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

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I will discuss recent progress in developing a framework for electronic structure calculations in correlated systems using auxiliary fields. The framework 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. Recent progress includes the treatment of solids with downfolded Hamiltonians [1], the use of frozen orbitals to eliminate pseudopotentials and to extend system sizes [2], method for excited states and many-body band structure [3], study of magnetic orders, and the treatment of spin-orbit coupling.

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