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Variational investigations of the electronic structure and energy of finite hydrogen systems with the Gutzwiller wave function within local correlation matrix renormalization approximation[1] YONGXIN YAO, JUN LIU, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University and Ames Laboratory-U.S. DOE
— We introduce the correlation matrix renormalization Hartree-Fock (CMR-HF) method in which the many-body Hamiltonian of a multi-electronic system is solved using a variational Gutzwiller-type wave-function. The Gutzwiller approximation is generalized to renormalize the one-electron density matrix and two-electron correlation matrix of the system. To achieve a clear presentation of the concept and methodology, we describe the detailed formalisms for a finite hydrogen system with minimal basis set. The resulting expectation value of the Hamiltonian have clear parallels to terms in the standard uncorrelated Hartree-Fock method, allowing an iterative self-consistent field solution of the many-electron problem analogous to the Hartree-Fock solution. We have applied the method to a series of hydrogen clusters to compare with the results of several other quantum chemical calculation methods.

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Yongxin Yao
Iowa State University and Ames Laboratory-U.S. DOE

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