Screened QED corrections in lithiumlike heavy ions in the presence of magnetic fields

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A rigorous evaluation of the complete gauge-invariant set of the screened one-loop QED corrections to the hyperfine structure and g factor in lithiumlike heavy ions is presented. The calculations are performed in both Feynman and Coulomb gauges for the virtual photon mediating the interelectronic interaction. As a result, the most accurate theoretical predictions for the specific difference between the hyperfine splitting values of H- and Li-like Bi ions as well as for the g factor of Li-like Pb ion are obtained.

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Investigations of the hyperfine splitting and the g factor in highly charged ions give an access to a test of bound-state QED in strongest electromagnetic fields available at present for experimental study. To date, accurate measurements of QED in strongest electromagnetic fields available at present can be substantially reduced [10, 11, 12]. Achievement of the required theoretical accuracy for the hyperfine structure and for the g factor in the case of Li-like ions is a very interesting and demanding challenge for theory.

At present, the theoretical accuracy of the specific difference of the hyperfine splitting values of H- and Li-like ions and of the g factor of Li-like heavy ions is highly limited by uncertainties of the screened QED and higher-order interelectronic-interaction corrections. In the present Letter we focus on one of the most difficult correction, namely, the screened QED correction in the presence of a magnetic field perturbation. State-of-the-art evaluations of the screened QED correction were performed with local screening potentials [13-15]. These calculations are based on the well-established technique developed for the evaluation of the one-loop QED corrections in the presence of an external potential [16]. However, the employment of a local screening potential does not allow one to take into account consistently all the contributing diagrams and to provide a reliable estimation of the uncertainty of the result. Therefore, a systematic description in the framework of QED requires the use of perturbation theory. This crucial step has been made now and in this Letter we report on our results of the rigorous evaluation of the complete gauge-invariant set of the screened one-loop QED corrections. As the most interesting application of these results towards tests of the magnetic sector of bound-state QED we present improved theoretical predictions for the specific difference between the ground-state hyperfine splitting values of H- and Li-like Bi ions and for the g factor of Li-like Pb ion.

The screened radiative correction in the presence of an external potential corresponds to the third-order perturbation theory terms. Nowadays, several approaches are used for derivation of the formal expressions from the first principles of QED: the two-time Green-function method [17], the covariant-evolution-operator method [18], and the line profile approach [19]. Here, we employ the two-time Green-function method. To simplify the derivation of formal expressions, we specify the formalism regarding the closed shell electrons as belonging to a redefined vacuum. It implies a modification of the 0-th-prediction in the electron propagator incorporating the closed-shell electrons. The corresponding shift of the Fermi-level does not affect the hyperfine structure and the g factor. In this way we have to consider all two-loop diagrams for the valence electron in the presence of magnetic perturbation, this is 27 nonequivalent diagrams. These diagrams merge the second-order interelectronic-interaction correction, the two-loop, and the screened one-loop radiative corrections. The generic types of the resulting screened self-energy diagrams are depicted in Fig. 1. The radiative correction to the hyperfine splitting \( x_{\text{rad}} \) can be written as the sum \( x_{\text{rad}} = x_{\text{QED}} + x_{\text{SQED}} \), where \( x_{\text{QED}} \) corresponds to the one-electron QED correction, and \( x_{\text{SQED}} \) stands for the screened radiative correction. The latter can be divided into self-energy (SE) and vacuum-polarization (VP) parts, \( x_{\text{SQED}} = x_{\text{SQED}}^{SE} + x_{\text{SQED}}^{VP} \). The screened SE correction can be distinguished according to so-called irreducible (irr) and reducible (red) parts. It appears...
as the sum of the following terms:

\[
\begin{align*}
\Delta^{A, \text{irr}}_{\text{SQED}} &= 2G_a \sum_b \sum_p (-1)^p \left\{ \sum_n \langle a | \Sigma (\varepsilon_a) | n \rangle \times \langle nb | I(\Delta) | \xi_{pa} P b \rangle + \langle n | T_0 | \eta_{pa} P b \rangle \right\}, \\
\Delta^{B, \text{irr}}_{\text{SQED}} &= 2G_a \sum_b \sum_p (-1)^p \left\{ \sum_n \langle \eta_{pa} | | \xi_{ea} P b \rangle \times \langle nb | I(\Delta) | \xi_{pa} P b \rangle \right\}, \\
\Delta^{C, \text{irr}}_{\text{SQED}} &= 2G_a \sum_b \sum_p (-1)^p \left\{ \sum_{n_1, n_2} \langle \eta_{pa} | | \xi_{ea} P b \rangle \sum_{n_1, n_2} \langle \xi_{pa} P b | I(\Delta) | n_2 \rangle \right\}, \\
\Delta^{D, \text{irr}}_{\text{SQED}} &= 2G_a \sum_b \sum_p (-1)^p \left\{ \sum_{n_1, n_2, n_3} \langle \xi_{ea} P b | I(\Delta) | n_3 \rangle \times \left\{ \sum_{n_1, n_2} \langle \xi_{pa} P b | I(\Delta) | n_3 \rangle \right\} \right\}, \\
\Delta^{E, \text{irr}}_{\text{SQED}} &= 2G_a \sum_b \sum_p (-1)^p \left\{ \sum_{n_1, n_2} \langle \xi_{ea} P b | I(\Delta) | Pa P b \rangle \times \langle nb | I(\Delta) | Pa \xi_{pa} P b \rangle \right\}.
\end{align*}
\]

