Electronic structure calculations in correlated materials: an auxiliary-field perspective*

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We will discuss recent progress in developing a framework for electronic structure calculations in correlated systems using auxiliary fields [1]. The framework, named as auxiliary-field quantum Monte Carlo, provides a natural extension for traditional independent-electron methods to better treat electron correlations. It casts the many-body problem, via an exact mapping, as a linear combination of mean-field solutions in external auxiliary fields. The wave function is then obtained by stochastic sampling of the auxiliary-field. This results in an accurate many-body solution, consisting of a statistical ensemble of Hartree-Fock or LDA solutions in the presence of fluctuating external fields. The method has been demonstrated to yield accurate results in many atomic, molecular, cluster, and extended systems. Recent progress includes the treatment of solids with downfolded Hamiltonians[2], the use of frozen orbitals to eliminate pseudopotentials and to extend system sizes [3], method for excited states and many-body band structure [4], study of magnetic orders (including bond stretching and bond breaking in Cr dimer [5]), and the treatment of spin-orbit coupling.

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