Auxiliary-field QMC: recent methodological developments and applications to real materials

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Phaseless auxiliary field quantum Monte Carlo (AFQMC) is a complementary method to diffusion Monte Carlo (DMC). It makes a different approximation to resolve the Fermion sign problem from fixed-node DMC, because its random walks take place in a manifold of Slater determinants. Applications show that this often reduces the reliance of the solution on the quality of the trial wave function and on the knowledge of many-body nodes. AFQMC can represent its random walkers by any single-particle basis, similar to DFT and other standard electronic structure methods. Planewaves with pseudopotentials are used for extended systems, while gaussian type orbitals (GTO's) are used for molecules. With GTO's, AFQMC can therefore be used as a high order quantum chemical method (configuration interaction and coupled cluster approaches), while gaining the scalability of QMC. Solid state and quantum chemistry applications will be presented. I will also discuss a newly developed post-processing finite-size error correction scheme, which generalizes our previous method to spin-polarized systems.

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