Auxiliary-Field Quantum Monte Carlo Calculations of Excited States and Strongly Correlated Systems

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I will describe our recent efforts to develop quantum Monte Carlo (QMC) approaches for excited states and for more systematic and accurate treatment of ground states of strongly correlated sytems and heavier elements. We use the auxiliary-field quantum Monte Carlo (AFQMC) framework, which is a many-body total energy method that looks like *many* coupled mean-field calculations. I will discuss this method's relations and differences with traditional density-functional and quantum chemistry methods, and with other forms of QMC. The AFQMC method uses importance-sampled random walks in the space of non-orthogonal Slater determinants to project out the many-body ground state, or excited state. The random walks are constrained by a trial wave function (TWF) to remove the so-called sign problem, giving approximate (but non-perturbative) results. With single-determinant TWFs from Hartree-Fock or density-functional theory (DFT), this approach can be thought of as a post-DFT method with no parameter. In this form, the accuracy is typically comparable to the quantum chemistry coupled-cluster CCSD(T) method near equilibrium geometries, and better than CCSD(T) when bonds are stretched. The computational cost of AFQMC scales as N^3 with characteristic size of the system. Its accuracy can be further improved at the cost of increased computing (releasing the constraint) or better TWF. With AFQMC, we can systematically target selected orbitals to correlate. This allows many-body calculations in solids with a frozen core, with down-folded Hamiltonians, or possibly embeded in a DFT calculations to extend scales. Results from a few on-going applications will be presented, including band structures in simple solids, magnetic phases in MnO, and Cobalt adsoption on graphene.

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