Role of Vortex Strings in the Three-Dimensional O(2) Model

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Using Monte Carlo techniques, we show that vortex strings are responsible for the phase transition in the three-dimensional planar model. The phase structure for a generalized planar model with vortex suppression is determined. This latter model has the unusual feature of long-range order in a ground state with finite, disordering entropy.

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The O(2) ($=XY$) model has the interesting and important feature that it supports topological defects which in $d=2$ dimensions are vortices. This property can be understood as a consequence of the fact that the first homotopy group $\pi_1(S^1)=Z$ is nontrivial. Indeed, according to the Kosterlitz-Thouless (KT) theory,[1] the phase transition in the 2D O(2) model occurs because of the dissociation of vortex-antivortex pairs as the temperature T increases through T_c. In general, defects of dimension p will occur if $\pi_{d-(p+1)}(G)$ is nontrivial,[2] where G is the space in which the order parameter lies. Thus, the 3D O(2) model has one-dimensional vortex strings. Several questions then arise. What role do these defects play? How is the behavior of the system altered if one suppresses, or indeed entirely removes, the vortex strings? These questions have considerable interest, since the 3D O(2) model is relevant to the critical behavior of a number of physical systems such as magnetic materials with planar spin Hamiltonians and the superfluid transition in liquid ^{4}He. We know of no theory in three dimensions analogous to the KT theory for two dimensions which predicts, from considerations of vortex-string interactions, such properties as how the correlation length diverges at the critical point, or the form of the singularity in the free energy. High-temperature series expansions[3] and the ϵ expansion[4] do predict the critical exponents, but they make no direct reference to the presence or absence of vortex strings in the model. Similarly, high-temperature series expansions, or equivalently, a $1/d$ expansion,[5] predict the value of the critical temperature (admittedly nonuniversal, but still of interest), and again make no reference to vortex strings. Nevertheless, it is expected,[6] on the basis of analysis of the Villain form of the model, that these objects do play a significant role in the phase transition. One is thus left with the somewhat unsettling situation that the quantitative knowledge of the critical behavior of the 3D O(2) model is based on analyses which do not involve vortex strings in sharp contrast to the KT theory of the 2D O(2) model. In this paper we report results which explicitly show that vortex strings are responsible for the phase transition in the former model.

The O(2) model in three dimensions is defined by (classical) spin-angle variables at vertices of a cubic lattice, which take values in the range $(-\pi,\pi)$, and by the following action and partition function:

$$S=-\sum_{\langle ij\rangle}\cos(\phi_i-\phi_j), \tag{1a}$$

$$Z=\prod_{\text{sites } i}\int\frac{d\phi}{2\pi}e^{-KS}, \tag{1b}$$

where $\langle ij\rangle$ denotes nearest-neighbor sites and $K\equiv J/k_\mathrm{B}T$ (here, we only consider the case $K\geqslant 0$). This model is known to have a second-order phase transition at[4] $K\approx 0.46$ from an ordered phase with nonzero magnetization to a disordered phase. To measure properties associated with vortices[7] we use the following definitions. Denote the discretized gradients of the spin angle around a square as $\Delta_i=\theta_i-\theta_{i+1}$, where $i=1,2,3,4$ labels the sites on this square. Each Δ_i can be decomposed into $\Delta_i=2\pi m_i+\bar{\Delta}_i$, where $m_i=\pm 1$ and the reduced gradient angle lies in the standard range $\bar{\Delta}_i\in(-\pi,\pi)$. Then since $\sum_i\bar{\Delta}_i=0$, it follows that $\sum_i\Delta_i=-2\pi v$, where the vortex charge $v=0,\ \pm 1$ (and, for a set of measure zero, ± 2). $|v|$ serves as a measure of the vortex string density. For periodic boundary conditions, which we use, the total vortex charge of the lattice vanishes.

