Density matrix quantum Monte Carlo

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This paper describes a quantum Monte Carlo method capable of sampling the full density matrix of a many-particle system, thus granting access to arbitrary reduced density matrices and allowing expectation values of complicated non-local operators to be evaluated easily. The direct sampling of the density matrix also raises the possibility of calculating previously inaccessible entanglement measures. The algorithm closely resembles the recently introduced full configuration interaction quantum Monte Carlo method, but works all the way from infinite to zero temperature. 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 and the concurrence of one-dimensional spin rings are compared to exact or well-established results. Finally, the nature of the sign problem in the method is 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. However, the use of QMC methods in the calculation of quantum information measures has been somewhat limited, largely due to their inability to sample reduced density matrices involving more than a few particles or lattice sites.

Entanglement, well established as an important concept in quantum information theory, has recently become a subject of active research in the condensed matter community, with various entanglement measures proving useful when studying how ground states change near quantum phase transitions [1]. In small systems the Lanczos method can be used to calculate exact entanglement measures, and in one-dimensional systems the density matrix renormalization group method is applicable [2]. However, the study of entanglement in large systems is more than one dimension is less straightforward. Relationships between reduced density matrices and spin correlation functions [2] allow QMC methods to access some entanglement measures in certain situations [3]. Moreover, Sandvik recently introduced a QMC method formulated in the valence-bond basis [3] that allowed certain new entanglement entropy measures to be evaluated [4, 7]. Hastings et al. showed that Renyi $S_2$ entanglement entropy can also be calculated [8]. However, in general, the inability of QMC methods to directly access the density matrix and reduced density matrices of systems has hindered their use in this area.

Projector QMC methods such as diffusion Monte Carlo [8] (DMC) and Green’s function Monte Carlo [8, 10] (GFMC) grant access to zero-temperature properties by stochastically applying a projection operator to some initial state such that a stochastic sampling of the ground-state wave function is eventually achieved. The fixed-node approximation [8] often allows accurate results to be obtained in systems with sign problems, with the accuracy of such results depending on the quality of the nodal surface used. Finite-temperature methods take a different approach. Path-integral Monte Carlo (PIMC) methods express the partition function, $Z = \text{Tr}(e^{-\beta H})$, as a sum over contributions from various paths in imaginary time [11]. With an appropriate update procedure, the paths can be sampled with the correct probabilities, thus allowing finite-temperature expectation values to be obtained. The stochastic series expansion (SSE) method [12] has much in common with this approach but begins by performing a Taylor expansion of the density matrix. The resulting terms in the expansion are then sampled in a similar manner. These methods also allow access to ground-state properties. However, the sign problem is, in many cases, insurmountable at low temperatures.

The full configuration interaction quantum Monte Carlo (FCIQMC) method recently introduced by Booth, Thom and Alavi [13] 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 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 [14] 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 [15, 16]. This has led to much interest in this di-
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.

In DMQMC, rather than sampling the components of the wave function in a discrete basis, the elements of the density matrix are sampled instead. It is then a simple task to calculate expectation values of arbitrary operators, even those that do not commute with the Hamiltonian. Such expectation values are usually difficult to calculate using other QMC methods \[21\]. Moreover, the ability to directly sample the density matrix means that many quantum information measures are accessible. These advantages cannot be expected to come without drawbacks, and, indeed, the systems to which we have successfully applied DMQMC to date are small by the standards of other finite-temperature methods. How- ever, the potential uses of a direct stochastic sampling of the density matrix are such that DMQMC deserves investigation. This paper demonstrate the use of DMQMC by studying the isotropic antiferromagnetic Heisenberg model, but DMQMC is a general method and is applicable to both bosonic and fermionic systems.

Section \(\text{II}\) summarizes the FCIQMC method, setting the stage for the description of DMQMC in Section \(\text{III}\). In Section \(\text{IV}\) an importance-sampling procedure is introduced. The DMQMC method is then applied to the isotropic antiferromagnetic Heisenberg model in Section \(\text{V}\) and used to calculate the energy and staggered magnetization of small square lattices and the concurrence of one-dimensional rings. The sign problem in DMQMC is investigated on the 4\(\times\)4 triangular lattice in Section \(\text{VI}\). We discuss our results and offer some concluding remarks in Section \(\text{VII}\). Hartree atomic units are used throughout.

## II. FULL CONFIGURATION INTERACTION QUANTUM MONTE CARLO

The DMQMC algorithm was formulated in analogy with the FCIQMC method. The two methods share many of the same features and it is often useful to compare them. We therefore begin by providing a brief summary of the FCIQMC method; for more detailed discussions readers are referred to Refs. \(\text{[13]}\) and \(\text{[14]}\).

