Nested Cluster Algorithm for Frustrated Quantum Antiferromagnets

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(Received 28 March 2008; revised manuscript received 15 May 2008; published 19 June 2008)

Frustrated antiferromagnets are important materials whose quantum Monte Carlo simulation suffers from a severe sign problem. We construct a nested cluster algorithm which uses a powerful strategy to address this problem. For the spin $\frac{1}{2}$ Heisenberg antiferromagnet on a kagome and on a frustrated square lattice the sign problem is eliminated for large systems. The method is applicable to general lattice geometries but limited to moderate temperatures.

DOI: 10.1103/PhysRevLett.100.247206 PACS numbers: 75.40.Mg, 75.10.Jm, 75.50.Ee

Numerous strongly correlated electron materials are governed by competing interactions. In particular, quantum antiferromagnets such as $Na_xCoO_2 \cdot yH_2O$ and $ZnCu_3(OH)_6Cl_2$ are geometrically frustrated. At present, the theoretical understanding of such materials from first principles is hindered by a very severe sign problem which prevents the application of standard quantum Monte Carlo methods. In this Letter we construct a nested cluster algorithm that solves the sign problem and, for the first time, allows us to simulate large frustrated antiferromagnets, at least at moderate temperatures. This is very useful, for example, for determining the couplings of frustrated magnets by comparison with experimental finite temperature data. To demonstrate the strength of the new method, we apply it to the spin $\frac{1}{2}$ Heisenberg antiferromagnet on kagome and frustrated square lattices of sizes never reached before in quantum Monte Carlo simulations of these systems.

Efficient cluster algorithms performing nonlocal updates were first developed by Swendsen and Wang for discrete classical Ising and Potts spins [1] and then generalized by Wolff [2] to classical spins with a continuous $O(N)$ symmetry. Improved estimators which average over an exponentially large number of configurations at polynomial cost are an additional benefit of cluster algorithms. The first cluster algorithm for the spin $\frac{1}{2}$ quantum Heisenberg model was developed in [3]. While that algorithm works efficiently only for quantum spin chains, the loop-cluster algorithm [4] is efficient also in higher dimensions, and was first applied to the 2D spin $\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice in [5]. The continuous-time variant of the algorithm eliminates the Suzuki-Trotter time-discretization error and can reach very low temperatures [6]. This method has also been used to simulate systems on very large lattices [7] and with very long correlation lengths [8]. An elegant and powerful related method based on stochastic series expansion is available as well [9].

Unfortunately, in many cases of physical interest, including frustrated quantum spin systems, quantum Monte Carlo calculations suffer from a very severe sign problem. Using an improved estimator, the sign problem of the 2D classical $O(3)$ model at vacuum angle $\theta = \pi$ has been addressed with a variant of the Wolff cluster algorithm [10]. In that case, some clusters are half-instantons also known as merons. Flipping a meron cluster leads to a sign change of the Boltzmann weight and hence to an exact cancellation between two configurations. As a consequence, only configurations without meron clusters contribute to the partition function. Restricting the simulation to those configurations eliminates the sign problem, since all configurations in the zero-meron sector have a positive sign. The meron concept has been generalized to fermionic systems [11] and the meron-cluster algorithm has been used to solve a number of very severe fermion sign problems [12–14]. Unfortunately, the meron-cluster algorithm is not generally applicable. In fact, as shown in [15], some sign problems are NP complete. Hence, a hypothetical method that can solve any sign problem would solve all NP-complete problems in polynomial time. This would imply the equality of the complexity classes NP = P. Since it is generally believed that NP ≠ P, it is expected that a universally applicable method that solves all sign problems cannot exist.

Let us consider the antiferromagnetic spin $\frac{1}{2}$ quantum Heisenberg model with the Hamiltonian

$$H = \sum_{x,y\in\Lambda} J_{xy}\vec{S}_x \cdot \vec{S}_y. \tag{1}$$

Here $\vec{S}_x$ is a quantum spin operator located at the site x of a lattice Λ, and $J_{xy} > 0$ is the antiferromagnetic exchange coupling between a pair of spins located at the sites x and y. Although our method can be applied directly in the Euclidean time continuum, in order to ease its implementation we work in discrete time. Depending on the lattice geometry, the Hamiltonian $H = H_1 + H_2 + \ldots + H_M$ is expressed as a sum of M terms H_i which leads to a Suzuki-Trotter decomposition of the partition function

$$\begin{aligned} Z &= \mathrm{Tr}\exp(-\beta H) \\ &= \lim_{\varepsilon\to 0}\mathrm{Tr}[\exp(-\varepsilon H_1)\exp(-\varepsilon H_2)\ldots\exp(-\varepsilon H_M)]^N. \end{aligned} \tag{2}$$

