The Density-Matrix Quantum Monte Carlo Method

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The density-matrix quantum Monte Carlo (DMQMC) method [1] is a finite-temperature generalization of the full-configuration-interaction quantum Monte Carlo (FCIQMC) method recently introduced by Booth, Thom and Alavi [2]. Like FCIQMC, DMQMC overcomes the fermion sign problem in small enough systems. Unlike FCIQMC, which is primarily a ground-state method, DMQMC samples the density operator of a many-particle system at finite temperature. The availability of the density matrix allows arbitrary reduced density matrix elements and expectation values of complicated non-local observables to be evaluated. This talk explains the theory behind DMQMC, describes the algorithm, and introduces an importance-sampling procedure to improve the stochastic efficiency. To demonstrate the potential of DMQMC, the energy and staggered magnetization of the isotropic antiferromagnetic Heisenberg model on small lattices, the concurrence of one-dimensional spin rings, and the Renyi S_2 entanglement entropy of various sublattices of the 6×6 Heisenberg model are calculated. We also present preliminary results for warm dense electron gas systems.

[1] N.S. Blunt, T.W. Rogers, J.S. Spencer, and W.M.C. Foulkes, Phys. Rev. B **89**, 245124 (2014)

[2] G.H. Booth, A.J.W. Thom, and A. Alavi, J. Chem. Phys. **131**, 054106 (2009)