Consider the imaginary-time Schrödinger equation

\[
\frac{d}{d\tau} \langle \Psi \rangle = -\hat{H} \langle \Psi \rangle. \tag{1}
\]

The general solution to this equation is

\[
\langle \Psi(\tau) \rangle = e^{-\tau \hat{H}} \langle \Psi(\tau = 0) \rangle, \tag{2}
\]
for some initial wave function \(\langle \psi(\tau = 0) \rangle\). If the initial wave function has a non-zero ground-state component, \(c_0(0)\), it is easy to see that \(\langle \Psi(\tau) \rangle\) will become proportional to the ground state in the limit of large \(\tau\),

\[
\langle \Psi(\tau \to \infty) \rangle = c_0(0)e^{-\tau E_0} \langle E_0 \rangle, \tag{3}
\]
where \(\langle E_0 \rangle\) is the ground state and \(E_0\) the ground-state energy. The factor of \(e^{-\tau E_0}\) can be removed by choosing the zero of energy such that \(E_0 = 0\). In practice, since \(E_0\) is usually unknown, we solve

\[
\frac{d}{d\tau} \langle \Psi \rangle = -\langle \hat{H} - S \hat{1} \rangle \langle \Psi \rangle = \hat{T} \langle \Psi \rangle, \tag{4}
\]
where we have defined \(\hat{T} = -\langle \hat{H} - S \hat{1} \rangle\). The energy shift \(S\) is adjusted slowly during the simulation to keep the normalization approximately constant. The long-time average of \(S\) gives another measure of the ground-state energy.

The above theory is common to all projector methods; the difference is how they achieve the evolution to the ground state. FCIQMC works in a discrete basis of kets \(\langle X_i \rangle\), which are normally Slater determinants for fermions or permanents for bosons. The components of the wave function in this basis are represented stochastically by a collection of markers. Following Anderson \(\text{[22] [23]}\), we refer to these markers as “psips”. Each psip has an associated sign, \(q = \pm 1\), which we refer to as its “charge”, and resides on a particular basis state \(\langle X_i \rangle\) (or on “site \(i\)”). The net psip charge on a basis state is interpreted as the amplitude of that state in the expansion of the wave function. At any point in a simulation, the distribution of psip charges does not need to provide an accurate representation of the wave function. Rather, the FCIQMC method only requires that the expectation values of the site charges represent the ground state \(\text{[17]}\). Thus, at any point in the simulation, the memory required to sample the wave function may be many orders of magnitude smaller than the memory required to store the whole state.

Booth and co-workers \(\text{[13]}\) introduced an algorithm to evolve the population of psips according to the imaginary-time Schrödinger equation. This can be summarized as follows. For each time step \(\Delta\tau\) we loop over the entire population of psips and perform the following steps:

1. **Spawning:** Allow a psip with charge \(q_i\) on site \(i\) to attempt to spawn onto a connected site \(j\), where \(T_{ij} \neq 0\) and \(i \neq j\), with probability \(|T_{ji}|\Delta\tau\). If the spawning attempt is successful, a psip is born at site \(j\) with charge \(q_j = \text{sign}(T_{ji})q_i\).

2. **Diagonal death/cloning:** Each psip has the chance to either clone or die with probability \(|T_{ii}|\Delta\tau\). The consequence of a successful death/cloning event depends on the sign of the diagonal matrix element: if \(T_{ii} > 0\) the psip is cloned; otherwise the psip is removed from the simulation.
3. Annihilation: Pairs of psips on the same site with opposite charges cancel out (“annihilate”) and are removed from the simulation, leaving a population of only a single charge type on each site.

The FCIQMC algorithm samples the solution of a first-order Euler finite-difference approximation to Eq. 4. Hence, the distribution of psips gives a stochastic representation of the wave function and, as $\tau \to \infty$, the psips settle down to sample the ground-state wave function.

The psip annihilation step does not alter the total charge on a site. However, it has been shown to be vital in order for the true ground-state wave function to emerge in systems with sign problems. Similar and more complex walker cancellation mechanisms have been attempted in continuum DMC and GFMC calculations with less success.

Walker cancellation in FCIQMC works better because psips are more likely to encounter each other in a discrete and finite Hilbert space.

The ability of FCIQMC to tackle the sign problem through the annihilation step is perhaps its most significant advantage. Annihilation leads to the characteristic population dynamics and allows the true ground state to emerge without any knowledge of the nodal structure of the ground-state wave function. At the start of an FCIQMC simulation, the shift is held constant at a value large enough to ensure that the psip population grows exponentially. Eventually, when a system-specific value large enough to ensure that the psip population anneals, the annihilation rate becomes equal to the spawning rate and the population spontaneously plateaus. During this plateau period the ground state of the correct Hamiltonian emerges, after which the population begins to grow again. The population can then be controlled by varying the shift. The psip population at the plateau must be a small fraction of the number of basis states in the Hilbert space in order for FCIQMC to be more (memory) efficient than an exact diagonalization.

The ground-state energy in FCIQMC can be calculated using a “projected estimator” based on the the expression

$$E_0 = \frac{\langle \Psi^T | H | \psi \rangle}{\langle \Psi^T | \psi \rangle} = \frac{\sum_{i,j} \psi_i^T H_{ij} \chi_j}{\sum_i \psi_i^T \chi_i}. \quad (5)$$

Here $|\Psi^T\rangle$ is an appropriate trial function with components $\psi_i^T$ in the many-particle basis, $|\chi\rangle$, and $\chi_i$ is a component of the exact ground state in this basis. The ground-state energy is obtained by averaging the numerator and denominator separately, with the total psip charge on each site, $q_i^{\text{tot}}$, used in the place of corresponding exact amplitude, $\chi_i$.