Here the inverse temperature $\beta = 1/T = N\varepsilon$ represents the extent of a periodic Euclidean time interval, which is divided into N discrete time steps of size ε. Each H_i is a sum of mutually commuting pair interactions $h_{xy} = J_{xy}\vec{S}_x \cdot \vec{S}_y$ on a set of disconnected bonds. Inserting complete sets of spin states $s_{x,t} = \pm\frac{1}{2} = \uparrow, \downarrow$ between the factors $\exp(-\varepsilon H_i)$ in Eq. (2), the partition function is expressed as a path integral over all spin configurations $[s]$ with the Euclidean action $S[s]$ [5]

$$Z = \sum_{[s]} \mathrm{Sign}[s] \exp(-S[s]). \tag{3}$$

The weight $\mathrm{Sign}[s]\exp(-S[s])$ of a spin configuration $[s]$ is a product of contributions from individual space-time plaquettes corresponding to the two-spin transfer matrix elements $\langle s_{x,t}s_{y,t}|\exp(-\varepsilon h_{xy})|s_{x,t+1}s_{y,t+1}\rangle$. In the basis $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ the two-spin transfer matrix reads

$$\exp(-\varepsilon h_{xy}) = \exp\left(\frac{\varepsilon J}{4}\right)\begin{pmatrix} A & 0 & 0 & 0 \\ 0 & A+B & -B & 0 \\ 0 & -B & A+B & 0 \\ 0 & 0 & 0 & A \end{pmatrix}, \tag{4}$$

with $A = \exp(-\varepsilon J_{xy}/2)$ and $B = \sinh(\varepsilon J_{xy}/2)$. The off-diagonal transfer matrix elements are negative. The product of the negative signs over all space-time plaquettes defines the total $\mathrm{Sign}[s] = \pm 1$ of a spin configuration. The remaining factor $\exp(-S[s])$ represents a positive Boltzmann weight which can be interpreted as a probability and thus can be used for importance sampling in a Monte Carlo simulation.

When one samples the system using the positive weight $\exp(-S[s])$, one must include $\mathrm{Sign}[s]$ in the measured observables $O[s]$ and expectation values are given by

$$\langle O\rangle = \frac{1}{Z}\sum_{[s]} O[s]\mathrm{Sign}[s]\exp(-S[s]) = \frac{\langle O\mathrm{Sign}\rangle_+}{\langle \mathrm{Sign}\rangle_+}. \tag{5}$$

Here the index $+$ refers to expectation values in the simulated ensemble with positive Boltzmann weights and partition function $Z_+ = \sum_{[s]}\exp(-S[s])$ such that

$$\begin{aligned}\langle \mathrm{Sign}\rangle_+ &= \frac{1}{Z_+}\sum_{[s]}\mathrm{Sign}[s]\exp(-S[s]) \\ &= \frac{Z}{Z_+} \sim \exp(-\Delta f \beta V).\end{aligned} \tag{6}$$

Here V is the spatial volume and Δf is the difference between the free energy densities of the original ensemble with the weight $\mathrm{Sign}[s]\exp(-S[s])$ and the simulated ensemble with the positive weight $\exp(-S[s])$. The expectation value of the sign is exponentially small in the space-time volume βV. Since it is obtained as a Monte Carlo average of contributions $\mathrm{Sign}[s] = \pm 1$, one needs an exponentially large statistics in order to accurately measure $\langle \mathrm{Sign}\rangle_+$. This is impossible in practice and gives rise to a very severe sign problem.

