Neél Order in Square and Triangular Lattice Heisenberg Models

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We show that the density matrix renormalization group can be used to study magnetic ordering in two-dimensional spin models. Local quantities should be extrapolated with the truncation error, not with its square root. We introduce sequences of clusters, using cylindrical boundary conditions with pinning fields, which provide for rapidly converging finite-size scaling. We determine the magnetization for both the square and triangular Heisenberg lattices with errors comparable to the best alternative approaches.

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Two-dimensional (2D) quantum lattice systems studied in condensed matter physics can be divided into two types: those with a sign problem in quantum Monte Carlo (QMC) simulations and those without one. This is because recent developments in QMC calculations [1–3] have enabled remarkably accurate large-scale studies of the latter systems, such as the square-lattice Heisenberg model (SLHM) [4]. In contrast, the former systems, such as the triangular lattice Heisenberg model (TLHM) and other models with geometric frustration, are often the subject of controversy even regarding questions of what type of order, if any, is present. For the TLHM, it is only recently that the rough agreement between several theoretical [5] and numerical [6–8] methods has made a convincing case that the model has three-sublattice, noncollinear 120° order.

The density matrix renormalization group (DMRG) [9] is not subject to the sign problem, it has an error which can be systematically decreased by increasing m, the number of states kept per block, and it is extremely accurate for one-dimensional systems. For 2D systems, the value of m needed in order to achieve a fixed accuracy, while weakly dependent on the system length L_x, grows exponentially with the width L_y. This effect is not immediately disastrous because the 1D accuracy is so high; systems with widths up to $L_y = 6 - 8$ have been studied with DMRG. Such widths are marginally useful for finite-size extrapolations, and even modest improvements would be useful. One such improvement is extrapolation in the truncation error (or discarded weight) ε, which is the sum of the discarded density matrix eigenvalues and is controlled by varying m. The extrapolation of the energy with $\varepsilon \to 0$ can improve its accuracy by nearly an order of magnitude [9–11]. However, for observables other than the energy, extrapolation has been more problematic and is much less used.

In this Letter we show that the difficulty in extrapolating local measurements A is due to the incorrect assumption that the error $\Delta A \sim \varepsilon^{1/2}$. In fact, the simplest way to measure local quantities within DMRG makes ΔA *analytic* in ε. The resulting extrapolations perform extremely well. A limitation of DMRG is a large loss of accuracy if periodic boundary conditions (BCs) are used lengthwise. To study the staggered magnetization M, we use an approach using cylindrical BCs on $L_x \neq L_y$ clusters and pinning magnetic fields. We show that with an appropriate choice of the aspect ratio $\alpha = L_x/L_y$, M scales much more rapidly to the thermodynamic limit than in widely used methods based on correlation functions on $L_x = L_y$ clusters with periodic BCs. Using these two improved extrapolation methods, our results for M are comparable to the best published QMC calculations [4,12] for the SLHM and to the best series expansion [8] and Green's function Monte Carlo [7] results for the TLHM.

We consider the $S = \frac{1}{2}$ Heisenberg model

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \tag{1}$$

with $J = 1$ on square and triangular lattices, where $\langle ij \rangle$ denotes nearest neighbor sites. We study $L_x \times L_y$ systems with periodic BCs in the y direction, and open BCs with pinning in the x direction. For the SLHM we consider both the standard orientation of the lattice and one tilted by 45°. In all cases we apply a staggered pinning field corresponding to infinite pinning on the edges of an auxiliary $(L_x + 2) \times L_y$ system, e.g., ± 0.5 for the standard orientation SLHM. Since our DMRG program conserves total S_z, for the TLHM it is not possible to pin all three sublattices simultaneously. Instead, we only pin in the z direction, pinning one sublattice (pointing down), with the other two free to rotate in a cone. Thus we expect one sublattice to exhibit $\langle S_z \rangle = -M$, and the other two $+M/2$.

We focus on the resulting on site magnetization $M_C = |\langle S_z \rangle|$ in the center column of the system. For any fixed $\alpha = L_x/L_y$, M_C approaches its thermodynamic limit M_0 as $L_x, L_y \to \infty$. For $L_x \gg L_y$, the system looks more one dimensional and we expect M_C to approach M_0 from below. For $L_y \gg L_x$, the strong pinning dominates and we expect an approach from above. We utilize intermediate α to accelerate the convergence with system size.