Calculating the ground-state expectation value of an operator $\hat{O}$ that does not commute with the Hamiltonian is more difficult because a projected estimator cannot be used. Instead, assuming that $|\psi\rangle$ is real, it is necessary to evaluate

$$\langle \hat{O} \rangle = \frac{\langle \psi | \hat{O} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\sum_{i,j} O_{ij} \chi_i \chi_j}{\sum_i \chi_i^2}, \quad (6)$$

where $O_{ij} = \langle X_i | \hat{O} | X_j \rangle$. Although $\langle \phi_i^{\text{tot}} \rangle = \chi_i$, the expectation value of a product is not equal to the product of the expectation values: $\langle \phi_i^{\text{tot}} \phi_j^{\text{tot}} \rangle \neq \chi_i \chi_j$. This means that $\chi_i \chi_j$ cannot be obtained by averaging the products of the instantaneous psip weights. One could in principle average $q_i^{\text{tot}}$ over many iterations to obtain $\chi_i$ before multiplying $\chi_i$ and $\chi_j$, but this would involve storing a number for every basis function, which is unfeasible due to memory limitations.

This problem is not easy to overcome and there is currently no way to evaluate general expectation values exactly within the FCIQMC framework. Indeed, the calculation of general expectation values in other Monte Carlo methods is often a difficult task.

III. DENSITY MATRIX QUANTUM MONTE CARLO

We now show how an FCIQMC-like dynamics can be used to sample both finite-temperature and ground-state density matrices. We first consider the thermal density matrix and how it can be evolved as a function of inverse temperature by solving the symmetrized Bloch equation. We then draw upon analogies with FCIQMC to formulate the DMQMC algorithm before discussing the calculation of estimators for a general quantum mechanical observable. This section ends with an explanation of how to sample a reduced density matrix in order to calculate estimators of entanglement measures.

A. Theory

Since the psip population (and hence the normalization) varies during a quantum Monte Carlo simulation, it is convenient to work with the unnormalized thermal density matrix

$$\hat{\rho}(\beta) = e^{-\beta \hat{H}}, \quad (7)$$

where $\hat{H}$ is the Hamiltonian operator and $\beta = 1/k_B T$ is the inverse temperature. The canonical partition function $Z(\beta)$ is given by:

$$Z(\beta) = \text{Tr} (\hat{\rho}(\beta)). \quad (8)$$

Differentiating $\hat{\rho}(\beta)$ with respect to $\beta$ shows that it obeys both the Bloch equation,

$$\frac{d\hat{\rho}}{d\beta} = -\hat{H} \hat{\rho}, \quad (9)$$

and the symmetrized Bloch equation,

$$\frac{d\hat{\rho}}{d\beta} = -\frac{1}{2} (\hat{H} \hat{\rho} + \hat{\rho} \hat{H}). \quad (10)$$

The symmetrized version turns out to be more useful for our purposes. Consider the general solution to
Annihilation: The familiar shift-update algorithm already used in FCIQMC, namely:

1. **Annihilation**: Pairs of psips inhabiting the same site \((i, j)\) with opposite charges annihilate and are removed from the simulation, leaving a population of only a single charge type on each site.

   The first three steps describe a stochastic algorithm to sample the solution of a first-order Euler finite-difference approximation to Eq. (10). The distribution of psip charges at \(\beta + \Delta \beta\) is thus proportional to the density matrix at this inverse temperature, provided that the distribution of charges at \(\beta\) was correct.

   The DMQMC method shares many similarities with FCIQMC, namely:
   - Annihilation does not alter the expected (normalized) psip distribution but serves to overcome the sign problem [13, 14].
   - The underlying finite-difference approximation is stable if \(0 < \Delta \beta < 2/(E_{\text{max}} - E_\beta)\), where \(E_{\text{max}}\) is the largest eigenvalue of the Hamiltonian matrix [14]. This is a sufficient condition to ensure correct projection onto the exact ground state, but the finite value of \(\Delta \beta\) leads to an error of \(O(\Delta \beta)\) in the density matrix at temperatures greater than zero. It is therefore necessary to check that finite-temperature results have converged with respect to \(\Delta \beta\).
   - The familiar shift-update algorithm already used in DMC [30] and FCIQMC [12] simulations is employed to modify \(S\) and thus to control the population. The shift, \(S\), is adjusted according to
     \[
     S(\beta + A \Delta \beta) = S(\beta) - \frac{\zeta}{A \Delta \beta} \ln \left( \frac{N_p(\beta + A \Delta \beta)}{N_p(\beta)} \right),
     \]
     where \(A\) is the number of \(\beta\)-steps between shift updates, \(\zeta\) is a shift damping parameter, and \(N_p(\beta)\) is the total number of psips at the inverse-temperature \(\beta\). During simulations, \(\zeta\) is chosen carefully to prevent large fluctuations in \(S\).
   - Rather than attempting all possible spawning events from a psip on a given site, it is computationally efficient to attempt just one (or a small

   We use the following algorithm to evolve a collection of psips according to Eq. (15). For a single step in inverse temperature of \(\Delta \beta\), we loop over the entire population of psips and perform the following steps:

