Auxiliary-field based trial wave functions in quantum Monte Carlo simulations[1] CHIA-CHEN CHANG, Univ of California - Davis, BRENDA RUBENSTEIN, MIGUEL MORALES, Lawrence Livermore National Laboratory — We propose a simple scheme for generating correlated multi-determinant trial wave functions for quantum Monte Carlo algorithms. The method is based on the Hubbard-Stratonovich transformation which decouples a two-body Jastrow-type correlator into one-body projectors coupled to auxiliary fields. We apply the technique to generate stochastic representations of the Gutzwiller wave function, and present benchmark resuts for the ground state energy of the Hubbard model in one dimension. Extensions of the proposed scheme to chemical systems will also be discussed.

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