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Monte Carlo studies of spin-stiffness fluctuations in the two-dimensional classical Heisenberg model

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A recent one-loop calculation has shown that, in the d-dimensional classical Heisenberg model at low temperatures, the absolute thermal fluctuations of the spin-stiffness constant are scale independent for $d<4$. We report the confirmation of this unexpected theoretical prediction by extensive Monte Carlo simulations in $d=2$. In addition, we find that the strength of the logarithmic correction for the relative fluctuations depends on the details of the boundary conditions.

I. INTRODUCTION

In a recent letter,[1] it was argued that the analog of the universal conductance fluctuations in a mesoscopic system[2,3] can be identified with the thermal fluctuations of the spin-stiffness constant in the classical Heisenberg model. In a mesoscopic sample, the length scale L is larger than the mean free path and smaller than the phase-coherence length of the conducting electrons. Using a one-loop calculation,[1] the absolute magnitude of the thermal fluctuations of the spin-stiffness constant was shown to be similar to that of the conductance fluctuations, i.e., independent of scale L for dimensions $d<4$ and relative fluctuations proportional to L^{4-2d} with logarithmic corrections in $d=2$. The calculation assumes mixed boundary conditions (fixed in the x direction and periodic for the remaining d-1 directions), low temperatures, and L is taken to be larger than the lattice spacing and smaller than the correlation length. These theoretical results are of fundamental interests and can, in principle, be tested by experiments on granular magnetic materials. Before such comparison can be unambiguously considered, one may need to resolve two important theoretical issues. First, one must ascertain that a calculation to one-loop order is adequate and second, the results may be sensitive to the specifics of the boundary condition and thus should be extended to isotropic boundary conditions, encountered in physical measurements.

In this paper, we address both of these issues by extensive Monte Carlo studies[4] of the spin-stiffness fluctuations in the finite two-dimensional classical Heisenberg model on a square lattice of $L\times L$ sites with three different sets of boundary conditions. A wide range of lattice sizes is used to probe the predictions of scale independence, with L up to 250 sites or 62 500 spins. Very long simulation with over-relaxation moves[5-7] is employed to ensure good statistics. We confirm the one-loop predictions for mixed boundary condition. We further find that the strength of the predicted logarithmic corrections depends on the details of the boundary condition. In contrast to the one-loop calculation with mixed boundary conditions, our results for a finite lattice with full periodic boundary condition is consistent with very small or no logarithmic term. The data for fixed boundary conditions in both the x and y directions are consistent with logarithmic corrections, but with a different amplitude.

II. MONTE CARLO METHOD

We consider a classical Heisenberg model on a finite $L\times L$ square lattice of spins $\{\mathbf{S}_i\}$. $\mathbf{S}_i$ is a spin vector at site i with unit length and parametrized by the three components in the x, y, and z directions. The spins interact with

$$H=-J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j=-J\sum_{\langle ij\rangle}S_iS_j\cos(\Omega_{ij})\ , \quad (1)$$

where the summation is over nearest-neighbor sites and Ω_{ij} is the planar angle between the two spin vectors. The model is ferromagnetic and J is positive. To implement fixed boundary conditions, the surface spins are coupled to a "wall" spin fixed at a constant unit vector taken to be $\mathbf{S}_{\text{wall}}=\hat{\mathbf{z}}$. The periodic boundary conditions are imposed by the standard torus topology. The spin stiffness or the helicity modulus in the $\hat{\boldsymbol{\mu}}$ direction can be sampled[8-11] as

$$\Upsilon_{\hat{\mu}}=(J/N)\left\langle\sum_{\langle ij\rangle}\cos(\Omega_{ij})(\hat{\boldsymbol{\epsilon}}_{ij}\cdot\hat{\boldsymbol{\mu}})^2\right\rangle -(1/N)(J^2/k_BT)\left\langle\left[\sum_{\langle ij\rangle}\sin(\Omega_{ij})\hat{\boldsymbol{\epsilon}}_{ij}\cdot\hat{\boldsymbol{\mu}}\right]^2\right\rangle\ , \quad (2)$$

where $N=L^2$ and $\hat{\boldsymbol{\mu}}$ are the bond directions $(\hat{\mathbf{x}},\hat{\mathbf{y}})$. $\hat{\boldsymbol{\epsilon}}_{ij}$ is the unit vector connecting nearest-neighboring sites i and j. Υ is obtained as an average over the two directions for cases where the boundary conditions are the same. We have used standard Monte Carlo sampling[4] with over-relaxation moves to reduce the correlation times.[5-7] One over-relaxation move is implemented for every ten Monte Carlo steps (MCS) for each spin and about $\leq 400\,000$ MCS per spin after equilibrium are used for averaging. Statistical errors are estimated by considering different runs (typically four independent runs) and block averaging. Using the temperature dependence of the correlation length (ξ) estimated by previous Monte Carlo studies,[12] we consider a temperature of $k_BT/J=0.4$ to obtain an

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estimated correlation length of $\xi \sim 211$ in units of the lattice spacing. This temperature will allow us to probe the scale dependence for $L/\xi \ll 1$ to ~ 1 by using L from 4 to 250. We also vary $k_B T/J$ for some runs and check that our general conclusions do not depend on the particular temperature used.

