THE CORRELATION MATRIX RENORMALIZATION METHOD FOR MOLECULAR AND LATTICE SYSTEMS

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ABSTRACT

We apply the correlation matrix renormalization (CMR) method [1,2,3] to G2 molecule set and simple lattice systems to assess the accuracy and efficiency of the approach. The CMR calculations are validated by the close agreement with full configuration interactions calculations based on the same quasi-atomic minimal basis set orbitals [4,5]. The results also compare favorably with the available experimental data. For lattice systems, the linear hydrogen chain is first used as a benchmark system, where the CMR calculations compare very well with the recent QMC results. We further study the equation of states of crystalline phases of atomic hydrogen, where the CMR method shows a better agreement with the available QMC data compared with LDA or Hartree-Fock calculations.

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