As has been noted previously,[8] magnetization cannot be meaningfully averaged on a finite lattice because, in a continuous spin system, there is no energy barrier preventing the spins from rotating as a whole. We use the definition for magnetization given in Ref. 8:

$$M=N_s^{-1}[\langle(\sum_i^{N_s}\cos\theta_i)^2\rangle+\langle(\sum_i^{N_s}\sin\theta_i)^2\rangle]^{1/2}. \tag{2}$$

For our Monte Carlo simulations, we used the method of Metropolis *et al.* Our runs were made on lattice sizes from 6^3 to 14^3. In most cases, a number N_T of sweeps were for thermalization and N_M were for measurement of expectation values, where one sweep means a sequential updating of all spins in the lattice. We denote this combination by (N_T,N_M). In an updating, a new spin θ' is obtained from the original spin

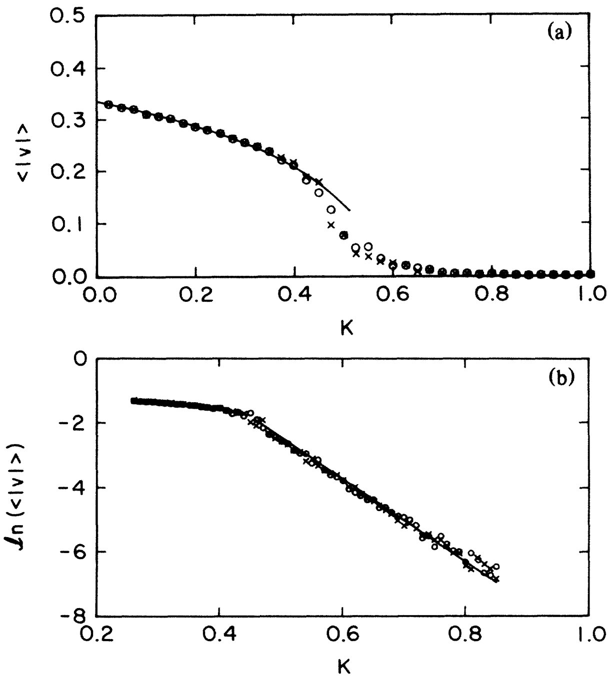

FIG. 1. (a) Vortex density plotted as a function of K. Measurements were made on an 8^3 lattice with (50,50) iterations. Also shown is the high-temperature series result, to quadratic order. (b) Logarithm of vortex density, measured on a 10^3 lattice with (50,50) iterations, as a function of temperature.

θ by

$$\theta' = \theta + \text{rand} \times I, \tag{3}$$

where rand is a random number in the interval $[-1,1]$, and I is chosen by the program to keep the number of rejections as close as possible to one half of the number of updates. This method of updating ensures fast thermalization.

As a test of the accuracy of our Monte Carlo data, we have measured the internal energy $U = \langle S \rangle$, vortex density, and magnetization and found them to be in good agreement with the analytic expansions for low and high temperatures. In Fig. 1(a), we plot results for $\langle |v| \rangle$ obtained on an 8^3 lattice using (50,50) iterations. The data from larger lattices give the same values, apart from small finite-size shifts in T_c and behavior very near T_c. Furthermore we have checked thermalization by performing (300,300) iterations. From these measurements, we determine the phase transition to occur at $K = 0.47 \pm 0.05$, which agrees with previous calculations.[4] In Fig. 1(a), we also plot the first three terms in a high-temperature expansion of the vortex density. It can be shown that the lowest-order term is exactly $\frac{1}{3}$, and the other terms can be evaluated by use of standard numerical integration techniques.

Note from Fig. 1(a) that the vortex density is large in the high-temperature region and small at low temperature, decreasing sharply as T decreases through T_c, which is consistent with the idea of vortex dissociation driving the phase transition as postulated in Ref. 6. In this reference, the Villain approximation was used to make computations in the O(2) model. In particular, one can compute the vortex density at low temperature, where the Villain approximation is thought to be applicable, and show that it has an exponential falloff with K.[9] In the three-dimensional planar model, where the lowest-energy excited configuration allowed is a loop of four vortices, we find, using the methods of Refs. 6 and 9 $\langle |v| \rangle = e^{-\kappa/K}$ where $\kappa = \frac{4}{3}\pi^2$. In Fig. 1(b), we plot the logarithm of vortex density as a function of temperature for low temperatures, measured on a 10^3 lattice. The solid line in this figure is the Villain result which is consistent with our data even in the region K slightly smaller than K_c.