First we discuss the convergence of DMRG with ε. If the truncation of density matrix states were made starting from the exact ground state ψ_0, then the truncation error and energy error would vary as (to leading order) $\varepsilon \sim \Delta E \sim |\Delta\psi|^2$, where $\Delta\psi = \psi - \psi_0$, and ψ is the new approximate

ground state [13]. For measurements of an operator $\hat{A}$ other than the Hamiltonian, standard variational arguments imply an error proportional to $\langle \Delta\psi|\hat{A}|\psi_0\rangle$, and thus $\propto \varepsilon^{1/2}$.

Consider the special situation where ψ is the lowest energy state within an incomplete basis B. Let C be the complement of B. Note that ψ is an exact eigenstate in the complete basis of a modified Hamiltonian in which the off-diagonal terms connecting B and C are set to zero. Label these coupling terms λV. Assuming ψ is close to the true ground state ψ_0, $\lambda V\psi$ is small, and one can consider λV as a small perturbation. The leading term in $\Delta\psi$, neglecting energy denominators, is $\propto \lambda V\psi$, which is in C.

Now consider a change of basis for C, negating each basis function. This sends $\lambda \rightarrow -\lambda$, but leaves the energy unchanged. Thus we expect analytic behavior for $E(\lambda^2)$. For the exact ground state ψ_0, the change of basis switches the sign of the C coefficients. The truncation error ε is (ideally [13]) the sum of the squares of these coefficients, and is therefore also an even function of λ. Consider an operator $\hat{A}$ which is block diagonal within the B/C split. Its expectation value would also be independent of the change of basis, and thus an analytic function of λ^2.

Within DMRG, the seemingly restrictive assumption that the operator $\hat{A}$ is block diagonal is easily satisfied for a local operator, such as S_z. Consider one particular DMRG step, and consider measuring an $\hat{A}$ which acts only on one or both of the central two sites, not part of the truncated left and right blocks. As part of the DMRG step, one finds the ground state ψ within the current reduced basis (B). Applying $\hat{A}$ on ψ creates a state which is exactly represented within this basis; therefore $\hat{A}$ is block diagonal. At this step only a few operators can be measured accurately, but as the algorithm sweeps through the lattice all local operators can be measured.

To utilize this analytic behavior in an extrapolation, one assumes that increasing m in successive sweeps corresponds to decreasing λ. (More accurately, increasing m moves states with large couplings from C to B.) Then, both the energy and central-site operators should have polynomial (i.e., analytic) dependence on the truncation error, and one can expect well-behaved polynomial extrapolations.

In Fig. 1, we show the behavior of $\langle S_z\rangle$ as a function of ε for two modest sized systems where essentially exact results could be obtained. The results show no signs of nonanalytic behavior as $\varepsilon \rightarrow 0$, and are fit nicely with a quadratic form. Using results from a number of similar modest sized systems we have devised a simple empirical ''recipe'' to reliably extrapolate to $\varepsilon \rightarrow 0$ for a local quantity such as $\langle S_z\rangle$, as is already commonly done with the total energy. Specifically, we utilize only the most accurate decade of data available, and fit it with a cubic polynomial. The error bars assumed for the purpose of the fit are proportional to ε. The extrapolation can be checked by a fourth order fit, or a quadratic fit over a smaller range. If these extrapolations agree well, the extrapolation is judged acceptable and we take as a rough error estimate the empirical parameter 0.2 times the size of the extrapolation from the last data point.

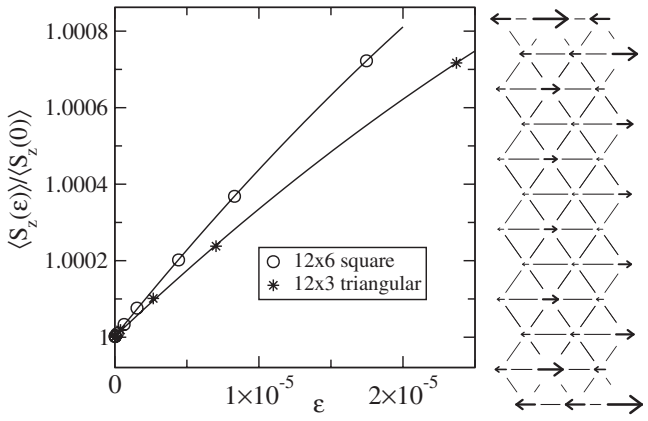

FIG. 1. $\langle S_z\rangle$ for a central site versus the truncation error ε, normalized to the $\varepsilon = 0$ result. The solid lines are quadratic fits. The 12×3 cluster, with true dimensions $6\sqrt{3} \times 3$, rotated 90°, is shown. The length of the arrows is proportional to $\langle S_z\rangle$, and pinning fields were $-0.25, -0.25, 0.5$.