III. MONTE CARLO RESULTS

We consider three sets of boundary conditions. First, we use the mixed boundary conditions (fixed in the x direction and periodic in the y direction) and calculate the spin stiffness and its fluctuations in the x and y directions separately. In Fig. 1, we present the finite-size (L) dependence of the ensemble average for the spin stiffness in the x direction ($\langle \Upsilon_{\hat{x}} \rangle$), absolute fluctuations ($\langle \Delta\Upsilon_{\hat{x}}^2 \rangle$), and the square root of the reciprocal of the relative fluctuations ($[\langle \Delta\Upsilon_{\hat{x}}^2 \rangle / \langle \Upsilon_{\hat{x}} \rangle^2]^{-0.5}$). For $1 \ll L \ll \xi$, the one-loop calculation predictions[1] are scale independence for the absolute fluctuations and a logarithmic term for the square root of the reciprocal of the relative fluctuations. This is indeed consistent with our numerical results and even the one-loop prediction of the amplitude for the logarithmic term ($1/\sqrt{2\pi}$) in the relative fluctuations is confirmed. [Note the dashed line in Fig. 1(c) for $L/\xi < 1$.] The data for the y direction is shown in Fig. 2. The one-loop calculation[1] does not give an explicit prediction for these quantities. The Monte Carlo results indicated smaller (if any) logarithmic corrections. For the relative fluctuations, the amplitude of the correction is <0.1 and has a different sign. It also occurs over a narrower range of L. Observe that all three sets of data approach weak or no scale dependence rapidly. (See Fig. 2.)

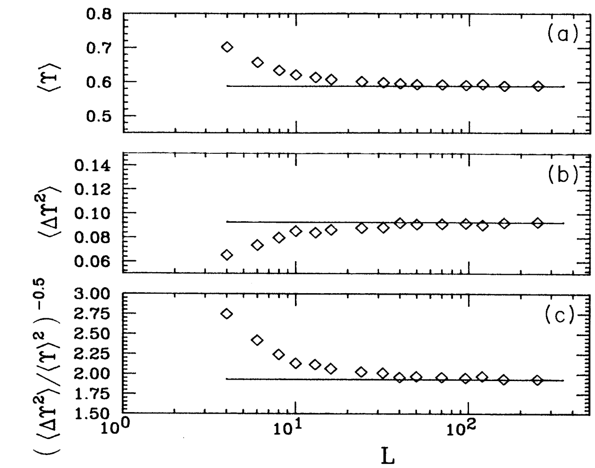

FIG. 2. Scale dependence of the Monte Carlo data for the spin stiffness (helicity modulus) Υ in the y direction. The mixed boundary conditions of fixed in the x direction and periodic in the y direction are used. This is the boundary condition used in the one-loop calculation (Ref. 1). The stiffness is in units of J and $k_B T/J = 0.4$. A is the thermal average of the spin stiffness, B is the absolute fluctuation, and C is related to the relative fluctuations. The solid and dash-dotted lines are guides to the eye only. The estimated errors are about or smaller than the size of the symbols. See Text.

We also study two sets of isotropic boundary conditions. Here, we can average our data over the x and y

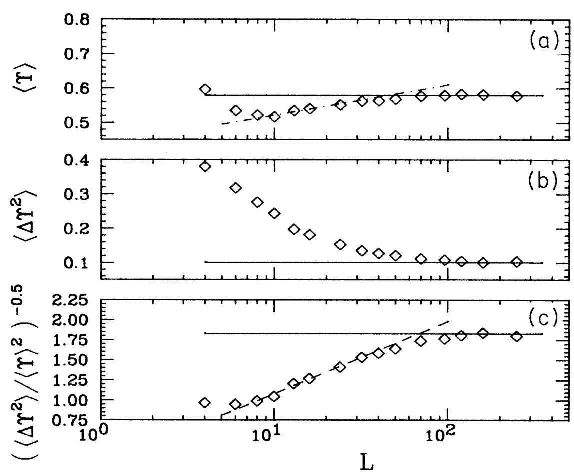

FIG. 1. Scale dependence of the Monte Carlo data for the spin stiffness (helicity modulus) Υ in the x direction. The mixed boundary conditions of fixed in the x direction and periodic in the y direction are used. This is the boundary condition used in the one-loop calculation (Ref. 1). The stiffness is in units of J and $k_B T/J = 0.4$. A is the thermal average of the spin stiffness, B is the absolute fluctuation, and C is related to the relative fluctuations. The solid and dash-dotted lines are guides to the eye only. The dashed line has the logarithmic amplitude predicted by the one-loop calculation of Ref. 1. The estimated errors are about or smaller than the size of the symbols. See text.

