THIRD-ORDER MANY-BODY PERTURBATION THEORY OF DIVALENT ATOMS AND IONS

Abstract

by

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Complete third-order MBPT formulae are presented for divalent systems. A total of 302 third-order Goldstone diagrams are organized into 12 one-body and 23 two-body terms. Third-order diagrams are presented and discussed. Applications are made to atoms and ions of the berylliumlike and magnesiumlike isoelectronic sequences. The energies of the ground-state and low-lying excited states are obtained in the no virtual-pair approximation (NVPA). The model potential is chosen to be a V^{N-2} Dirac-Hartree-Fock potential, and B-spline basis functions in a cavity of finite radius are employed. The Breit correction is included up to second order of MBPT only.

A detailed breakdown of MBPT contributions from the third-order diagrams is presented for the ground-state energies of both sequences. Dominant classes of diagrams are found to be the quadruple excitation one and one class of folded diagrams. They both correspond to valence-valence interactions only. Diagrams associated with core polarizations and core-core correlations are found to be less important for divalent systems.

The computed energies are in excellent agreement with experiment and accuracy is obtained at the 0.2% level on average for both Be-like and Mg-like ions.

Comparisons are also made to previous second-order MBPT results and results from other theories. The third-order correction is shown to be important. It improves the correlation energies by an order of magnitude as compared to the second order. Our results also compare well with those obtained from the large-scale configuration interaction (CI) and the combined CI+MBPT methods.