The implications of the analytic behavior in ε are significant: local measurements for finite ε are more accurate than previously thought, and the extrapolation $\varepsilon \rightarrow 0$ improves results and provides error estimates.

We now turn to finite-size effects. Previous QMC studies of the magnetization M have utilized correlation functions measured in periodic $L \times L$ systems, and extrapolation in $1/L$ for the quantity M_0^2. The leading term varies as $1/L$ with a substantial coefficient. The expansion in $1/L$ for the periodic $L \times L$ SLHM is known in detail from chiral perturbation theory, allowing Sandvik to determine $M_0 = 0.3070(3)$ using only systems up to $L = 16$ [4]. For the TLHM, chiral perturbation results are not available, and less robust QMC methods must be used, making extrapolation to $L \rightarrow \infty$ much more difficult. For example, Capriotti *et al.* extrapolated Green's function Monte Carlo results with $M^2 \geq 0.13$ for $L \leq 10$ down to $M_0^2 \sim 0.04$ for $L \rightarrow \infty$ to obtain $M_0 = 0.205(10)$. Other estimates [5] range as high as $M_0 = 0.266$.

The leading $1/L$ scaling of the order parameter M in the 2D Heisenberg systems is universal and is determined by the long-wavelength spectrum of the problem, namely, by the massless spin waves [14]. We have analyzed the effect of the aspect ratio $\alpha = L_x/L_y$ on the scaling for pinned cylindrical and for periodic clusters using both finite-size scaling within an effective σ model and finite-size spin-wave theory (FSSWT). A key conclusion from both methods is that the coefficient in the $1/L$ correction to M depends on α and, for special aspect ratios α_c, vanishes, leaving corrections of order $O(1/L^2)$. The two methods agree exactly on the values of α_c for nontilted and tilted square-lattice clusters: for periodic systems, $\alpha_c = 7.0555$, while for cylindrical systems, for M_C in the middle of the cluster, $\alpha_c = 1.7639$, almost exactly 4 times smaller. The values of α_c are controlled by the cluster geometry and

BCs through the placement of the allowed wave vectors near the zeros of spin-wave energy: for periodic SLHM systems, one has $\mathbf{k} = (2\pi i/L_x, 2\pi j/L_y)$, whereas for the cylindrical-pinned geometry case, $\mathbf{k} = [\pi i/(L_x + 1), 2\pi j/L_y]$. The factor of 4 improvement in the aspect ratio for the latter is due to the shift by $\pi/(L_x + 1)$ away from the ordering vector. The effective-model analysis determines the $1/L$ correction term up to an unknown factor, but the zero crossing is independent of it.

The FSSWT produces approximate results for $M = |\langle S_z \rangle|$ for all sites. Figure 2(a) shows $M(x)$ vs x for two representative clusters. Because of suppression of the long-wavelength spin fluctuations the magnetization is enhanced near the boundary. The asymptotic falloff of the magnetization away from the edge can be shown to be $M(x) \approx M_0 + a/x$. These FSSWT results are in a good agreement with the DMRG data for the SLHM in the nontilted clusters shown in Fig. 3(a). One can see that already for the $L_x \times 6$ clusters M_C provides a good estimate of the asymptotic 2D value M_0 when the aspect ratio is near $\alpha = 2$.