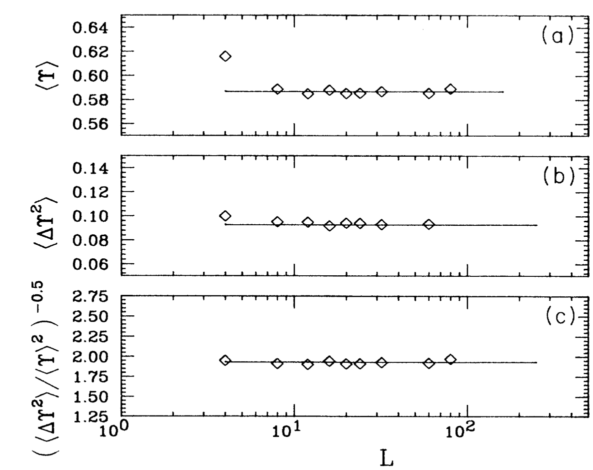

FIG. 3. Scale dependence of the Monte Carlo data for the spin stiffness (helicity modulus) Υ averaged over the x and y directions. The full periodic boundary condition for both the x and y directions is used. The stiffness is in units of J and $k_B T/J = 0.4$. A is the thermal average of the spin stiffness, B is the absolute fluctuation, and C is related to the relative fluctuations. The solid line is a guide to the eye only. The estimated errors are about or smaller than the size of the symbols. See text.

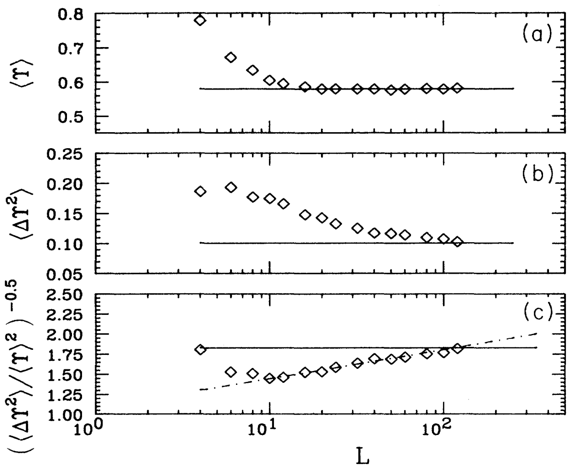

FIG. 4. Scale dependence of the Monte Carlo data for the spin stiffness (helicity modulus) Υ averaged over the x and y directions. The full fixed boundary conditions for both the x and y directions are used. The stiffness is in units of J and $k_B T/J = 0.4$. A is the thermal average of the spin stiffness, B is the absolute fluctuation, and C is related to the relative fluctuations. The solid and dash-dotted lines are guides to the eye only. The estimated errors are about or smaller than the size of the symbols. See text.

directions. Initially, we eliminate surface effects by using full periodic boundary conditions in the x and y directions. The data given in Fig. 3 indicates small or no logarithmic correction and consistent with scale independence. Finally, we present the data for the fixed boundary condition in both x and y directions. (See Fig. 4.) The data for the relative fluctuations is now again consistent with logarithmic behaviors but with an amplitude of 0.16 ± 0.026, very different from $(1/\sqrt{2\pi} \sim 0.4)$ for the mixed boundary conditions.[1]

IV. REMARKS

We have presented extensive Monte Carlo simulation results for the spin-stiffness fluctuations in the finite two-dimensional classical Heisenberg model over a wide range of lattice sizes and with three sets of boundary conditions. Theoretical one-loop calculations are available only for the mixed boundary conditions and indeed our results are consistent with the predictions. We confirm the predictions of the logarithmic term in the relative fluctuations and scale independence for the absolute fluctuations of the spin stiffness in the directions with fixed boundary conditions. For the directions with periodic boundary conditions, our data indicate smaller or no logarithmic correction. This is also found in systems with full periodic boundary condition, in contrast to the results of full fixed boundary condition where the data is again consistent with logarithmic term. These data appear to indicate that the logarithmic term may be sensitive to the details of the boundary condition. We have no rigorous theoretical explanation for these possibilities and refrain from speculations. These numerical results should stimulate further theoretical investigations and encourage experimental measurements.

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