A pedagogical program in MATLAB for auxiliary-field quantum Monte Carlo

Huy Nguyen, Jie Xu, and Shiwei Zhang

Department of Physics, College of William and Mary Williamsburg, VA, USA

We describe CPMC-m, a pedagogical MATLAB program for learning the constrained-path and phase-free auxiliary-field Monte Carlo methods [1]. The package illustrates the constrained-path Monte Carlo method for the Hubbard model in any dimensions, with a graphical interface. The ground-state energy is calculated using importance sampling and implementing the algorithmic details of a total energy calculation. This tool allows users to experiment with various model and run parameters and visualize the results. It provides a direct and interactive environment to learn the method and study the code with minimal overhead for setup.

- [†] Supported by NSF (REU) and DOE (SciDAC and CMCSN).
- S. Zhang, J. Carlson and J. E. Gubernatis, Phys. Rev. B 55, (12) (1997); S. Zhang and H. Krakauer, Phys. Rev. Lett. 90, 136401 (2003)

65