Figures 2(b) and 3(b) show M_C vs $1/L_y$ for cylindrical BCs, obtained by the FSSWT and DMRG, respectively. Also shown are the results for the $L \times L$ systems with periodic BCs, in Fig. 2(b) by FSSWT from this work and from Ref. [15], and in Fig. 3(b) by QMC calculations using standard correlation function methods, Ref. [4]. Clearly, even for the same aspect ratio, the finite-size effects in the cylindrical BC clusters are 3–4 times smaller than in the periodic systems. The FSSWT agrees precisely with the effective theory on the value of $\alpha_c = 1.7639$ for eliminating the leading $1/L$ term. This is in a good qualitative agreement with the DMRG data, but the DMRG data seem to indicate consistently higher values of $\alpha_c \approx 1.9$. We have also performed QMC calculations [16] for the SLHM with periodic BCs. With the largest clusters up to 20×160 the "magic" aspect ratio is $\alpha_c \approx 7.5$, also higher than the effective theory value 7.0555. While we cannot exclude a change in the behavior on larger lattice sizes, this seems to indicate some insufficiency of the effective theory analysis.

In Fig. 3(b) DMRG results for M_C are shown. For the largest system, 20×10, up to $m = 2400$ states were kept, with the run taking about 40 h single-core time on a 2.6 GHz Mac Pro. This yielded a truncation error of order 10^{-6}, a variational energy with an accuracy of a part in 10^4, an extrapolated energy accurate to a few parts in 10^5, and an uncertainty in M_C of about 0.0007 [17].

More accurate DMRG results can be obtained for 45° tilted lattices [18], allowing more detailed fits. For example, on a $32/\sqrt{2} \times 8\sqrt{2}$ system, the energies and M_C were roughly 2 times more accurate than for the 20×10 nontilted system, and the finite-size effects were smaller. The improved behavior comes from how DMRG sees the width of the system (the number of sites on the boundary of the left or right block) versus the physical dimension—the greater spacing by a factor of $\sqrt{2}$ in the tilted case accounts for the improvement. In Fig. 4(a) we show results for M_C vs $\alpha = L_x/L_y$ for various L_y near the value $\alpha = 1.925$ where the curves nearly intersect. The intersection of such curves as $L_y \to \infty$ provides a simple determination of both α_c and M_0. The resulting value of α_c, based on the available sizes, is somewhat larger than that given by FSSWT and the continuum analysis. The values of α are discrete because we have integral lattice dimensions. Performing a least squares fit of these data to the expression

$$M_C(\alpha, L_y) = M_0 + a(\alpha - \alpha_c)/L_y \qquad (2)$$

we obtain $M_0 = 0.3067$, $\alpha_c = 1.9252$, and $a = -0.1580$. In Fig. 4(b), the solid lines are based on this fit; the points for $\alpha = 1.9$ and $\alpha = 1.925$ are obtained from linear extrapolation along the lines shown in Fig. 4(a). The result for

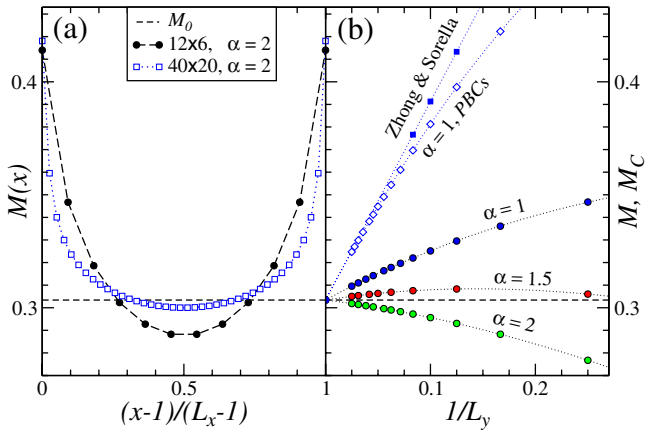

FIG. 2 (color online). (a) FSSWT results for the SLHM showing the position dependence of the magnetization $M(x)$. $M_0 = 0.3034$ is the spin-wave theory bulk value. (b) M_C (M) vs $1/L_y$ by FSSWT for periodic BCs (upper two sets) and cylindrical BCs (lower sets). In Ref. [15] M was extracted from the correlation function, and so differs in $(1/L^2)$ terms.