Here, \( a \) and \( b \) denotes the valence and core electron states, respectively, the sum over \( b \) runs over all closed-shell states, \( P \) is the permutation operator, giving rise to the sign \((-1)^p\) of the permutation, and the notation \((a \leftrightarrow b)\) stands for the contribution with interchanged labels \( a \) and \( b \). The SE operator \( \Sigma (\varepsilon) \), the interelectronic-interaction operator \( I(\omega) \), and
their derivatives (indicated by primes) are defined similar as in Ref. [17], \( u = 1 - \frac{1}{Z} \) preserves the proper treatment of poles of the electron propagators. The energy difference \( \Delta \) is defined as \( \Delta = \varepsilon_a - \varepsilon_p \) and, accordingly, \( \Delta = \varepsilon_b - \varepsilon_p \) in terms \( (a \leftrightarrow b) \). \( T_0 \) 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 wavefunctions \( |\xi_a\rangle \), \( |\xi'_a\rangle \), and \( |\xi'_b\rangle \) are defined as follows

\[
|\xi_a\rangle = \sum_n \frac{\varepsilon_a - \varepsilon_n}{n} \langle n | T_0 | a \rangle,
\]

\[
|\xi'_b|P_aP_b\rangle = \sum_n \frac{\varepsilon_a - \varepsilon_n}{n} \langle n | (\Delta) | P_aP_b \rangle,
\]

and \( |\xi'_a\rangle = \frac{\partial}{\partial \varepsilon_a} |\xi_a\rangle \), \( |\xi'_b|P_aP_b\rangle = \frac{\partial}{\partial \varepsilon_a} |\xi_b|P_aP_b\rangle \).

The expressions compiled in Eqs. (10) and (11) contain ultraviolet divergences. We separate out the divergent zero- and one-potential terms in Eqs. (1), (2), (5), and zero-potential terms in Eqs. (6), (7), and 8 and evaluate these terms in the momentum space, where the divergences can be removed analytically (see, e.g., Ref. [20]). The remaining many-potential terms are ultraviolet finite and calculated in coordinate space. The infrared divergences which occur in the terms of the Eqs. (3), (4), (6), (7), and 9 are regularized by introducing a nonzero photon mass and canceled analytically.

The numerical evaluation is based on employing the dual-kinetic-balance finite basis set method [21] with basis functions constructed from B-splines [22]. The Fermi model for the nuclear charge density and the sphere model for the magnetic moment distribution have been employed. In what follows we present our result for the case of Li-like Bi utilizing the corresponding values for the nuclear properties: \( \mu_B = 5.5211 \text{ nm}^{-1} \text{f}^{-1} \), \( f^* = 9/2 - \frac{1}{2} \), and \( \mu = 4.1106(2) \mu_N \) [24]. The calculations have been performed in Feynman and Coulomb gauges for the photon propagator describing the electron-electron interaction, thus providing an accurate check of the numerical procedure. The obtained results for the screened SE correction for the hyperfine splitting of the Li-like Bi are presented in Table I in both gauges, respectively. Finally, we have calculated the screened SE correction within local screening potentials: Kohn-Sham 0.0012 and core-Hartree 0.0013. The results are in reasonable agreement with the rigorous evaluation \( x_{\text{SQED}}^{\text{SE}} = 0.00111 \).

We have also calculated the screened VP correction in the presence of a magnetic field employing the Uehling approximation for the VP loop. The results have been checked utilizing the Feynman and Coulomb gauges for the photon propagator mediating the interelectronic interaction. The electric-loop part of the screened Wichmann-Kroll (WK) contribution has been calculated by means of the approximate formulas for the WK potential from Ref. [23]. As concerns the screened WK magnetic-loop part we have employed the hydrogenic 2s value from Ref. [26], assuming that it enters with the same screening ratio as the Uehling terms. Accordingly, our value for the screened VP correction is \( x_{\text{VP}}^{\text{SQED}} = -0.00054(2) \).

