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**Recent advances in auxiliary-field methods — simulations in lattice models and real materials**[1]
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We have developed an auxiliary-field (AF) quantum Monte Carlo (QMC) method for many-body simulations. The method takes the form of a linear superposition of independent-particle calculations in fluctuating external fields. "Entanglement" of the different field configurations leads to random walks in Slater determinant space. We formulate an approximate constraint on the random walk paths to control the sign/phase problem, which has shown to be very accurate even with simple mean-field solutions as the constraining trial wave function. The same method can be applied to both simplified lattice models and real materials. For realistic electronic Hamiltonians, each random walk stream resembles a density-functional theory (DFT) calculation in random local fields. Thus, the AF QMC method can directly import existing technology from standard electronic structure methods into a many-body QMC framework. We have demonstrated this method with calculations in close to 100 systems, including Si solid, first- and second-row molecular systems, molecules of heavier post-d elements, transition-metal systems, and ultra-cold atomic gases. In these we have operated largely in an automated mode, inputting the DFT or Hartree-Fock solutions as trial wave functions. The AF QMC results showed consistently good agreement with near-exact quantum chemistry results and/or experiment. I will also discuss additional algorithmic advances which can further improve the method in strongly correlated systems.

[1]In collaboration with W. A. Al-Saidi, Henry Krakauer, and Wirawan Purwanto