   1. **Spawning along columns of the density matrix**: Allow a psip with charge \(q_{ij}\) on site \((i, j)\) to attempt to spawn onto connected sites \((k, j)\), where \(T_{ik} \neq 0\) and \(i \neq k\), with probability \(\frac{1}{2} |T_{ik}| \Delta \beta\). If the spawning attempt is successful, a psip is born at \((k, j)\) with charge \(q_{kj} = \text{sign}(T_{ik}) q_{ij}\).
The algorithm is highly parallelizable — only the statistically large number of statistically independent data points. Another advantage is that a single simulation can provide better at high temperature than at low temperature. An- other advantage is that a single simulation can provide data across the entire temperature range being studied. It is not uncommon to have to average over a sufficiently large number of estimates obtained using a given number of psips. Consider a composite quantum system \( C \), which greatly reduces the density matrix would be very poorly sampled. However, the dimension of the Hilbert space, \( D \), rises exponentially with the number of particles or sites, \( N \), so that \( D \propto e^{nN} \) and thus \( D^2 \propto e^{o(2N)} \). The doubling of the exponent implies that a DMQMC simulation for an \( N/2 \)-site lattice model requires approximately the same number of psips as an \( N \)-site FCIQMC simulation to achieve the same sampling quality. Moreover, DMQMC estimators for operators that do not commute with the Hamiltonian often have significantly smaller variance than the forward-walking or other estimators required to evaluate the ground-state expectation values of such operators in FCIQMC.

C. Entanglement measures

It straightforward to obtain a stochastic representation of any reduced density matrix (RDM) from a stochastic representation of the full density matrix. Reduced density matrices are required to calculate entanglement measures such as the concurrence described in Appendix A. As a result, configurations in which the average energy of the psip population happens to be less negative than usual are effectively given too large a weight. This problem is particularly severe in DMQMC because the results at each temperature are obtained by averaging over separate \( \beta \)-loops, and thus, for each quantity contributing to a given estimator, the corresponding shift (and hence population) profiles can be very different.

The population bias can be greatly reduced using a method suggested by Umrigar et al. in the context of DMC [13], in which each sampled quantity proportional to the psip population is multiplied by the factor

\[
\Pi(\beta, B) = \prod_{m=0}^{\tilde{B}-1} e^{-S(\beta-m\Delta\beta)},
\]

where \( B \) is some chosen number of factors and \( \tilde{B} = \min(\frac{\beta}{\Delta\beta}, B) \). By multiplying by this factor, we remove the last \( \tilde{B} \) factors of \( e^{\Delta\beta S} \) introduced by varying the shift. As \( B \to \infty \) the population control bias should be completely removed. The population control bias can also be reduced by using a larger population of psips.

Another concern is that the number of elements in the density matrix is the square of the dimension of the Hilbert space of many-particle states. At first glance it seems that, without dramatically increasing the number of psips, the density matrix would be very poorly sampled. However, the dimension of the Hilbert space, \( D \), increases exponentially with the number of particles or sites, \( N \), so that \( D \propto e^{nN} \) and thus \( D^2 \propto e^{o(2N)} \). The doubling of the exponent implies that a DMQMC simulation for an \( N/2 \)-site lattice model requires approximately the same number of psips as an \( N \)-site FCIQMC simulation to achieve the same sampling quality. Moreover, DMQMC estimators for operators that do not commute with the Hamiltonian often have significantly smaller variance than the forward-walking or other estimators required to evaluate the ground-state expectation values of such operators in FCIQMC.
sublattice $A$ is defined by taking the partial trace of the full density matrix, $\rho_C$, over all the sites on sublattice $B$: 

$$\rho_A = \text{Tr}_B(\rho_C).$$  \hfill (19)

Our implementation of DMQMC represents the many-particle basis functions as bit strings $\text{B1}$, where each bit refers to the state of a single spin. To evaluate $\rho_A$ we construct a mask, $I_B$, which only has bits set which correspond to spins in subsystem $B$. The $(i,j)$ density matrix element of $\rho_C$ contributes to $\rho_A$ if the result of the logical $\text{AND}$ operation of the $i$ string with the $I_B$ mask is identical to that of the $j$ string. The corresponding element in the RDM can be found by taking $\text{AND}$ with an analogous $I_A$ mask.

We calculate the desired entanglement measure from the unnormalized stochastic RDM along with its trace at the desired temperature, as discussed in Appendix $\text{A}$ for the case of concurrence. The entanglement measure and trace are averaged over multiple $\beta$-loops, or, for ground-state properties, over many iterations starting from a sufficiently low temperature.

Depending on the specific Hamiltonian, psip population and temperature, it may be that only a few psips survive the masking process to contribute to the RDM. In such cases it is necessary to increase the psip population or accumulate the RDM over several $\beta$-loops before making a single estimate. The use of translational and other symmetries can improve the quality of the sampling of an RDM, although symmetry was not exploited in this work.

Any reduced density matrix can be obtained using DMQMC, but this does not necessarily allow any entanglement measure to be calculated. For example, calculating the von Neumann entropy involves taking the logarithm of the RDM, which requires the full RDM to be represented and diagonalized. This places a limit on the size of the reduced subsystem but not on the full system. Fortunately, many useful entanglement measures involve subsystems containing only a small number of spins.

**IV. IMPORTANCE SAMPLING**

This article considers the application of DMQMC to the $S = 1/2$ antiferromagnetic Heisenberg model,

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j,$$  \hfill (20)

where $J > 0$ and the $\langle i,j \rangle$ implies that the summation is over nearest-neighbor pairs of spins only. Periodic boundary conditions are applied. We work in the standard basis set where the many-spin states are tensor products of the one-spin eigenstates, $|\uparrow\rangle$ and $|\downarrow\rangle$, of the $\hat{S}_z$ operator.

