Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Efficient heat-bath sampling in Fock space[1] ADAM HOLMES, Laboratory of Atomic and Solid State Physics, Cornell University, HITESH CHANGLANI, University of Illinois at Urbana-Champaign, CYRUS UMRIGAR, Laboratory of Atomic and Solid State Physics, Cornell University — We introduce an algorithm for sampling many-body quantum states in Fock space. The algorithm efficiently samples states with probability approximately proportional to an arbitrary function of the second-quantized Hamiltonian matrix elements connected to the current state. We apply the new sampling algorithm to the recently-developed Semistochastic Full Configuration Interaction Quantum Monte Carlo method (S-FCIQMC), a semistochastic implementation of the power method for projecting out the ground state energy in a basis of Slater determinants. The heat-bath sampling requires modest additional computational time and memory compared to uniform sampling but results in newly-spawned weights that are approximately of the same magnitude, thereby greatly improving the efficiency of projection. A comparison in efficiency between uniform and approximate heat-bath sampling is performed on the all-electron nitrogen dimer at equilibrium in Dunning's cc-pVXZ basis sets with $X \in \{D, T, Q, 5\}$, demonstrating a large gain in efficiency that increases with basis set size.

[1]This work was supported in part by grants NSF CHE-1112097, DOE DE-SC0006650, and NSF ACI-1534965.

Adam Holmes
Laboratory of Atomic and Solid State Physics, Cornell University

Date submitted: 06 Nov 2015 Electronic form version 1.4