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\sum_{n_1,n_2,n_3}{}'\frac{\langle Pan_2|I(\omega)|n_1Qb\rangle\langle n_3|T_0|n_2\rangle\langle Pbn_1|I(\omega-\Delta_{PaQa})|n_3Qa\rangle}{(\varepsilon_{Pa}-\omega-u\varepsilon_{n_1})(\varepsilon_{Qb}-\omega-u\varepsilon_{n_2})(\varepsilon_{Qb}-\omega-u\varepsilon_{n_3})}, \quad (8)$$

where the prime on the sums indicates that in the summation we omit the reducible and infrared-divergent terms, namely, those with $\varepsilon_{n_1}+\varepsilon_{n_2}=\varepsilon_a+\varepsilon_b$ in the ladder-W diagrams, with $\varepsilon_{n_1}=\varepsilon_{Pa}$, $\varepsilon_{n_2}=\varepsilon_{Qb}$ in the direct parts of the cross-W diagrams, with $\varepsilon_{n_1}=\varepsilon_{n_2}=\varepsilon_a$, ε_b in the exchange parts of the cross-W diagrams, with $\varepsilon_{n_1}+\varepsilon_{n_2}=\varepsilon_a+\varepsilon_b$ and $\varepsilon_{n_1}+\varepsilon_{n_3}=\varepsilon_a+\varepsilon_b$ and $\varepsilon_{n_2}=\varepsilon_{n_3}=\varepsilon_{Qb}-\Delta_{PaQa}$ in the ladder-S diagrams, with $\varepsilon_{n_1}=\varepsilon_{Pa}$, $\varepsilon_{n_2}=\varepsilon_{Qb}$ and $\varepsilon_{n_1}=\varepsilon_{Pa}$, $\varepsilon_{n_3}=\varepsilon_{Qb}$ and $\varepsilon_{n_2}=\varepsilon_{n_3}=\varepsilon_{Qb}$ in the direct parts of the cross-S diagrams, with $\varepsilon_{n_1}=\varepsilon_{n_2}=\varepsilon_a$, ε_b and $\varepsilon_{n_1}=\varepsilon_{n_3}=\varepsilon_a$, ε_b and $\varepsilon_{n_2}=\varepsilon_{n_3}=\varepsilon_a$, ε_b in the exchange parts of the cross-S diagrams. In Eqs. (1)–(8), a and b refer to the valence- and core-electron states, respectively; the sum over b runs over all closed-shell states, P and Q are the permutation operators giving rise to the signs $(-1)^P$ and $(-1)^Q$ of the permutation, respectively. $I(\omega)$ is the interelectronic-interaction operator [19], $u=1-i0$ preserves the proper treatment of poles of the electron propagators. The energy difference $\Delta_{n_1n_2}$ is defined as $\Delta_{n_1n_2}=\varepsilon_{n_1}-\varepsilon_{n_2}$. T_0 is the electronic part of the hyperfine-interaction operator and G_a is the multiplicative factor depending on the quantum numbers of the valence electron (see, for details Ref. [15]). The modified wave function $|\xi\rangle$ is defined as follows

$$|\xi_a\rangle = \sum_n^{\varepsilon_n\neq\varepsilon_a}\frac{|n\rangle\langle n|T_0|a\rangle}{\varepsilon_a-\varepsilon_n}. \quad (9)$$

We refer to all contributions, where the energies of intermediate states and the reference state coincide, the infrared-divergent contributions, and the nondiagrammatic terms as the remaining reducible part. Formal expressions for this part, which are rather bulky, will be published elsewhere. Following the treatment of Ref. [22] we introduce a nonzero photon mass. In such a way we regularize the infrared divergences and cancel them analytically.

Now let us discuss the numerical evaluation procedure. The infinite threefold summations over the spectrum of the Dirac equation have been performed employing the dual-kinetic-balance finite basis set method [23] with basis functions constructed from B splines [24]. The Fermi model for the nuclear charge density and the sphere model for the magnetic moment distribution have been utilized. The summations over magnetic substates have been performed analytically by means of standard formulas and also numerically as an independent check. The most problematic part has consisted in evaluation of the two-electron terms, which contain the integration over the energy of the virtual photon ω. In order to avoid strong oscillations arising for large real values of ω, we have performed a Wick rotation of the integration contour, as it was done in the calculations of two-photon exchange corrections to the Lamb shift Refs. [25–27], and have employed the integration contours such as in Ref. [27]. However, special care should be taken for the identification of the pole structure of the integrands, because they are essentially more complicated than in the case of the two-photon exchange corrections to the energy levels.