Finally, the total value for the screened QED correction to the ground-state hyperfine structure in Li-like Bi results as \( x_{\text{SQED}}^{\text{SE}} = 0.00057(2) \).

Probing the influence of QED effects on the hyperfine splitting of highly charged ions is impeded by the uncertainty of the nuclear magnetization distribution correction [the Bohr-Weisskopf (BW) effect]. In this context, it was proposed to consider a specific difference of the ground state hyperfine splitting in H- and Li-like ions [16]: \( \Delta' E = \Delta E^{(2s)} - \xi \Delta E^{(1s)} \), where \( \Delta E^{(1s)} \) and \( \Delta E^{(2s)} \) are the hyperfine splittings of H- and Li-like ions, respectively, the parameter \( \xi \) is chosen to cancel the BW correction. In this specific difference the nuclear corrections almost vanish completely. We have recalculated the energy shift \( \Delta' E \) employing the most accurate result obtained for the screened QED correction. The interelectronic-interaction corrections have been evaluated to first-order in \( 1/Z \) within the QED perturbation theory and to higher-orders within the large-scale configuration-interaction Dirac-Fock-Sturm method. Extracting numerically the contribution of the BW effect in different terms we found that the cancellation appears with \( \xi \) chosen to be \( \xi = 0.16886 \) for the case of Bi. In Table II we present obtained result for the specific difference between the hyperfine structure values of H- and Li-like Bi ions. The Dirac value incorporates also the finite nuclear size correction. The nuclear-polarization correction to the 1s hyperfine splitting calculated in Ref. [27] yields \( \xi (E^{(1s)}_{\text{NP}}) = 0.009 \text{ meV} \). However, since all nuclear corrections have the similar scaling dependence upon the principal quantum numbers, we expect the strong cancellation between 1s and 2s nuclear-polarization corrections in the specific difference. The same is valid for the second-
order one-electron QED contributions. Comparing with the results for the specific difference $\Delta E$ presented in Ref. [10] we have increased the accuracy for the screened QED part and performed more elaborate calculations for the higher-order interelectronic-interaction correction. Further rigorous evaluation of the higher-order electron-electron interaction corrections will provide a test of bound-state QED at strongest electric and magnetic fields.

Similar calculations have been performed for the g factor of Li-like heavy ions. Here, we present our results for the case of $^{208}$Pb$^{79+}$ with the following value for the nuclear charge radius $<r^2>^{1/2} = 5.5010$ fm [23]. The rigorous evaluation of the screened SE correction gives $\Delta_{\text{SE}}^{\text{QED}} = -3.1(1) \times 10^{-6}$. The previous value obtained with local screening potentials was $-3.5(1.2) \times 10^{-6}$ [14]. Thus, the uncertainty of the screened SE correction has been reduced by an order of magnitude. The screened VP contribution has been calculated within the Uehling approximation. As to the WK part, we have employed the approximate formulas for the electric-loop potential [25], while the magnetic-loop value has been taken from Ref. [28], assuming the same screening ratio as for the Uehling term. Accordingly, we have obtained $\Delta_{\text{VP}}^{\text{QED}} = 1.5 \times 10^{-6}$. In Table III we have updated the value for the g factor of Li-like $^{208}$Pb$^{79+}$ previously reported in Ref. [14] employing the result obtained for the screened QED correction. Further extensions of these calculations to the g factor of B-like heavy ions may serve for an independent determination of the fine structure constant from QED at strong fields [12].

In summary, we have rigorously calculated the screened QED correction to the hyperfine splitting and g factor of heavy Li-like ions. We have increased the theoretical accuracy for the specific difference between the hyperfine splitting values of H- and Li-like bismuth as well as for the g factor of Li-like lead. The rigorous calculation of the higher-order interelectronic-interaction correction will be the next step towards the unprecedented accuracy for the stringent test of the bound-state QED in the presence of magnetic fields.

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TABLE III: Individual contributions to the ground-state g factor of Li-like $^{208}$Pb$^{79+}$.

| Contribution                  | Value          |
|-------------------------------|----------------|
| Dirac value (point nucleus)   | 1.932002904    |
| Finite nuclear size           | 0.0007858(13)  |
| Interel. inter.               | 0.002140(7)    |
| QED, $\sim \alpha$            | 0.002411(7)    |
| QED, $\sim \alpha^2$          | -0.0000036(5)  |
| Screened QED                  | -0.0000016(1)  |
| Nuclear recoil                 | 0.0000025(35)  |
| Nuclear polarization          | -0.00000004(2) |
| Total                         | 1.9366289(28)  |

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