

Density matrix quantum Monte Carlo

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We present a quantum Monte Carlo method capable of sampling the full density matrix of a many-particle system at finite temperature. This allows arbitrary reduced density matrix elements and expectation values of complicated non-local observables to be evaluated easily. The method resembles full configuration interaction quantum Monte Carlo but works in the space of many-particle operators instead of the space of many-particle wave functions. One simulation provides the density matrix at all temperatures simultaneously, from $T = \infty$ to $T = 0$, allowing the temperature dependence of expectation values to be studied. The direct sampling of the density matrix also allows the calculation of some previously inaccessible entanglement measures. We explain the theory underlying the method, describe the algorithm, and introduce an importance-sampling procedure to improve the stochastic efficiency. To demonstrate the potential of our approach, 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. The nature of the sign problem in the method is also investigated.

I. INTRODUCTION

Quantum Monte Carlo (QMC) methods are well established as vital tools in the study of complex many-body quantum systems, often providing highly accurate results. Projector methods such as diffusion Monte Carlo [1, 2] (DMC) and Green's function Monte Carlo [3, 4] (GFMC) grant access to zero-temperature properties by stochastically applying a projection operator to a starting wave function to obtain a statistical sampling of the ground state. The fixed-node approximation [5–8] allows projector QMC to be applied to systems with sign problems and often produces very good results, but its accuracy depends on the quality of the trial nodal surface and is difficult to assess. Another drawback of projector QMC is that expectation values of quantum mechanical observables that do not commute with the Hamiltonian are difficult to calculate [1, 2, 9, 10].

Finite-temperature QMC methods take a different approach. Path-integral Monte Carlo (PIMC) calculations express the partition function, $Z = \text{Tr}(e^{-\beta H})$, as a sum of contributions from paths through Hilbert space [11]. With an appropriate update procedure, the paths can be sampled with the correct probabilities, thus allowing finite-temperature expectation values to be evaluated. The stochastic series expansion (SSE) method [12] has much in common with PIMC. These algorithms also allow access to ground-state properties in principle, but in practice the sign problem is often insurmountable at low temperatures.

The full configuration interaction quantum Monte Carlo (FCIQMC) method recently introduced by Booth, Thom and Alavi [13, 14] is a projector method for studying zero-temperature properties, and, as such, has much in common with DMC and GFMC. However, unlike

DMC and GFMC, where the sampling of the ground-state wave function is performed in real space, FCIQMC samples the components of the wave function in a discrete basis. Crucially, no prior knowledge of the nodal structure of the ground-state wave function is required to reach the exact ground state. Rather, the sign problem manifests itself in the large but system-specific population of quantum Monte Carlo walkers required in order for the ground state of the Hamiltonian to emerge [15] from the background noise. The system sizes accessible to FCIQMC are limited by the amount of memory available to store these walkers. However, the method has proven highly successful in many chemical systems, reducing the memory needed to achieve FCI-quality results by several orders of magnitude [16–20]. This has led to much interest in this direction and research into fundamental improvements and new applications of the algorithm continues [17, 21].

This article presents a closely-related QMC method, which we call density matrix quantum Monte Carlo (DMQMC). Like the path-integral and SSE methods, DMQMC allows finite-temperature results to be calculated. However, it uses a projection approach to achieve this and thus has more in common with zero-temperature QMC methods. DMQMC was inspired by FCIQMC and shares many of its features, but samples the elements of the density matrix instead of the components of the wave function in a discrete basis. This enables expectation values of arbitrary quantum mechanical observables to be calculated easily, even when the operator corresponding to the observable does not commute with the Hamiltonian. Such expectation values are difficult to calculate using other QMC methods [1, 2, 9, 10]. Moreover, the ability to directly sample the density matrix means that many quantum information measures are accessible.

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