Interaction of Variational Localised Correlation Functions for Atomic Properties of Be I

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Synopsis We present some progress associated to the localised correlation function interaction (LCFI) method. In this report, the LCFI method is tested not only for total energy but also for the specific mass shift operator, the hyperfine structure parameters and the transition probabilities. These properties are computed for the three lowest electronic states of the beryllium atom. These calculations illustrate the importance of the contraction effects.

Variational methods are used for targeting specific correlation effects by tailoring the configuration space. Independent sets of correlation orbitals, embedded in the localised correlation functions (LCFs), are produced from the multiconfiguration Hartree-Fock (MCHF) or Dirac-Hartree-Fock (MCDHF) calculations [1,2]. These non-orthogonal functions are then coupled to each other by solving the associated generalised eigenproblem. The Hamiltonian and overlap matrix elements are evaluated using the biorthonormal orbital transformations and efficient counter-transformations of the configuration interaction eigenvectors [3]. This method was successfully applied for describing the total energy of the ground state of beryllium [4]. Moreover it has been shown that the energy convergence is faster than with the usual SD-MCHF method for which a single set of orthonormal one-electron orbitals spanning the complete configuration space is optimised.

In the present work, we investigate the interaction of localised correlation functions (LCFI), not only for the $1s^2 2s^2$ ^1S state of beryllium but also for the first two excited states: $1s^2 2s 2p$ $^3P^o$ and $1s^2 2s 2p$ $^1P^o$. For these three states, we evaluate the total energy, the specific mass shift (SMS), the hyperfine structure (HFS) parameters and the transition probabilities. The comparison between the SMS and HFS results obtained using the LCFI method and the traditional MCHF one stresses the importance of the mixing coefficients contraction within each LCF function. We demonstrate that this unwanted contraction effect can be bypassed by enlarging the associated generalised eigenproblem.

The beryllium atom is a system for which it is still possible to saturate a single orthonormal orbital set through the complete active space MCHF expansions. As such, it constitutes the perfect benchmark for the LCFI method. For larger systems, it becomes hopeless to saturate a single common set of orthonormal orbitals, the LCFI method should be a good alternative for reaching a full-correlated wave function. The present study is a first step in the current development of the extension of both ATSP2K and GRASP2K packages [1,2] that will adopt the biorthonormal treatment for energies, isotope shifts, hyperfine structures and transition probabilities.

References

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