Order Parameter Profiles in a Twisted Heisenberg Model

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We present the results of Monte Carlo simulations of the 3-D Heisenberg model with twisted boundary conditions. The boundaries are chosen to have a saturated magnetization in equal and opposite directions which imposes a twist on the order parameter profile centered at the midpoint of the sample. The magnetization profiles are distinct from mean field theory. We present a detailed examination of the magnetization profile and suggest experiments which can verify the finite size scaling forms we observe.

Index Terms—**Critical phenomenon, domain walls, ferromagnetism, Monte Carlo.**

THE DOMAIN walls which typically occur in a ferromagnetic material are the result of dipolar fields, which produce the demagnetization field. However, artificial domain walls can also be created by tailoring the structure of a material in such a way that the magnetization profile contains a twist. One successful method involves rotating a crystal about an applied magnetic field during growth [1], producing an artificial magnetic spiral [1]–[3]. While the stability of the spin spiral depends on the details of the anisotropy field, the theoretical study of magnetic twists is usually undertaken by imposing opposing surface fields at the boundaries of a model, such as an Ising [4] or Heisenberg [5]–[7] ferromagnetic model. A major prediction [6] of mean field theory is that at T_C the order parameter profile for a model with continuous Heisenberg spins is identical to that of a model with discrete Ising spins, implying that the anisotropy is irrelevant at T_C.

This result is surprising since, intuitively, one might expect that a Heisenberg model with opposing boundary conditions will produce a Bloch like domain wall, where the magnetization rotates uniformly between the "up" and "down" surface fields [5]. However, mean field theory predicts that, at criticality, a sharp twist of the magnetization occurs, confined to the midpoint of the sample [6]. The predictions of mean field theory are, however, not valid in three dimensions, and so one could expect important differences when fluctuations become important. Indeed, one reason to study the model is that the critical fluctuations at T_C in a binary alloy with opposing surface fields (modeled as a twisted Ising ferromagnet) produce long-range forces analogous to the electromagnetic Casamir force [6].

In order to gain a better understanding of the magnetization profiles in twisted Heisenberg models, we have simulated the model using a Monte Carlo algorithm. The Hamiltonian for the classical Heisenberg model is $\mathcal{H} = -\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$, where the sum runs over nearest neighbor, unit vector, Heisenberg spins on a simple cubic lattice. We use periodic boundary conditions in the $\hat{x}$ and $\hat{y}$ directions, and to simulate the twist we impose surface fields which interact with the fluctuating spins at $z = 1$ and $z = L$, where L is the linear dimension of the sample.

There are several types of surface fields used in the study of twisted Heisenberg models. One type [6] is to impose infinite and opposite surface fields on the two boundaries in the $\hat{z}$ direction. We simulate this by considering finite crystals of size $L \times L \times L$, with the plane of free and fluctuating spins at $z = 1$ and $z = L$ coupled to a rigid and unfluctuating plane of spins with $\mathbf{S}(z = 0) = +\hat{z}$ and $\mathbf{S}(z = L + 1) = -\hat{z}$ respectively.

To measure the twist imposed on the magnetization we have simulated the model using a conventional Metropolis Monte Carlo update method along with overrelaxation updates [8]. The details of our implementation of the method can be found elsewhere [9], where it was demonstrated that the overrelaxation update eliminated the critical slowing down in a frustrated Heisenberg model. We have varied the number of Monte Carlo updates from 5000 to 25 000 per site and have not detected any significant differences between important measures, indicating that the sample independence time has been greatly exceeded. We have been able to simulate large lattices with $4 \leq L \leq 64$ both with and without the twist. As an indication of the accuracy we achieve, in the case of the untwisted model, we have calculated the critical exponent ratios $\beta/\nu = 0.519(8)$ and $\gamma/\nu = 1.965(26)$, in good agreement with the accepted values [10] $\beta/\nu = 0.514(5)$ and $\gamma/\nu = 1.975(4)$.

