Abstract Submitted
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Symmetry-projected Hartree-Fock wave functions in quantum Monte Carlo calculations[1] HAO SHI, The College of William and Mary, CARLOS HOYOS, RAYNER RODRIGUEZ, GUSTAVO SCUSERIA, Rice University, SHIWEI ZHANG, The College of William and Mary — Symmetry-projected Hartree-Fock wave functions provide an ansatz which accounts for static correlations while preserving symmetry. We implement such wave functions in constrained path (CP) auxiliary-field quantum Monte Carlo (AFQMC) calculations as the trial wave function. Unlike usual multi-determinant trial wave functions obtained from a configuration interaction picture, the computational cost of this class of trial wave functions can be made to scale as a low power with system size. A systematic test is carried out in the two-dimensional Hubbard model on the accuracy of the approach. It is found that the accuracy of the calculated ground-state energy increases as more symmetries are restored, while the statistical variance decreases. We find that wave functions with space group and spin symmetry significantly reduce the CP systematic error in AFQMC compared to simple Hartree-Fock trial wave functions. Essentially all the correlation energy is recovered by the AFQMC when the fully symmetry-projected trial wave function is used. Correlation functions are accurately predicted.

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