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Evaluation of higher-order correlation effects in highly charged ions

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Abstract

The structure and dynamics properties of highly charged ions (HCIs) up to an extremely high precision are described ab initio by quantum electrodynamics (QED), which is currently considered to be one of the most accurate theories of the fundamental interactions. Compared to neutral atoms or light ions, many physical phenomena are greatly enhanced in HCIs. Relativistic and Breit-interaction effects, QED corrections as well as violations of various selection rules are known to become increasingly important and influential in the structure and radiative properties of HCIs. Since extraordinary precision of QED offers unique scientific opportunities, e.g., in the search for "new" physics, its stringent experimental tests remain to be of high importance. HCI are actively studied experimentally at heavy ion storage rings and small-scale Electron-Beam-Ion-Trap facilities.

High-precision evaluations of the structure and dynamics properties of highly relativistic, tightly bound electrons in HCIs represent one of the most challenging tasks in modern theoretical atomic physics. Achieving the required theoretical accuracy in the case of few-electron HCIs is a very important and complicated problem. The calculation techniques used for high-Z ions are generically different from those used for low-Z ions, because the nuclear-strength parameter αZ (α is the fine-structure constant) is not small. Therefore, it cannot be employed as an expansion parameter, instead, the calculations have to be performed to all orders in αZ. The corresponding method of calculation for the QED contributions of the first- and second-order diagrams are developing and applying actively, however, the technical complexity of direct calculations of QED corrections grows rapidly with increasing order of perturbation theory and the number of electrons, making them practically impossible on a large scale. In this regard, simple approximate methods for taking these corrections into account are employed [1, 2]. Further improvement of the accuracy of theoretical calculations can be achieved by developing methods that allow us to use the advantages of the exact and approximate approaches. Meanwhile, there are many experimental data whose

accuracy exceeds the theoretical one, e.g., for Li-like [3], B-like [4, 5], and F-like [6, 7] ions.

To improve the theoretical predictions obtained by the rigorous QED methods (but only in the lowest orders) the correlation contributions of the higher orders can be taken into account within the lowest relativistic approximation through solution of the Dirac-Coulomb-Breit equation (DCB). The calculations can be performed both for single levels [8, 9], and in the framework of the quasidegenerate perturbation theory to rigorously account for the mixing of close levels of the same symmetry [10, 11].

In such a manner to improve prediction of the QED screening corrections we will employ an approximate approach based on the model QED operator. This can be done by isolating the higher orders of the interelectronic interaction from the QED screening results obtained with the model operator. For this purpose, we will add a small parameter in front of the interelectronic-interaction operator in the calculations with the effective QED operator [1], which will allow us to numerically decompose the QED screening correction by this parameter. Then, separating the contributions of lower orders from the total value, we will find the contribution of higher orders, which will be added to the exact QED values. The accuracy of the results obtained can be estimated from the scatter of the final values, depending on the initial approximation of the perturbation theory on the interelectronic interaction (depending on the initial screening potential).

In the present work we demonstrate merges of the rigorous QED treatment up to the second order of perturbation theory with the higher-order electron-correlation contributions evaluated within the Breit approximation and model QED operator in HCIs. To account for correlation effects in the Breit approximation, the relativistic Dirac-Fock-Sturm configuration interaction method (CI-DFS) in combination with the many-body perturbation theory [12] is utilized.

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