How can one increase the statistics by an exponential factor without investing more than a polynomial numerical effort? The meron-cluster algorithm [10,11] achieves this by constructing an improved estimator for the sign. Like the meron-cluster algorithm, the method presented here is based on the loop-cluster algorithm [4] which decorates a spin configuration with bonds connecting spins to closed loop clusters. The four spins on a space-time plaquette are connected in pairs. In fact, A and B in Eq. (4) represent weights of two possible bond configurations on a space-time plaquette. The weight A corresponds to bonds connecting the spins $s_{x,t}$ and $s_{y,t}$ with their timelike neighbors $s_{x,t+1}$ and $s_{y,t+1}$, while B corresponds to spacelike bonds connecting $s_{x,t}$ with $s_{y,t}$ and $s_{x,t+1}$ with $s_{y,t+1}$. Sites connected by bonds form a closed oriented loop cluster. Up to an overall spin-flip of the entire cluster, the spin configuration on a cluster is determined by the cluster geometry. Timelike bonds connect parallel spins, while spacelike bonds connect antiparallel spins. Integrating out the spins, the partition function can be expressed as a sum over bond configurations $[b]$

$$Z = \sum_{[b]} \mathrm{Sign}[b] A^{n_A} B^{n_B} 2^{N_C}. \tag{7}$$

Here n_A is the number of timelike and n_B is the number of spacelike plaquette breakups, while N_C is the number of loop clusters. The factor 2^{N_C} arises because each cluster has two possible spin orientations. The partition function can be sampled by a Metropolis update of the plaquette breakups. Remarkably, while the original cluster algorithm which operates on spins and bonds never changes the sign and is thus not ergodic [16], the algorithm which operates only on bonds (after the spins have been integrated out) is ergodic and still avoids unnatural freezing. Interestingly, $\mathrm{Sign}[s]$ remains invariant under cluster flips; i.e., all clusters are nonmerons. However, in this case the meron-cluster algorithm does not solve the sign problem because almost half of the configurations in the zero-meron sector have a negative sign [16]. Since it does not change under spin flips, $\mathrm{Sign}[s] = \mathrm{Sign}[b]$ is uniquely determined by the bond configuration. It is important to note that the sign can be expressed as a product of cluster signs $\mathrm{Sign}[b] = \prod_C \mathrm{Sign}_C$. Depending on the orientation of a cluster, each spacelike breakup contributes a factor $\pm i$ to the two clusters traversing the corresponding space-time plaquette. By construction, each cluster traverses an even number of spacelike breakups, and hence $\mathrm{Sign}_C = \pm 1$.

We distinguish space-time plaquettes shared by two different clusters from internal plaquettes belonging entirely to one cluster. Updating the breakup on a space-time plaquette shared by two different clusters does not lead to a sign change. Only updates of cluster-internal plaquettes may change the sign. We apply the following method to

construct an improved estimator for the sign. Once a statistically independent bond configuration has been produced by the cluster algorithm, we perform an inner Monte Carlo simulation by updating only the cluster-internal plaquette breakups. Each cluster $\mathcal{C}$ defines the set of lattice sites $\Lambda_{\mathcal{C}}$ contained in $\mathcal{C}$. The inner Monte Carlo algorithm generates clusters with different orientations that visit all sites of $\Lambda_{\mathcal{C}}$ in different orders, thus contributing different values of $\mathrm{Sign}_{\mathcal{C}}$. In this process, breakups that lead to the decomposition of $\Lambda_{\mathcal{C}}$ into separate clusters must be rejected. The inner Monte Carlo algorithm estimates an average $\langle \mathrm{Sign}_{\mathcal{C}} \rangle_i$ for each set of sites $\Lambda_{\mathcal{C}}$. Since the different sets are independent, the improved estimator of the sign is given by

$$\langle \mathrm{Sign} \rangle_i = \prod_{\Lambda_{\mathcal{C}}} \langle \mathrm{Sign}_{\mathcal{C}} \rangle_i. \tag{8}$$

Remarkably, the nesting of an outer and an inner cluster algorithm achieves exponential error reduction at a cost linear in the volume (as long as the cluster size remains fixed). A similar strategy was very successfully applied to the measurement of exponentially suppressed Wilson loops in lattice gauge theory [17] as well as to quantum impurity models [18]. Correlation functions and susceptibilities can also be measured with improved estimators. Let us consider the staggered magnetization operator $\vec{M}_s = \sum_x z_x \vec{S}_x$. Here z_x is a stagger factor depending on the sublattice to which the site x belongs. The corresponding staggered susceptibility