The algorithm described in section II allows a stochastic sampling of the exact finite-temperature density matrix, assuming $\Delta \beta$ is sufficiently small. However, for the antiferromagnetic Heisenberg model, the sampling method described is found to be insufficient for all but the smallest systems. The ground-state wave function is highly delocalized over the states in the basis set, and thus the ground-state density matrix, $\rho = |E_0\rangle \langle E_0|$, has many off-diagonal elements with magnitudes comparable to the diagonal elements. As a result, when the density matrix is sampled via the DMQMC algorithm, only a small fraction of psips reside on or near diagonal elements. Estimators for the expectation values of most operators of interest only receive contributions from psips on or near the diagonal, so very few psips contribute and these estimators suffer from large statistical errors at low temperatures. Importance sampling can greatly improve the sampling quality.

We start by defining the excitation level between basis states $|X_i\rangle$ and $|X_j\rangle$ to be the smallest number of pairs of opposite spins that must be flipped in order to reach $|X_i\rangle$ from $|X_j\rangle$. For the Heisenberg model, Eq. (20), the excitation level can change by at most $\pm 1$ in a single application of the Hamiltonian.

One straightforward way to improve the quality of sampling is to reduce the probability of psips spawning far from the diagonal of the density matrix. Psips that do reside on higher excitation levels are given a correspondingly larger weight, so that expectation values of operators are unchanged. However, the increase in the population of low-weight psips near the diagonal of the density matrix reduces the stochastic error in near-diagonal expectation values.

With this motivation in mind, we define the following importance-sampling procedure: a more rigorous formulation is given in Appendix $\text{B}$. Every time a psip on excitation level $\gamma$ attempts to spawn a new psip on excitation level $\delta$, the probability of successful spawning is altered by a factor $P_{\gamma\delta}$. Thus, if a psip on a diagonal element attempts to spawn a new psip onto the first excitation level, the probability of successful spawning is altered by a factor $P_{01}$, where $P_{01} < 1$. The first excitation level will thus be occupied by $P_{01}$ times as many psips as it would have been with unaltered spawning probabilities. The reduced (relative) population must be accounted for by giving all psips in the first excitation level a weight of $W_1 = 1/P_{01}$ when evaluating estimators. The number of spawning events from the first to the second excitation level is also altered by a factor $P_{01}$ (due to the reduced number of psips at level 1) and the chance of successful spawning for each attempt is multiplied by the factor $P_{12}$. Hence, the weight given to the second excitation level must be $W_2 = 1/P_{01} P_{12}$. Furthermore, since there are $P_{01}$ times as many psips on the first excitation level, the probability of spawning from the first excitation level to the diagonal elements must be enhanced by a factor $1/P_{01}$ in order to achieve consistent spawning dynamics.

In general $P_{\gamma\delta} = 1/P_{\delta\gamma}$ and the weight given to a psip
as if you were reading it naturally. Do not hallucinate.

RAW TEXT START

FIG. 1. (Color online.) The imaginary-time dependence of the fractions of psips on the first four excitation levels during a DMQMC simulation of a 4×4 square antiferromagnetic Heisenberg lattice. A single β-loop was carried out using an initial population of 10^5 psips on the diagonal elements. The results shown in (a) were obtained without importance sampling. The results shown in (b) were obtained using importance sampling to ensure that every excitation level had a roughly equal number of psips at zero temperature.

The estimator for an expectation value, \( \langle \hat{O} \rangle \), is thus

\[
\langle \hat{O} \rangle = \frac{\sum_{i,j} \hat{O}_{ij} \rho_{ij}}{\sum_{ii} \rho_{ii}},
\]

(22)

where \( E(i,j) \) is the excitation level between \( |X_i\rangle \) and \( |X_j\rangle \), and \( \hat{\rho}_{ij} \) is the importance-sampled density matrix. The expected value of the importance-sampled psip charge on site \( (i,j) \) is proportional to \( \hat{\rho}_{ij} \).

There is clearly some freedom in the numerical values chosen for the factors \( P_{\gamma,\delta} \). In this study we adjust \( P_{\gamma,\delta} \) such that all excitation levels have similar psip populations in the ground state. Whilst this choice is not necessarily optimal, it successfully increases the quality of ground-state estimates by many orders of magnitude whilst still allowing the entire density matrix to be sampled. Figures 1(a) and 1(b) show the fractions of psips on the first four excitation levels for the 4×4 square Heisenberg lattice as obtained without and with importance sampling. Both simulations used an initial population of 10^5 psips and a single β-loop. It is clear that importance sampling greatly assists in keeping a non-negligible population on the lower excitation levels.

In practice, the values of \( P_{\gamma,\delta} \) are very small for small \( \gamma \) and \( \delta \) and decrease in magnitude as the lattice size increases. In order to avoid an unnecessarily large suppression of psip spawning from the diagonal at high temperatures, we introduce the weights \( W_\gamma \), and probabilities \( P_{\gamma,\delta} \) gradually from \( \beta = 0 \) until they reach their desired final values at \( \beta_{\text{target}} \). For \( \beta < \beta_{\text{target}} \), the weight at excitation level \( \gamma \) is set equal to \( W_\gamma \beta/\beta_{\text{target}} \); for \( \beta > \beta_{\text{target}} \), the weight is held constant. The value of \( \beta_{\text{target}} \) is chosen to be the imaginary time at which the ground state is deemed to have been reached. However, the value of this parameter is not critical for the quality of the sampling.

