Abstract Submitted for the MAR17 Meeting of The American Physical Society

Self-Learning Monte Carlo Method in Fermion Systems HUITAO SHEN, JUNWEI LIU, YANG QI, Massachusetts Institute of Technology, ZI YANG MENG, Institute of Physics, Chinese Academy of Sciences, LIANG FU, Massachusetts Institute of Technology — As a new general-purpose Monte Carlo method, self-learning Monte Carlo (SLMC) has been numerically demonstrated in boson systems. In this work, we propose a new type of update algorithm, dubbed cumulative update, which could be naturally integrated into SLMC. Based on many local updates in the self-learned effective model, cumulative update efficiently proposes a global move with a high acceptance probability in the original model. Cumulative update can reduce the conventional computational cost of a full sweep $O(N^4)$ to $O(N^3)$, and also effectively reduce the auto-correlation time to be 1. We numerically show its efficiency through the well-known double-exchange model. With cumulative update, the SLMC could be several hundreds of times faster than the conventional local update method. By employing the cumulative update, SLMC can be generally used in any sign-problem-free Fermion systems and maximize the performance of Monte Carlo simulation.

> Huitao Shen Massachusetts Institute of Technology

Date submitted: 11 Nov 2016 Electronic form version 1.4