

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Efficient heat-bath sampling in Fock space¹ 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.

¹This 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