Calculation of higher-order correlation effects in highly charged ions

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The properties of highly charged ions (HCIs), including both their structure and dynamics, are rigorously described from first principles by quantum electrodynamics (QED), widely acknowledged as one of the most precise theories of fundamental interactions. In comparison to neutral atoms or light ions, HCIs exhibit significantly enhanced physical phenomena. Relativistic effects, Breit interactions, QED corrections, and deviations from various selection rules are notably pronounced in HCIs, exerting considerable influence on their structural and radiative characteristics. The remarkable precision offered by QED theory presents unique scientific opportunities, particularly in the exploration of "new" physics, underscoring the ongoing necessity for rigorous experimental verification. HCIs are actively investigated experimentally utilizing heavy ion storage rings and Electron-Beam-Ion-Trap facilities of varying scales.

Precisely evaluating the structure and dynamic properties of highly relativistic, tightly bound electrons within HCIs presents one of the most formidable challenges in contemporary theoretical atomic physics. Achieving the required theoretical accuracy in the case of few-electron HCIs is a very important and complicated problem. Methodologies employed for calculating high-Z ions fundamentally differ from those used for low-Z ions due to the non-small nuclear-strength parameter αZ (where α denotes the fine-structure constant), rendering it unsuitable as an expansion parameter. Consequently, calculations necessitate consideration of all orders in αZ. The methodologies for calculating the QED contributions from first- and second-order diagrams are actively evolving and being applied. However, the technical intricacy of directly computing QED corrections escalates rapidly with the order of perturbation theory and the number of electrons, rendering large-scale computations practically infeasible. Consequently, simplified approximate methods are often employed to incorporate these corrections [1,2]. Enhancing the precision of theoretical calculations entails the development of methodologies that leverage the benefits of both exact and approximate approaches. Nonetheless, numerous experimental datasets exhibit greater precision than their theoretical counterparts, notably for Li-like [3], B-like [4,5], and F-like [6,7] ions.

To enhance the theoretical accuracy achieved through rigorous QED methods (limited to the lowest orders), higher-order correlation contributions can be incorporated within the lowest relativistic approximation by solving the Dirac-Coulomb-Breit equation (DCB). These calculations are feasible for both individual levels [8,9] and within the framework of quasidegenerate perturbation theory to rigorously address the mixing of closely spaced levels with the same symmetry [10,11].

To refine the prediction of QED screening corrections, we propose employing an approximate method based on the model QED operator. This entails isolating higher-order interelectronic interactions from the QED screening outcomes derived with the model operator. To achieve this, we will introduce a small parameter scaling the interelectronic interaction operator in calculations conducted with the effective QED operator [1]. This parameter enables a numerical decomposition of the QED screening correction by this parameter. By segregating the lower-order contributions from the total value, we can deduce the higher-order contributions, which will be incorporated into the exact QED values. The accuracy of the results obtained can be gauged by the dispersion of

the final values, contingent upon the initial approximation of the perturbation theory regarding the interelectronic interaction (determined by the initial screening potential).

In this study, we illustrate the integration of rigorous QED calculations up to the second order of perturbation theory with higher-order electron-correlation contributions assessed within the Breit approximation and model QED operator in HCIs. To account for correlation effects within the Breit approximation, we employ the relativistic Dirac-Fock-Sturm configuration interaction method (CI-DFS) in conjunction with many-body perturbation theory [12].

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References

[1] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, Phys. Rev. A **88**, 012513 (2013).
[2] V. V. Flambaum and J. S. M. Ginges, Phys. Rev. A **72**, 052115 (2005).
[3] M. Lestinsky *et al.*, Phys. Rev. Lett. **100**, 033001 (2008).
[4] S. A. King *et al.*, An Optical Atomic Clock Based on a Highly Charged Ion, Nature **611**, 43 (2022).
[5] X. Liu, X. P. Zhou, W. Q. Wen, Q. F. Lu, C. L. Yan, G. Q. Xu, J. Xiao, A. V. Volotka, Y. S. Kozhedub, M. Y. Kaygorodov, Z. K. Huang, W. L. Ma, S. X. Wang, and X. Ma, Phys. Rev. A **104**, 062804 (2021).
[6] G. O'Neil, S. Sanders, P. Szypryt, *et al.*, Phys. Rev. A **102**, 032803 (2020).
[7] Q. Lu, C. L. Yan, G. Q. Xu, N. Fu, Y. Yang, Y. Zou, A. V. Volotka, J. Xiao, N. Nakamura, and R. Hutton, Phys. Rev. A **102**, 042817 (2020).
[8] Y. S. Kozhedub, A. V. Volotka, A. N. Artemyev, D. A. Glazov, G. Plunien, V. M. Shabaev, I. I. Tupitsyn, and Th. Stoehlker, Phys. Rev. A **81**, 042513 (2010).
[9] J. Sapirstein and K.-T. Cheng, Phys. Rev. A **83**, 012504 (2011).
[10] Y. S. Kozhedub, A. V. Malyshev, D. A. Glazov, et. al, Phys. Rev. A **100**, 062506 (2019).
[11] A. V. Malyshev, D. A. Glazov, Y. S. Kozhedub, I. S. Anisimova, M. Y. Kaygorodov, V. M. Shabaev, and I. I. Tupitsyn, Phys. Rev. Lett. **126**, 183001 (2021).
[12] I. I. Tupitsyn *et al.*, Phys. Rev. A **68**, 022511 (2003); I. I. Tupitsyn *et al.*, Phys. Rev. A **72**, 062503 (2005).