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Pfaffian wavefunctions with pairing orbitals for electronic structure quantum Monte Carlo MICHAL BAJDICH, GABRIEL DROBNY, LUCAS K. WAGNER, Center for High Performance Simulation and Department of Physics, North Carolina State University, KEVIN E. SCHMIDT, Arizona State University, LUBOS MITAS, Center for High Performance Simulation and Department of Physics, North Carolina State University — The trial wavefunction nodal structure determines the accuracy of electronic structure calculations by the fixed-node quantum Monte Carlo (QMC). Wavefunctions based on Hatree-Fock (HF) or multi-reference HF provide about 95% of correlation energy in real systems such as molecules and solids. On the other hand, antisymmetrized product of pairing orbitals (geminals) is a variationally richer form which can describe effects absent in HF such as electron singlet and triplet pairing. One of such forms is the BCS pairing wavefunction with singlet pairing which can be expressed as a determinant. An extension of BCS includes also triplet pairing and therefore requires a pfaffian. We explore the variational freedom of pfaffian wavefunctions and evaluate improvements of fixed-node QMC energies for cases of atomic, molecular and solid systems.

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