The most important quantities of interest are the magnetizations profiles, $\mathbf{m}(\mathbf{z})$. The instantaneous value of the magnetization components in the $k = \hat{x}, \hat{y}$, and $\hat{z}$ directions are

$$m_k(z) = \sum_i S_{i,k}(z) \quad (1)$$

where the sum is restricted to the $n = L^2$ spins in the plane at z. The instantaneous value of the total magnetization for each plane is thus

$$m(z) = [m_{\hat{x}}(z)^2 + m_{\hat{y}}(z)^2 + m_{\hat{z}}(z)^2]^{1/2}. \quad (2)$$

The instantaneous angle made by the magnetization and the $\hat{z}$ direction is

$$\theta(z) = \cos^{-1}[m_{\hat{z}}(z)/m(z)]. \quad (3)$$

The three magnetization components, the total magnetization, and the angle between the magnetization

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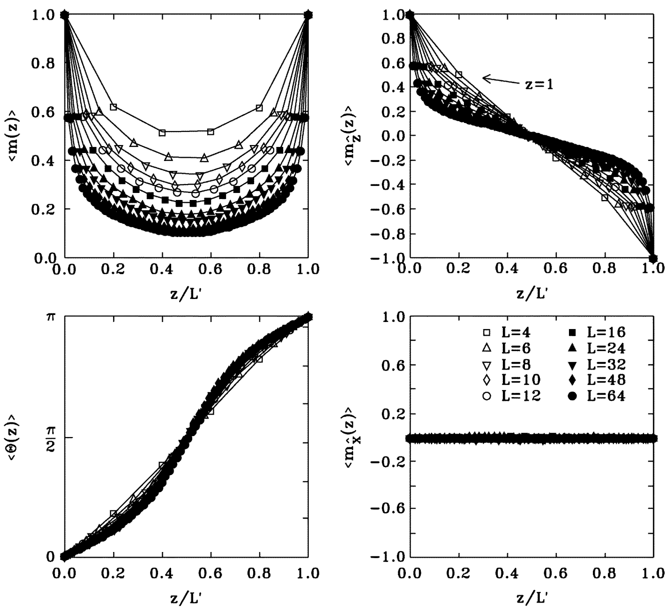

Fig. 1. Magnetization profiles for the twisted Heisenberg model ($m(0) = +1$ and $m(L+1) = -1$). Clockwise from top left, magnetization/site $m(z)$, $\hat{z}$ axis projection of the magnetization/site $m_{\hat{z}}(z)$, $\hat{z}$ axis projection of the magnetization/site $m_{\hat{x}}(z)$, and the angle between the magnetization and the $\hat{z}$ axis $\theta(z)$. The arrow (top right) is a guide to the eye, pointing through $\langle m_{\hat{z}}(z=1)\rangle$.

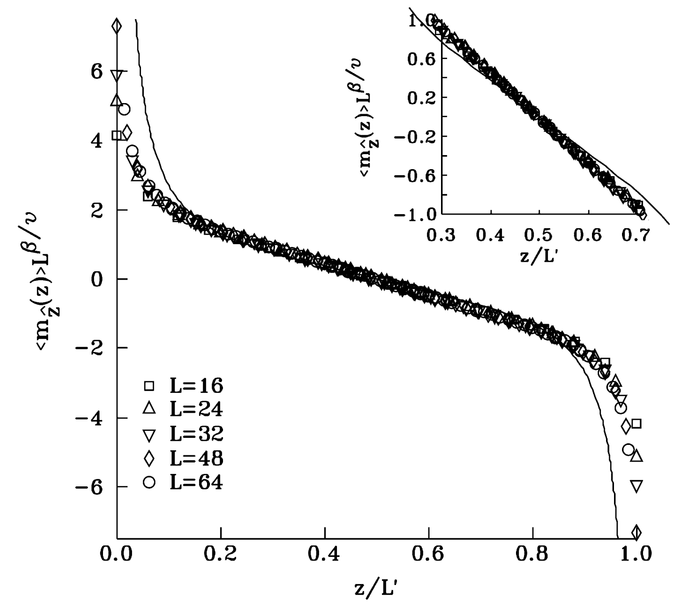

Fig. 2. Scaling plot of the $\hat{z}$ component of the magnetization with $\beta/\nu = 0.514$ appropriate for the 3-D Heisenberg model. Solid line is the scaling function $h_{+,-}$ from mean field theory. Inset shows the behavior near the midpoint of the sample, demonstrating that mean field theory fails everywhere.

and the $\hat{z}$ axis are all averaged over time, yielding $\langle m_{\hat{x}}(z)\rangle, \langle m_{\hat{y}}(z)\rangle, \langle m_{\hat{z}}(z)\rangle, \langle m(z)\rangle$, and $\langle\theta(z)\rangle$.

It is important to note that the time average of the x and y projections of the magnetization, $\langle m_{\hat{x}}(z)\rangle$ and $\langle m_{\hat{y}}(z)\rangle$ must be zero due to ergodicity. Physically, this results from the fact that left- and right-handed twists of the magnetization occur with equal probability, and as such the magnetizations in the transverse directions tend to cancel. For example, a particular state could be a spin structure with $\mathbf{S}(z) = (\sin\theta, 0, \cos\theta)$ or $\mathbf{S}(z) = (-\sin\theta, 0, \cos\theta)$ with $\theta = \pi z/L'$ and $0 \le z \le L$. Since the two twists have the same energy but mirror symmetry, the x axis projection of the magnetization cancels.

