A stochastic independent-electron approach for correlated systems ⋆

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We have been developing an auxiliary-field Monte Carlo method for many-body calculations. The method takes the form of a linear superposition of independent-electron calculations in fluctuating external fields. "Entanglement" of the different field configurations leads to a formally exact many-body solution. Computationally, this is realized by random walks in the space of mean-field solutions. Each random walk stream resembles a density-functional theory (DFT) calculation in a local external potential. We formulate an approximate constraint on the random walk paths to control the sign/phase problem. Often, simple mean-field solutions taken directly from DFT or Hartree-Fock (HF) have been used as the constraining wave function. This approach, in ~ 100 molecular and solid systems tested to date [1], has given results at or near chemical accuracy. I will briefly describe the conceptual framework, its connection with DFT and HF, computational scalability, and report on the latest effort toward larger system sizes and stronger correlations, and excited states.

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[1] See `http://physics.wm.edu/~shiwei` under publications.