V. RESULTS

For this first study of DMQMC we focus primarily on reproducing some exact and well-established results. It is generally the case that QMC simulations of the antiferromagnetic Heisenberg model on square lattices of even dimensions do not suffer from the sign problem. In the FCIQMC and DMQMC methods this is because all psips spawned on any specific site have the same sign and no annihilation occurs [14]. This system is therefore particularly convenient to study.

In order to calculate real finite-temperature properties, it is necessary to include contributions from all \( M_S \) (total spin) subspaces. The Heisenberg Hamiltonian conserves \( M_S \), so different subspaces can be studied using separate simulations, which is an embarrassingly parallel computational task. Combining results for different values of \( M_S \) is straightforward but requires additional calculations and reveals nothing of interest about the performance of DMQMC. We therefore present results for the \( M_S = 0 \) subspace only.

We first consider the example of the 4×4 lattice, which is small enough that an exact diagonalization can be performed, thereby allowing a direct check of our DMQMC results. Figure 2(a) shows the energy as a function of temperature using an initial population of 100 psips at the start of each β-loop and accumulating statistics over 1000 such loops. The shift was allowed to vary throughout the simulation and there were typically 700–800 psips in the simulation by the end of each β-loop. No importance sampling was applied, and so statistical fluctuations increase with inverse temperature as explained in Sec. II.

The agreement with the exact results is very good. Increasing the initial population to 10^5 psips (Fig. 2(b)) reduces the statistical errors such that the agreement with the exact results is essentially perfect.

The square of the staggered magnetization is represented by the operator

\[
\hat{M}^2 = \hat{M} \cdot \hat{M}, \quad \text{with} \quad \hat{M} = \frac{1}{N} \sum_i (-1)^{x_i+y_i} \hat{S}_i,
\]

(23)

where \( x_i \) and \( y_i \) denote the coordinates of the square lattice. This operator does not commute with the Hamiltonian. Its expectation value, \( \langle \hat{M}^2 \rangle \), is plotted as a function of \( \beta \) in Fig. 3 for an 8×8 lattice; a ground-state
The importance-sampling procedure described in the main text was applied. The DMQMC value of $\langle \hat{M}^2 \rangle$ is plotted every 50th iteration. Error bars, where not visible, are smaller than the size of the markers.

The ground-state concurrence, $C_{gs}$, for neighboring spins (qubits) on an antiferromagnetic Heisenberg ring was studied by Wootters and O’Connor in 2001 [37]. They showed that, for an even number of spins, $C_{gs}$ has a simple relationship with the ground-state energy,

$$C_{gs} = \frac{1}{2}(4E_0/N + 1).$$

The exact results calculated from this formula provide a useful test of our DMQMC estimates of $C_{gs}$, which are obtained from the sampled reduced density matrix (see Appendix A).

The DMQMC estimates of $C_{gs}$ are presented in Table I along with Wootters and O’Connor’s exact analytic values for up to $N = 10$ sites. A ring with $N = 36$ sites was also studied, using FCIQMC to calculate $E_0$ and then Eq. (24) to obtain a value of $C_{gs}$ for comparison with the DMQMC results. For lengths up to $N = 10$, the calculation of the concurrence can easily be carried out using other methods and provides a straightforward test of the DMQMC algorithm. The $N = 36$ chain is far from trivial, and it is promising that such accurate results can be obtained.

We note that the DMQMC estimates of $C_{gs}$ were obtained by sampling the reduced density matrix for a single pair of spins. Due to translational invariance, these estimates could have been improved by sampling the reduced density matrix for every neighboring pair and combining the results.

VI. THE SIGN PROBLEM IN DMQMC

As discussed in Sec. II, the annihilation step in FCIQMC leads to the characteristic population dynamics, whereby the sign problem can only be overcome once a critical psip population (the ‘plateau’) has been exceeded. Since the annihilation steps in FCIQMC and DMQMC are identical, we would expect DMQMC to possess similar population dynamics. The annihilation rate for a given psip population in DMQMC will be significantly smaller than in FCIQMC because the number of density matrix elements is the square of the number of basis functions. As such, it is to be expected that the plateau height for a given Hamiltonian will be higher in DMQMC than in FCIQMC.
The full density matrix of the recurrence for rings up to \( N \) responds to a Hilbert space of \( N^2 \) elements. The density matrix was sampled using \( N_p \) psips, and statistics accumulated over \( N_I \) \( \beta \)-loops. Exact results for the energy and recurrence of one-dimensional spin rings by directly sampling reduced density matrices. In all cases investigated, the sign problem in the antiferromagnetic Heisenberg model on a 4 \( \times \) 4 triangular lattice is severe in both FCIQMC and DMQMC calculations. A fixed shift was used and a single \( \beta \)-loop performed. Panel (a) shows the emergence of a plateau in the psip population and (b) shows the exact energy and the DMQMC estimate of the energy as functions of \( \beta \). Once the plateau has been exited, the DMQMC energy is in good agreement with the exact results. The severity of the sign problem increases with inverse temperature.

To investigate this, we considered the antiferromagnetic Heisenberg model on a 4 \( \times \) 4 triangular lattice, for which an exact diagonalization is easily carried out. The triangular lattice is the archetypal example of a frustrated lattice and has a severe sign problem. We carried out a single \( \beta \)-loop and allowed the population to grow with a fixed shift whilst simultaneously investigating the accuracy of the DMQMC energy estimate. Figure 4(a) demonstrates that the population plateaus as expected. Figure 4(b) shows the accuracy of the energy estimate throughout the plateau period.