In Fig. 1 we show the calculated magnetization profiles for a selection of lattice sizes at the inverse critical temperature [10] $\beta_C = 1/T_C = 0.6930$. The data are presented as functions of $\bar{z} = z/L'$, with $L' = L+1$, so that the boundaries appear at $\bar{z} = 0$ and $\bar{z} = 1$ respectively. We do not show $\langle m_{\hat{y}}(\bar{z})\rangle$ since, owing to time reversal symmetry, it must be zero, like $\langle m_{\hat{x}}(\bar{z})\rangle$ as shown in Fig. 1. It is clear that the magnetization (for finite samples) rotates smoothly about the $\hat{z}$ axis, with $\langle\theta(\bar{z} = 1/2)\rangle = \pi/2$. Furthermore, the magnetization is decreasing to zero in the bulk, as should be expected for a finite system at criticality.

Mean field theory predicts that the magnetization is restricted to the $\hat{z}$ direction at T_C, and

$$\langle m_{\hat{z}}(\bar{z}) >= L^{-\beta/\nu} h_{+,-}(\bar{z}) \tag{4}$$

where β and ν are the usual scaling exponents, and $h_{+,-}(\bar{z})$ is a scaling function [6]. Of course, since we work in three dimensions we must use the exponents $\beta = 0.362$ and $\nu = 0.704$ appropriate for the 3-D Heisenberg universality class [10]. In Fig. 2 we show a plot of $\langle m_{\hat{z}}(\bar{z})\rangle L^{\beta/\nu}$ versus $\bar{z}$ and compare this with the predicted $h_{+,-}(\bar{z})$ from mean field theory.[1] The fact that the scaling function does not perfectly capture the actual physics in three dimensions is unsurprising. The scaling function is, however, quite adequate for $1/4 < \bar{z} < 3/4$, although on close inspection it is clear that the slope is wrong, as shown in the inset to Fig. 2.

In the limit $\bar{z} \to 0$ with L large, mean field theory predicts that [6], [7] $h_{+,-}(\bar{z}) \sim \bar{z}^{-1}$. It is clear from Fig. 1 that $\langle m_{\hat{z}}(z)\rangle$ approaches a finite value in the limit of large L (which we can resolve for the first six planes or so). This polarization of the magnetization near the boundaries implies a very specific form for the actual scaling function $h_{+,-}(\bar{z})$ near $z = 0$. Setting $\langle m_{\hat{z}}(z)\rangle$ equal to a constant for in (4) shows that, in the limit $z/L \to 0$, $h_{+,-} \sim (z/L)^{-\beta/\nu}$. Mean field theory predicts the same form, except the exponents take mean field values $\beta = \nu = 1/2$.

Mean field theory does not, however, predict the correct order parameter profile, even qualitatively. The main prediction is that, at T_C, we should have $\langle m(z)\rangle = |\langle m_{\hat{z}}(z)\rangle|$. We do *not* find this to be the case. Instead, $\langle m(z)\rangle \ge |\langle m_{\hat{z}}(z)\rangle|$, as can be seen by comparing Figs. 2 and 3. In the regime $0 \le \bar{z} < 0.1$ (and by symmetry $0.9 < \bar{z} \le 1$) $\langle m(z, L=\infty)\rangle = |\langle m_{\hat{z}}(z, L=\infty)\rangle|$, which we show in the inset to Fig. 3 for the largest ($L = 64$) sample, and where the finite size differences between $\langle m(z)\rangle$ and $\langle m_{\hat{z}}(z)\rangle$ are almost negligible. It is important to note though that $\langle\theta(z)\rangle$, is *not* related to the ratio $\langle m_{\hat{z}}(z)\rangle/\langle m(z)\rangle$, and so while $m(z) = m_{\hat{z}}(z)$ for $0 \le \bar{z} < 0.1$ and L large, $\theta(z) \ne 0$ for the finite samples.

[1]For the comparison, we use the mean field scaling function from [7] rather than that of [6] as it fits our data better. However, both mean field calculations predict the same limiting behavior of the magnetization near the boundaries, and are in this sense equivallent.