$$\chi_s = \frac{\langle M_s^2 \mathrm{Sign} \rangle_+}{\beta V \langle \mathrm{Sign} \rangle_+} = \frac{\langle \langle M_s^2 \mathrm{Sign} \rangle_i \rangle_+}{\beta V \langle \langle \mathrm{Sign} \rangle_i \rangle_+} \tag{9}$$

is obtained from an improved estimator which is given in terms of $M_s = \sum_{\mathcal{C}} M_{s\mathcal{C}}$ with $M_{s\mathcal{C}} = \sum_{(x,t)\in\mathcal{C}} z_x s_{x,t}$ as

$$\langle M_s^2 \mathrm{Sign} \rangle_i = \sum_{\Lambda_{\mathcal{C}}} \langle M_{s\mathcal{C}}^2 \mathrm{Sign}_{\mathcal{C}} \rangle_i \prod_{\Lambda_{\mathcal{C}'} \neq \Lambda_{\mathcal{C}}} \langle \mathrm{Sign}_{\mathcal{C}'} \rangle_i. \tag{10}$$

In which cases will the nested cluster algorithm eliminate or at least substantially reduce the sign problem? Since some sign problems are NP hard, it is expected that any method will fail at least in those cases. The nested cluster algorithm fails to solve the sign problem when a cluster fills almost the entire volume, because then the inner Monte Carlo algorithm becomes inefficient. Since large clusters necessarily arise in the presence of large correlation lengths, the nested cluster algorithm does not work efficiently in low-temperature ordered phases.

Even in the absence of long-range order, cluster algorithms may become inefficient if the clusters grow to unphysically large sizes beyond the physical correlation length. This potential problem is prevented when there is a reference configuration that limits cluster growth [14]. For the antiferromagnet on the square lattice the reference configuration is given by the classical Néel state; i.e., all spins in a loop cluster are in a staggered pattern. The

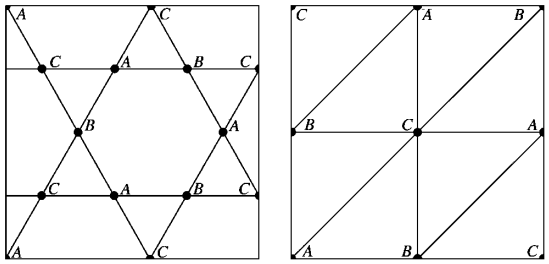

FIG. 1. Kagome lattice (left) and frustrated square (or anisotropic triangular) lattice (right) consisting of three sublattices A, B, C.

cluster size squared is then tied to the staggered susceptibility which protects the clusters from growing to unphysically large sizes. Also for frustrated systems it is natural to consider a classical ground state as a reference configuration. When one quantizes the spins along a local quantization axis in the direction of the spin orientation in the classical ground state, an interesting algorithm with open string clusters emerges. The spins in each cluster are in the reference configuration and hence these clusters are protected from becoming unphysically large. However, the meron concept does not apply to the open string clusters; i.e., when these clusters are flipped, they are not independent but affect each other in their effect on the sign. As will be explained elsewhere, one can still integrate out the spins analytically. This glues the open string clusters together to the closed loop clusters of the algorithm discussed before. While typical closed loop clusters are hence larger than the correlation length corresponding to the classical order, they still represent physical correlated regions. In fact, they grow up to the length scale at which the signs, which are a manifestation of quantum entanglement, decorrelate.

Even if the typical cluster size is moderate, the inner Monte Carlo algorithm may not lead to an efficient cancellation of signs. For example, there are cases in which the improved estimator $\langle \mathrm{Sign} \rangle_i$ is not positive. Still, if such cases are rare, the sign problem is substantially reduced. To optimize the performance of the algorithm, the numerical

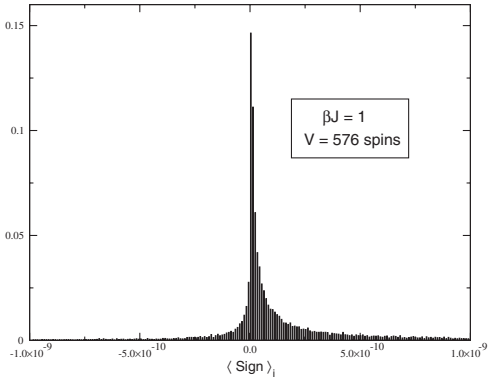

FIG. 2. Probability distribution of $\langle \mathrm{Sign} \rangle_i$ for the kagome lattice with $V = 576$ spins and $\beta J = 1$.