At high temperatures accurate results are obtained. This is also the case in other finite-temperature methods, where it is generally found that the sign problem is less severe for small \( \beta \); indeed, there is no sign problem at all at infinite temperature. However, at lower temperatures the energy estimates suffer large fluctuations, and it is not until the population exceeds the plateau that a good agreement with exact results is once again obtained. The plateau height occurs at \( \beta J \approx 0.45 \). For comparison, the plateau population in an FCIQMC calculation of the same system is at \( \approx 1.25 \times 10^4 \) psips. We find (in this case) that the DMQMC plateau height is approximately the square of the plateau height in FCIQMC, matching the increase in the size of the space being sampled. It is possible to obtain accurate results for the entire temperature range simply by starting the simulation with an initial population greater than that of the plateau. Moreover, even if the plateau cannot be reached due to memory restrictions, one can nevertheless systematically reach lower temperatures by increasing the population of psips.

The sign problem in the antiferromagnetic Heisenberg model on a triangular lattice is severe in both FCIQMC and DMQMC [14]. However, the efficiency of the annihilation procedure in FCIQMC varies substantially with the system studied and with the basis set used [14]. Furthermore, the initiator approximation (i-FCIQMC) proposed by Cleland et al. [16], has been shown to reduce the memory requirements for FCIQMC calculations by several orders of magnitude in many cases. In i-FCIQMC, spawning events onto previously unoccupied sites are forbidden unless the psip population of the parent site exceeds a threshold. This increases the annihilation rate relative to FCIQMC and ameliorates the sign problem at the expense of introducing a systematically improvable approximation. We have yet to investigate the DMQMC equivalent of the initiator method. It is expected that ground-state properties will be available, but it is not yet clear to what extent the modified spawning will affect finite-temperature results.

| \( C_{gs} \) | \( E_0/N \) | \( E_0/N \) Exact [37] | \( N_p \) | \( N_I \) | \( D \) |
|---|---|---|---|---|---|
| 4 | -0.5000 | 0.5000 | 0.5005(4) | 2.5 \( \times \) 10\(^4\) | 250 | 6 |
| 6 | -0.4671 | 0.4343 | 0.4342(5) | 2.5 \( \times \) 10\(^4\) | 1 \( \times \) 10\(^3\) | 20 |
| 8 | -0.4564 | 0.4128 | 0.4129(5) | 1 \( \times \) 10\(^4\) | 1 \( \times \) 10\(^3\) | 70 |
| 10 | -0.4515 | 0.4031 | 0.4031(4) | 4 \( \times \) 10\(^3\) | 1 \( \times \) 10\(^3\) | 252 |
| 36 | -0.4473(4) | 0.3874(8) | 0.3873(8) | 1 \( \times \) 10\(^6\) | 12 | 9.08 \( \times \) 10\(^9\) |

TABLE I. DMQMC estimates of the ground-state concurrence, \( C_{gs} \), for antiferromagnetic spin rings containing \( N \) sites in the absence of an external magnetic field. Each ring corresponds to a Hilbert space of \( D \) basis functions. The density matrix was sampled using \( N_p \) psips, and statistics accumulated over \( N_I \) \( \beta \)-loops. Exact results for the energy and concurrence of rings up to \( N = 10 \) are taken from Ref. [37]. An FCIQMC calculation was used to find the energy of the \( N = 36 \) chain, from which an “exact” value of \( C_{gs} \) was determined using Eq. [23]. The full density matrix of the \( N = 36 \) chain has approximately \( D^2 = 8.24 \times 10^{19} \) elements.

VII. DISCUSSION

This article has described DMQMC, a quantum Monte Carlo method that allows direct sampling of the finite-temperature and ground-state density matrices in a discrete basis. The validity of the method has been verified by reproducing exact and well-established results for some small systems, including the calculation of the concurrence of one-dimensional spin rings by directly sampling reduced density matrices. In all cases investigated, DMQMC has proved capable and accurate.

The introduction of an importance-sampling procedure allows larger lattices to be investigated — the largest system that we have simulated successfully to date is a.
10\times10 antiferromagnetic Heisenberg model. Larger systems could easily be tackled at high temperatures, but it is unlikely that our very simple approach to importance sampling will allow simulations of lattices of more than 10\times10 sites over the entire range of temperatures from infinity to zero. If a better importance-sampling procedure can be devised, as we believe likely, many more avenues will be opened.

Like FCIQMC, DMQMC uses an annihilation procedure that allows it to overcome the sign problem if a system-specific population of psips is reached. In FCIQMC the sign problem can often be ameliorated, for example by changing to a more appropriate basis set [14, 28] or by applying the initiator approximation [16]. Given the similarities between DMQMC and FCIQMC, it is likely that these ideas and future developments in FCIQMC will also apply to DMQMC. Due to the relative youth of FCIQMC, the rate of theoretical and algorithmic improvements is rapid [16, 20].

The lattices studied with DMQMC so far are small by the standards of path-integral quantum Monte Carlo methods. However, the unique and defining feature of DMQMC is that it samples the full density matrix. Given the prominent role of the density matrix in the study of quantum information measures and the wide applicability of DMQMC, we hope that DMQMC will prove useful enough to justify further development.