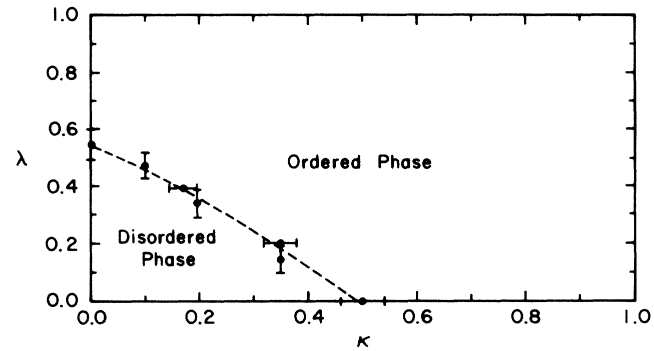

FIG. 2. Phase diagram in the K-λ plane.

While the measurements of vortex density are consistent with the transition being driven by vortices, they do not by themselves prove it. To investigate the question further, we introduce a term into the action to suppress or enhance vortices[10]:

$$-KS \rightarrow -KS - \lambda \sum_{\text{plaq}} |v|. \tag{4}$$

With this action, we map out the phase diagram in the two parameters λ and K. The rationale behind this procedure is that, if the phase transition in K disappears when we suppress vortices sufficiently, then vortices are responsible for this transition. The result is shown in Fig. 2. This phase diagram was mapped by use of heating and cooling measurements of magnetization, vortex density, and internal energy. An example of these measurements is shown in Fig. 3, for $K = 0$. Again, as a check that our Monte Carlo program is correct, we plot in Figs. 3(a) and 3(c) the linear terms in an expansion of internal energy and vortex density, respectively. The agreement with the Monte Carlo calculation is excellent. An interesting feature is that for large λ, M saturates at ≈ 0.47, substantially less than 1. As a check on the measurement

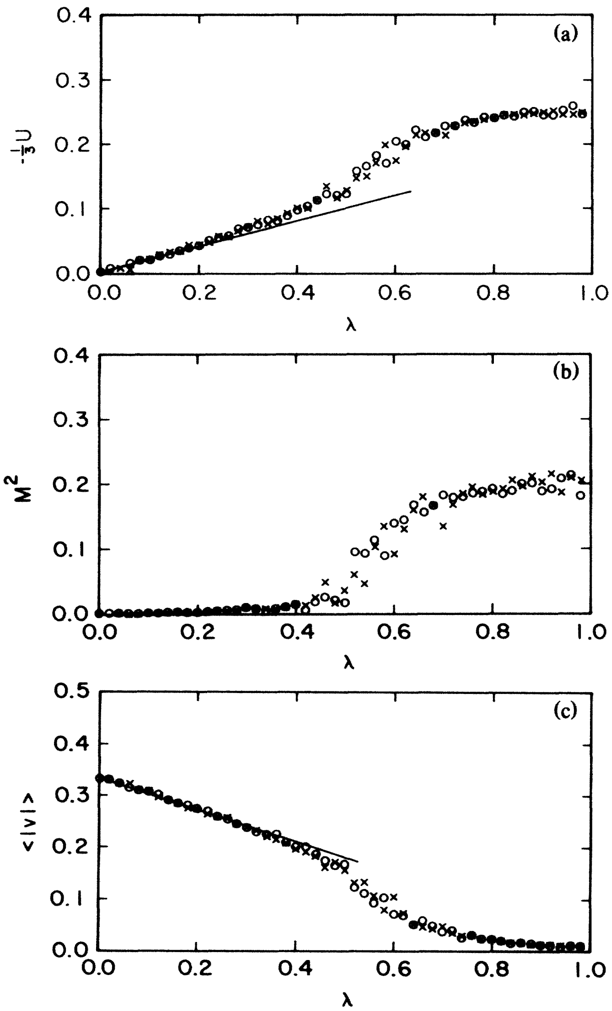

FIG. 3. Various thermodynamic quantities plotted as a function of λ for $K=0$. Measurements were made on an 8^3 lattice with (50,50) iterations. (a) Reduced internal energy. Also shown is the small-λ series result, to linear order. (b) Magnetization. (c) Vortex density. Also shown is the small-λ series result, to linear order.

