Recent developments in auxiliary-field quantum Monte Carlo: magnetic orders and spin-orbit coupling *

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We discuss several recent developments in auxiliary field quantum Monte Carlo (AFQMC) for treating magnectic orders and systems with spin-orbit coupling (SOC). Symmetry properties can be preserved via proper choices of the Hubbard-Stratonovich transformation and the trial wave function, to greatly increase the accuracy and efficiency. For example, a generalized Hartree-Fock (GHF) trial wave funtion which perserves symmetry in spin-z direction is shown to further improve the AFQMC accuracy in the Hubbard model compared to standard Hartree-Fock (HF) trial wave functions. We determine the magnetic orders in the ground state of the doped Hubbard model. A formally related development allows AFQMC to treat many-body Hamiltonians with SOC. The random walkers become GHF Slater determinants instead of the usual HF form. With this and several algorithmic advances, we calculate exact properties of the strongly interacting Fermi gas with a Rashba SOC. The interplay between superconductivity and SOC coupling is examined.

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