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Title: Frozen core method in auxiliary-field quantum Monte Carlo

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We describe the implementation of the frozen-core approximation in phaseless auxiliary-field quantum Monte Carlo method (AFQMC). Since AFQMC random walks take place in a many-electron Hilbert space spanned by a chosen one-particle basis, this can be achieved without introducing additional approximations, such as pseudopotentials. In parallel to many-body quantum chemistry approaches, tightly-bound inner electrons occupy frozen canonical orbitals, which are determined from a lower level of theory, e.g. Hartree-Fock or CASSCF. This provides significant computational savings over fully correlated all-electron treatments, while retaining excellent transferability and accuracy. Results for several benchmark systems will be presented. This includes the notoriously difficult Cr2 molecule, where for a small basis set near-exact DMRG results are available [Y. Kurashige and T. Yanai, J. Chem. Phys. 130, 234114 (2009)]. (Research is supported by DOE, NSF, and ONR.)