Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Semi-stochastic full configuration interaction quantum Monte Carlo[1] ADAM HOLMES, FRANK PETRUZIELO, MIHIR KHADILKAR, HITESH CHANGLANI, Laboratory of Atomic and Solid State Physics, Cornell University, M.P. NIGHTINGALE, Department of Physics, University of Rhode Island, C.J. UMRIGAR, Laboratory of Atomic and Solid State Physics, Cornell University — In the recently proposed full configuration interaction quantum Monte Carlo (FCIQMC) [1,2], the ground state is projected out stochastically, using a population of walkers each of which represents a basis state in the Hilbert space spanned by Slater determinants. The infamous fermion sign problem manifests itself in the fact that walkers of either sign can be spawned on a given determinant. We propose an improvement on this method in the form of a hybrid stochastic/deterministic technique, which we expect will improve the efficiency of the algorithm by ameliorating the sign problem. We test the method on atoms and molecules, e.g., carbon, carbon dimer, N2 molecule, and stretched N2.

[1] Fermion Monte Carlo without fixed nodes: a Game of Life, death and annihilation in Slater Determinant space. George Booth, Alex Thom, Ali Alavi. J Chem Phys 131, 050106, (2009).
[2] Survival of the fittest: Accelerating convergence in full configuration-interaction quantum Monte Carlo. Deidre Cleland, George Booth, and Ali Alavi. J Chem Phys 132, 041103 (2010).

[1]NSF CHE-1112097, DOE DE-FG02-07ER46365

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

Date submitted: 16 Dec 2011 Electronic form version 1.4