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Fast Update Algorithm for Quantum Monte Carlo Simulations of the Hubbard Model PHANI K.V.V. NUKALA, THOMAS A. MAIER, MICHAEL S. SUMMERS, GONZALO ALVAREZ, Oak Ridge National Laboratory, THOMAS C. SCHULTHESS, ETH Zurich — This paper presents an efficient algorithm for computing the transition probability in auxiliary field quantum Monte Carlo simulations of strongly correlated electron systems using a Hubbard model. This algorithm is based on a low-rank updating of the underlying linear algebra problem, and results in significant computational savings. The computational complexity of computing the transition probability and Green's function update reduces to $O(k^2)$ during the k-th step, where k is the number of accepted spin flips, and results in an algorithm that is faster than the competing delayed update algorithm. Moreover, this algorithm is orders of magnitude faster than traditional algorithms that use naive updating of the Green's function matrix.

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