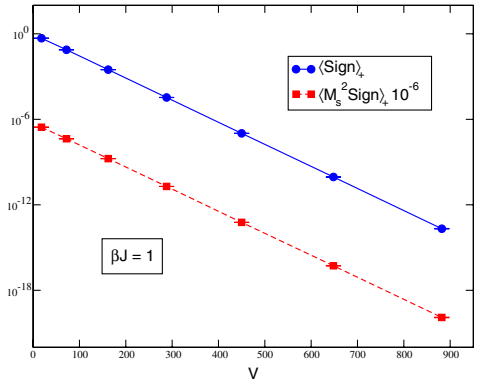

FIG. 3 (color online). Volume-dependence of $\langle \mathrm{Sign} \rangle_+$ and $\langle M_s^2 \mathrm{Sign} \rangle_+$ (rescaled by 10^{-6}) for the kagome lattice with $\beta J = 1$.

effort invested in the inner and outer Monte Carlo procedures must be properly balanced against each other. It pays to invest a larger number of inner Monte Carlo sweeps on the larger sets Λ_C. In any case, the efficiency of the nested cluster algorithm must be investigated on a case-by-case basis.

We now consider the Heisenberg antiferromagnet with uniform nearest-neighbor coupling $J_{xy} = J$ on the lattices illustrated in Fig. 1. The frustrated square lattice has an additional coupling J' along the diagonals. We have simulated large kagome lattices with up to $V \approx 1000$ spins at moderate temperatures with $\beta J \approx 1$. Figure 2 shows the probability distribution of the improved estimator $\langle \mathrm{Sign} \rangle_i$. Although sometimes it is negative, it still leads to an accurate determination of the average sign. We consider M_s with $z_x = 1, -1, 0$ on sublattice A, B, C, respectively, which may signal coplanar spin order. As shown in Fig. 3, with increasing volume V both $\langle \mathrm{Sign} \rangle_+$ and $\langle M_s^2 \mathrm{Sign} \rangle_+$ decrease dramatically over numerous orders of magnitude, but are still accurately accounted for by the nested cluster algorithm. For example, with $V = 882$ spins $\langle \mathrm{Sign} \rangle_+ = 2.09(8) \times 10^{-14}$. A brute force approach would require an astronomical statistics of about 10^{30} sweeps in order to achieve a similar precision. Figure 4 shows the coplanar staggered susceptibility χ_s compared to the collinear Néel susceptibility χ_N. On the square lattice, frustration reduces the Néel order, while (at least for $J' = J/4$) the coplanar order is as weak as on the kagome lattice (and practically indistinguishable from it in Fig. 4).

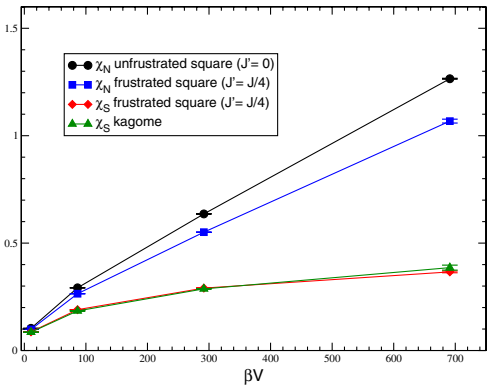

FIG. 4 (color online). Coplanar staggered susceptibility χ_s and collinear Néel susceptibility χ_N as functions of the space-time volume βV for the kagome as well as the frustrated ($J' = J/4$) and unfrustrated ($J' = 0$) square lattice at fixed space/time aspect ratio $\sqrt{V}/\beta J = 20$.

To conclude, in contrast to other Monte Carlo methods, the nested cluster algorithm is capable of eliminating very severe sign problems for large systems, at least at moderate temperatures. As we have demonstrated, by studying appropriate susceptibilities one may obtain valuable insights concerning possible types of order. Applications to frustrated antiferromagnets on various lattice geometries are currently in progress.

U.-J. W. likes to thank S. Chandrasekharan for a long-lasting fruitful and very inspiring collaboration on the sign problem. We also have benefited from interesting discussions with M. Troyer. This work was supported by the Schweizerischer Nationalfonds.

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