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Improvements and Applications of Semistochastic Quantum Monte Carlo[1] ADAM HOLMES, HITESH CHANGLANI, Laboratory of Atomic and Solid State Physics, Cornell University, MIGUEL MORALES, Lawrence Livermore National Laboratory, M.P. NIGHTINGALE, Department of Physics, University of Rhode Island, C.J. UMRIGAR, Laboratory of Atomic and Solid State Physics, Cornell University — Fully stochastic quantum Monte Carlo (QMC) methods, such as the full configuration interaction quantum Monte Carlo (FCIQMC) [1,2] allow one to compute the ground state of a Hamiltonian in a far larger Hilbert space than is possible using deterministic iterative diagonalization techniques. However, QMC methods suffer from the sign problem and may have large statistical errors. Recently we have shown [3] that these problems can be greatly alleviated by using a semistochastic quantum Monte Carlo (SQMC) approach, wherein the iterative projector is applied deterministically for a small subset of the Hilbert space states and stochastically elsewhere. In addition, the initiator bias, which is introduced to tame the sign problem in FCIQMC, is often greatly reduced. We explore further improvements to SQMC and apply it to a subset of the G2 set of molecules [4]. [1] George Booth, Alex Thom, Ali Alavi. J Chem Phys 131, 050106, (2009). [2] Deidre Cleland, George Booth, and Ali Alavi. J Chem Phys 132, 041103 (2010). [3] F. R. Petruzielo, A. A. Holmes, Hitesh J. Changlani, M. P. Nightingale, and C. J. Umrigar. Phys Rev Lett (Accepted 5 Oct 2012). [4] L. A. Curtiss, K. Raghavachari, G. W. Trucks, and J. A. Pople, J Chem Phys 94, 7221 (1991).

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

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