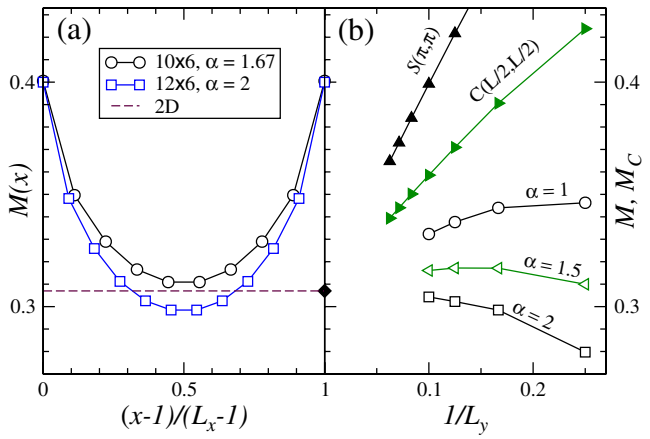

FIG. 3 (color online). (a) DMRG results for $M(x)$ vs x for the SLHM. The line labeled "2D" and the solid diamond are the QMC $L \to \infty$ extrapolated result, $M_0 = 0.3070(3)$ [4]. (b) M_C vs $1/L_y$ results from DMRG for the SLHM. The upper two curves are periodic QMC $\alpha = 1$ results for M [4].

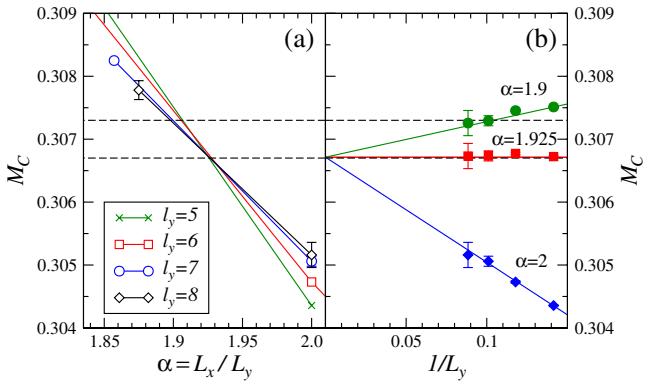

FIG. 4 (color online). DMRG results for the 45° tilted SLHM. (a) The solid lines are straight segments connecting the discrete data points from different lattice sizes, with $L_y = l_y\sqrt{2}$. The two dashed lines show the bounds on the QMC result [4]. (b) A three parameter fit to the data from (a), as discussed in the text.

M_0 is consistent with, and of comparable accuracy to, the best QMC result.

For the triangular lattice, we have studied a variety of clusters and pinning fields; these results consistently supported that the triangular system has the three-sublattice 120° order found in other studies. The cluster orientation shown in Fig. 1 seems to be the most convenient and efficient for a DMRG analysis to obtain M_0. Our DMRG results for comparable lattice sizes are only slightly less accurate than for the SLHM.

Unfortunately, the finite-size analysis for the TLHM is much less accurate. The allowed widths in the preferred geometry must be multiples of 3, and our results for $L_y = 12$ are of low accuracy, leaving only $L_y = 3, 6, 9$. Currently, we do not have comparable analytical guidance, such as predictions for the optimal aspect ratio, for the triangular case. In Fig. 5 we show results for the TLHM with this orientation and also for lattices rotated by 90°. The scaling behavior appears to be quite similar to the SLHM, but with a somewhat smaller $\alpha_c \sim 1.6$–1.7. Assuming this behavior, we estimate $M_0 = 0.205(15)$,

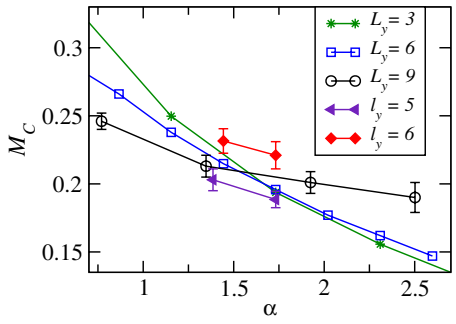

FIG. 5 (color online). M_C versus aspect ratio for various widths for the TLHM, from DMRG. The two curves labeled with l_y come from clusters rotated by 90°, with $L_y = l_y\sqrt{3}$.

consistent with recent QMC calculations and series expansions [7,8]. The results for the rotated clusters seem to have larger finite-size effects and are less useful.

In conclusion, we have developed improved techniques for studying ordering in 2D lattice systems using DMRG, making DMRG competitive with QMC calculations and series expansions for the SLHM and TLHM systems. These techniques include proper scaling of local quantities with the discarded weight, and the use of nontraditional cluster geometries and BCs to improve finite-size scaling.

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