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Modification of the configuration interaction plus many-body perturbation theory approach for calculations of atomic structure of ions with partly filled d and f shells

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At present, there are several methods for relativistic calculations of atomic structure and properties, such as multiconfiguration Dirac-Fock, coupled cluster, configuration interaction (CI), many-body perturbation theory (MBPT), their combination, and others. Generally, these approaches can provide accurate and reliable results for atoms and ions with a small number of valence electrons. Calculations of the spectra of ions with many valence electrons, like lanthanides and actinides, are very difficult and usually not so accurate. To account for strong electron correlations in these species a very large configuration space is required. Such a huge configuration space makes calculations very expensive.

The proposed modification of the original CI+MBPT method [1] uses different splitting of the problem into the CI and MBPT parts [2]. In particular, it is suggested to account for double excitations from the valence subspace to virtual using the MBPT and to include single excitations in the CI space. Moreover, the same idea of dividing into parts with single and double excitations, which are then handled differently, can also be used for treating the core-valence correlations.

[1] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **54**, 3948 (1996).
[2] M. G. Kozlov, I. I. Tupitsyn, A. I. Bondarev, and D. V. Mironova, Phys. Rev. A **105** 052805 (2022).

Primary author: Dr BONDAREV, Andrey (GSI Darmstadt/HI Jena)

Presenter: Dr BONDAREV, Andrey (GSI Darmstadt/HI Jena)

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