Abstract Submitted for the MAR16 Meeting of The American Physical Society

Auxiliary-field based trial wave functions in quantum Monte Carlo simulations¹ 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.

¹This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, 15-ERD-013

> Chia-Chen Chang Univ of California - Davis

Date submitted: 06 Nov 2015

Electronic form version 1.4