In what follows we present our result for the case of Li-like Bi utilizing the following values for the nuclear

TABLE I. Individual contributions to the two-photon exchange correction $C(\alpha Z)/Z^2$ for the ground-state hyperfine structure of the Li-like $^{209}Bi^{80+}$.

Contr.	Feynman	Coulomb
3el, A	0.001 685	0.002 229
3el, B	−0.001 942	−0.002 489
3el, C	0.001 154	0.001 036
3el, D	0.003 781	0.003 914
2el, lad-W	0.003 401	0.003 960
2el, cr-W	0.000 363	−0.000 019
2el, lad-S	0.001 155	0.001 226
2el, cr-S	0.000 207	−0.000 001
reducible	−0.009 063	−0.009 116
Total	0.000 740	0.000 740

properties: $\langle r^2\rangle^{1/2} = 5.5211$ fm [28], $I^\pi = 9/2-$, and $\mu = 4.1106(2)\mu_N$ [29]. We have performed calculations in both Feynman and Coulomb gauges and the corresponding individual contributions to the $C(\alpha Z)/Z^2$ are presented in Table I. The total result is gauge independent on the level of the numerical accuracy, that serves as an accurate check for both the derived formulas and the numerical procedures. As an additional check, we have reproduced the third-order many-body perturbation theory (MBPT) result, considering the Breit approximation in the derived expressions. Finally, we have found that the result of the rigorous QED evaluation of the two-photon exchange correction 0.000 740 is in reasonable agreement with the $1/Z^2$ term 0.000 75 extracted from the large-scale configuration-interaction Dirac-Fock-Sturm calculation.

Now let us come to the consideration of the specific difference between the ground-state hyperfine splitting values for H-like and Li-like Bi. The cancellation of the Bohr-Weisskopf effect appears with $\xi = 0.168\,86$ for the case of Bi. In Table II we present the current status of individual contributions to the specific difference. The rigorous evaluation of the two-photon exchange corrections improves the accuracy of the interelectronic-interaction term by an order of magnitude in comparison with previous calculations [11,12]. The accuracy of the screened QED contribution has been also increased due to recent rigorous evaluations of the Wichmann-Kroll parts of the electric and magnetic loops [30], which was accounted for in Refs. [11,12] within some approximations. Thus, the remaining theoretical uncertainty for the specific difference comes from the uncalculated Wichmann-Kroll parts of the screened vacuum-polarization correction and from the $1/Z^3$ and higher orders interelectronic-interaction term. The second uncertainty in the total value of $\Delta' E$ arises from the uncertainty of the nuclear magnetic moment, the nuclear polarization corrections [31], and other nuclear effects, which do not completely cancel in the specific difference. It should be noted that the nuclear magnetic moment uncertainty can be larger due to a chemical shift [32]. Employing the experimental value of the $1s$ hyperfine splitting $\Delta E^{(1s)}_{\rm exp} = 5.0840(8)$ eV [1] and the theoretical result for the specific difference, one can easily find the hyperfine splitting for Li-like Bi $\Delta E^{(2s)} = 797.16(14)$ meV, where the accuracy is fully determined by the uncertainty of the experimental value. As one can see from Table II, the one-electron QED corrections are strongly canceled in the specific difference and the dominant QED contributions comes from the many-electron effects. Therefore, the theoretical accuracy achieved now for the specific difference allows us to test the many-electron QED effects on the few percent level, provided the hyperfine splittings in H- and Li-like bismuth are measured with a relative accuracy of about 10^{-6}. When the QED corrections will be tested and found to be valid, the comparison between the theoretical and experimental values will enable the determination of the nuclear magnetic moments and their volume distribution.

TABLE II. Individual contributions to the specific difference $\Delta' E$ for ^{209}Bi in meV.

	$\Delta E^{(2s)}$	$\xi\Delta E^{(1s)}$	$\Delta' E$
Dirac value	844.829	876.638	−31.809
Interelectronic-interaction			
$\sim 1/Z$	−29.995		−29.995
$\sim 1/Z^2$	0.258		0.258
$\sim 1/Z^3$ and higher-orders	−0.003(3)		−0.003(3)
QED	−5.052	−5.088	0.036
Screened QED	0.193(2)		0.193(2)
Total			−61.320(4)(5)

In summary, we have rigorously calculated the two-photon exchange correction to the hyperfine splitting in heavy Li-like ions. As a result we have significantly increased the accuracy of the specific difference, thus providing the theoretical prerequisite for a test of many-electron QED effects at strongest electromagnetic fields. Further extensions of these calculations to the g factor of Li-like and B-like heavy ions may also serve for an independent determination of the fine structure constant from QED at strong fields [33].

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