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Variationally Optimized Slater-Jastrow Wave Functions for Constrained Path Quantum Monte Carlo[1] JEONG-PIL SONG, LEONARD SPRAGUE, Brown Univ, CHIA-CHEN CHANG, Univ of California - Davis, BRENDA RUBENSTEIN, Brown Univ — Real space Quantum Monte Carlo techniques, such as Diffusion Monte Carlo, have long employed optimized Slater-Jastrow wave functions as starting points for more accurate calculations. In this work, we present Constrained Path Quantum Monte Carlo calculations on the two-dimensional Hubbard model that make use of variationally optimized Slater-Jastrow trial wave functions. The Jastrow factors employed are determined through a stochastic optimization technique, as first pioneered for the variational optimization of tensor network states. The stability and accuracy of the algorithm with respect to the size of the variational parameter space are assessed. The systematic and statistical errors of the CPMC results obtained are compared to those obtained using mean field wave functions and unoptimized multideterminant expansions. We end with a discussion of how this algorithm can be generalized to produce optimized wave functions to be used as starting points for electronic structure calculations performed with Auxiliary Field Quantum Monte Carlo.

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