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### Appendix A: Concurrence

For the special case of a two-qubit mixed state, the entanglement of formation can be calculated from a quantity known as the “concurrence”. Given a reduced density matrix \( \rho_A \), where in this case \( A \) refers to a subsystem of two qubits, the concurrence is defined as

\[
C(\rho_A) \equiv \max(0, \gamma_1 - \gamma_2 - \gamma_3 - \gamma_4),
\]

where \( \gamma_1 > \gamma_2 > \gamma_3 > \gamma_4 \) are the eigenvalues of the matrix

\[
R = \sqrt{\rho_A \hat{\rho}_A \rho_A},
\]

and

\[
\hat{\rho}_A = (\sigma_y \otimes \sigma_y)\rho_A^* (\sigma_y \otimes \sigma_y),
\]

with \( \sigma_y \) the Pauli spin matrix for the \( y \)-direction. This expression is only valid in the standard basis set.

The value of the concurrence \( C \) ranges from zero to one and is monotonically related to the entanglement of formation [39]; the concurrence can therefore be regarded as a measure of entanglement. The entanglement of formation for two qubits [40] is given by

\[
E(C) = h\left(\frac{1 + \sqrt{1 - C^2}}{2}\right),
\]

where

\[
h(x) = -x \log_2 x - (1 - x) \log_2 (1 - x).
\]

If the Hamiltonian and thus the reduced density matrix are real (as is the case in the Heisenberg model), the calculation of \( C \) reduces to the calculation of the moduli of the eigenvalues of \( R = \rho_A (\sigma_y \otimes \sigma_y) \).

Since \( R \) is a \( 4 \times 4 \) matrix, it is trivial to compute the concurrence by direct diagonalization once \( \rho_A \) is known.

Using DMQMC, it is possible to sample the unnormalized reduced density matrix as described in Sec. III and thus to estimate the concurrence using

\[
\langle C \rangle = \frac{\max(0, \gamma_1 - \gamma_2 - \gamma_3 - \gamma_4)}{\text{Tr}(\rho_A)},
\]

where \( \rho_A \) is now the unnormalized reduced density matrix and \( \{\gamma_i\} \) are the eigenvalues of the unnormalized matrix \( R \).

### Appendix B: Importance sampling

The DMQMC evolution equation is

\[
\frac{d\hat{\rho}_{ij}}{d\beta} = \frac{1}{2} \sum_k (T_{ik}\rho_{kj} + \rho_{ik}T_{kj}),
\]

where \( \rho_{ij} \) is an element of \( \hat{\rho} \) in the many-particle basis chosen for the simulation. Instead of \( \rho_{ij} \), we would like to sample the importance-sampled density matrix

\[
\hat{\rho}_{ij} = \frac{\rho_{ij}}{W_{E(i,j)}},
\]

where \( E(i,j) \) is the excitation level of the pair \( (i,j) \) and \( W_a \) is defined in Eq. (21). Following the standard procedure of importance sampling, we introduce a trial function

\[
\rho_{ij}^T = \frac{1}{W_{E(i,j)}},
\]

This matrix is symmetric, \( \rho_{ij}^T = \rho_{ji}^T \), as \( E(i,j) = E(j,i) \). The importance-sampled density matrix then has components \( \hat{\rho}_{ij} = \rho_{ij}^T \rho_{ij} \), where no summation is performed.
over indices. Multiplying Eq. (B1) by $\rho_{ij}^T$ yields the following evolution equation for $\tilde{\rho}_{ij}$:

$$\frac{d(\rho_{ij}^T\tilde{\rho}_{ij})}{d\beta} = \frac{1}{2} \sum_k \left( \left( \rho_{ij}^T T_{ik} \frac{1}{\rho_{kj}} + \rho_{ik} T_{kj} \tilde{\rho}_{kj} \right) \rho_{ij}^T \tilde{\rho}_{kj} + \left( \rho_{ik}^T T_{kj} \frac{1}{\rho_{ik}} + \rho_{kj} T_{ik} \tilde{\rho}_{ik} \right) \rho_{ij}^T \tilde{\rho}_{ik} \right) \right) \right) \right)$$

$$\Rightarrow \frac{d\tilde{\rho}_{ij}}{d\beta} = \frac{1}{2} \sum_k \left( (\rho_{ij}^T T_{ik} \frac{1}{\rho_{kj}}) \tilde{\rho}_{kj} + \tilde{\rho}_{ik} (\rho_{ij}^T T_{kj} \frac{1}{\rho_{ik}}) \right).$$

The above differential equation is entirely analogous to the standard DMQMC algorithm: the extra factors of $\rho^T$ simply act to alter the spawning probabilities. Consider the case where the excitation level of $(i, j)$ is $\gamma$ and excitation level of $(k, j)$ is $\gamma - 1$. The probability that a spawning attempt from $(k, j)$ to $(i, j)$ is successful is altered by the factor

$$\rho_{ij}^T \frac{1}{\rho_{kj}^T} = \frac{W_{E(k,j)}}{W_{E(i,j)}} = \frac{W_{\gamma-1}}{W_{\gamma}} = P_{\gamma-1,\gamma},$$

where Eq. (21) has been used to simplify the expression. Similarly, when spawning in the opposite direction, the probability is altered by the reciprocal of this factor. Spawning events that do not alter the excitation level are unaffected.