Atomic calculations of the low-lying states of ions with two valence electrons within the configuration-interaction plus all-order method

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In recent years, the configuration-interaction plus all-order (CI+all-order) method [1, 2] has been widely used for precision calculations of atoms with two-three valence electrons. However, there are still some details of this method that are not fully studied. The CI+all-order method is based on the Brillouin-Wigner perturbation theory, where effective Hamiltonian depends on the energy. The effect of this dependence on the results was studied for the earlier version of the method, namely the CI plus many-body perturbation theory (CI+MBPT) method. On the other hand, all calculations within the CI+all-order method have been made neglecting this dependence. At the same time, the consistent treatment of the high orders requires accurate account of the energy dependence of the effective Hamiltonian.

The technique of approximate treatment of the energy dependence of the effective Hamiltonian was suggested in [3] within the CI+MBPT method. This technique can be also applied in the CI+all-order method. It is implemented in our computer package, which is based on the programs of W. R. Johnson and I. I. Tupitsyn (see [2, 4] and the references therein).

High accuracy atomic calculations are important for many areas of atomic physics. Spectra of multiply charged ions are observed in astrophysics and plasma physics, where one of the main problems is the identification of these spectra. Accurate calculations of the atomic spectra are also important for studies of the possible variation of fundamental constants in the laboratory experiments and in the astrophysical observations. Accurate calculations of atomic spectra are necessary for the development of the new frequency standards and for studies of the fundamental symmetries in atomic experiments. For high-precision calculations the accurate treatment of electronic correlations is most important. The CI+all-order method allows accounting for the valence-valence, valence-core, and core-core correlations in a most effective manner.

In this work we study the isoelectronic sequence of magnesium. The magnesium atom is suitable for the test calculations as it has two valence electrons and three core shells that allow studying the method in full operation. We calculate the valence energies for several low-lying atomic states and determine the size of the corrections from the energy dependence of the effective Hamiltonian.

References:

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