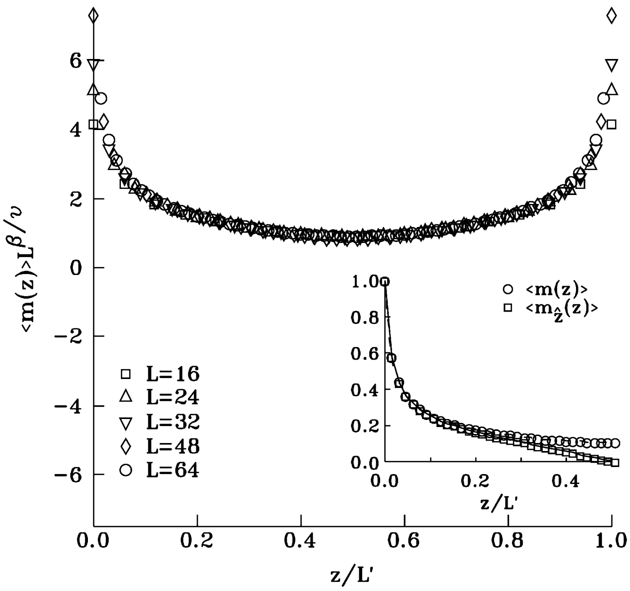

Fig. 3. Scaling plot of the total magnetization with $\beta/\nu = 0.514$ appropriate for the 3-D Heisenberg universality class. The inset shows both $m(z)$ and $|m_{\hat{z}}(z)|$ for $L = 64$ which are unequal near the midpoint of the sample.

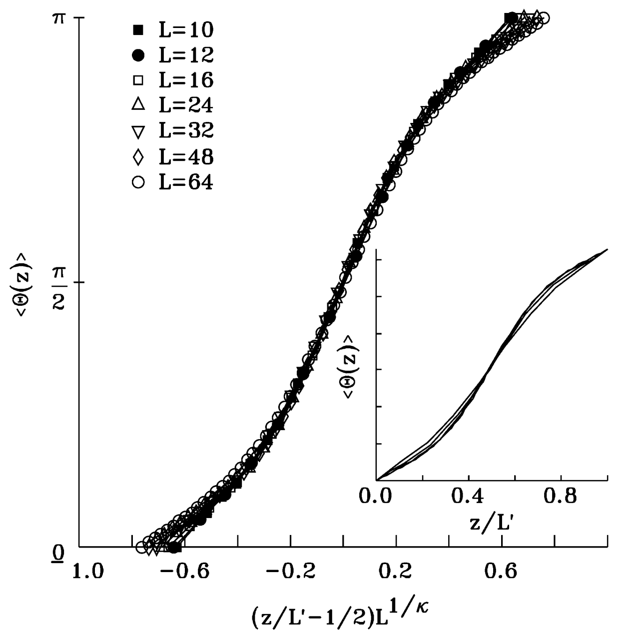

Fig. 4. Scaling plot of $\theta(z)$ with $\kappa \sim 10$. The large value of κ indicated that the sharpening of the domain wall with increasing L is slow, as shown in the inset where we plot $\langle\theta(\bar{z})\rangle$ for $L = 8, 16, 32$ and 64.

Within the confines of mean field theory, $\langle\theta(z)\rangle$ is a step function [6] with $\langle\theta(z)\rangle = 0$ for $\bar{z} < 1/2$ and $\theta(z) = \pi$ for $\bar{z} > 1/2$. In a finite sample this step is rounded, and one might expect that at the midpoint of the sample $d\langle\theta(z)\rangle/d\bar{z}$ should diverge with increasing L. We find that $d\langle\theta(z)\rangle/d\bar{z}|_{\bar{z}=1/2} \sim L^{1/\kappa}$ with $\kappa \sim 10$. This is shown in Fig. 4 where we have plotted $\langle\theta(\bar{z})\rangle$ versus $(\bar{z} - 1/2)L^{1/\kappa}$, with $1/\kappa = 0.1$.

The large value of κ indicates that the increase of slope with increasing L is slow, as shown in the inset to Fig. 4 where we have plotted $\langle\theta(\bar{z})\rangle$ more clearly than in Fig. 1, by omitting the labelling. Furthermore, since $1/\kappa < 1$, the experimentally relevant quantity $d\langle\theta(z)\rangle/dz \sim L^{-0.9}$, and so the sharp twist predicted here will not explicitly occur; it can only be observed in the reduced units of z/L'. However, the fact that the slope of $\langle\theta(\bar{z})\rangle$ diverges at the midpoint of the sample confirms the qualitative picture given in mean field theory where an abrupt domain wall is created at criticality. Experimentally, polarized neutron reflectometry can measure the magnetization profiles modeled here [2], [3], and it would be interesting to compare the real profiles occurring in artificial magnetic structures [1] of varying sizes at T_C with the theoretical predictions.

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