Correlation matrix renormalization method for correlated-electron systems

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We developed a correlation matrix renormalization (CMR) method which extends the commonly adopted Gutzwiller approximation for the evaluation of the one particle density matrix to treat the evaluation of the two-particle correlation matrix of strongly correlated-electron systems. This approach allows the expectation value of the many-electron Hamiltonian with a variational many-body wave function of the Gutzwiller form to be evaluated with reduced computational complexity. We have applied the method to the study of dissociation behavior of Hydrogen clusters with single correlated orbital and Nitrogen clusters with multiple-correlated orbitals. The results compare favorably with sophisticated quantum chemical calculations. We believe our approach can serve as an alternative starting point for building up the exchange-correlation energy functional for an improved density functional theory description of systems with strong electron correlations.