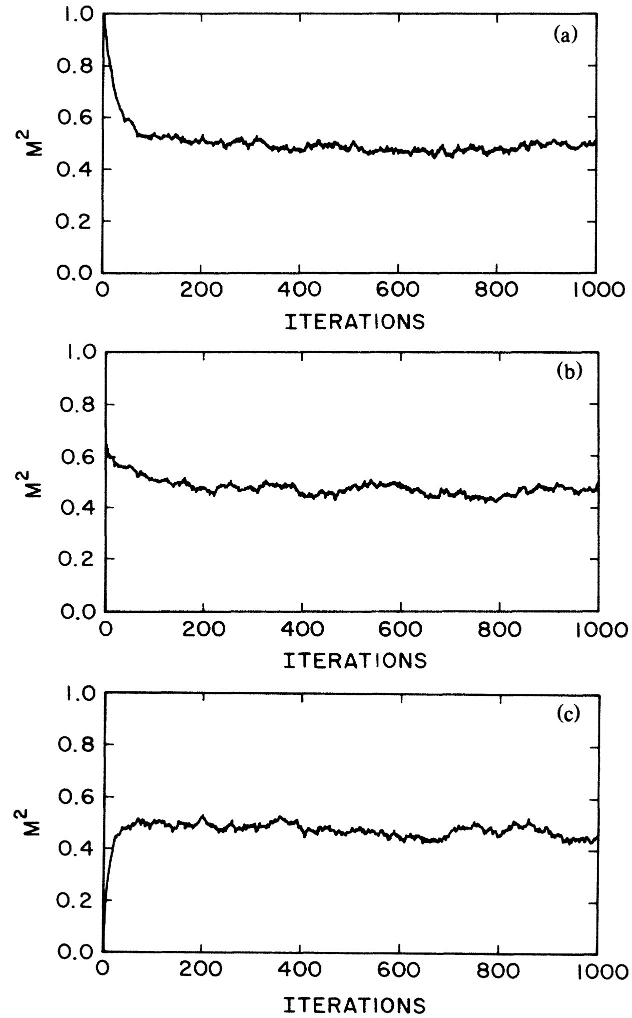

FIG. 4. Magnetization as a function of iteration number for different starts, at $\lambda=3$. (a) Ordered start. (b) Random start. (c) Start with zero magnetization *and* vorticity.

of M, runs were made with three quite different starting configurations: ordered, random, and a configuration in which $v=0$ for all squares and $M=0$; as shown in Fig. 4, these all converge to the same value $M \simeq 0.47$ at $\lambda=\infty$.

What makes this result especially interesting is that the long-range order is present even in the absence of any direct ferromagnetic spin-spin coupling. Clearly, a sufficiently aligned ferromagnetic spin configuration has zero vortex-string density. However, the converse is false; one can easily produce configurations with $v=0$ for all squares, but nevertheless $M=0$. Indeed, starting with a completely ferromagnetic ordered configuration, one can, with zero expenditure of internal energy, reverse the spins in half of the lattice. This is in contrast to the situation with a usual spin-spin interaction Hamiltonian. Our model (2) thus exhibits what we believe is a qualitatively new mechanism of ordering, caused by an interaction which even as $\lambda \rightarrow \infty$ allows a great amount of spin rotation at each site.

Our model contradicts the common belief that long-range order is incompatible with finite ground-state disordering entropy S. To our knowledge, it is the first such counterexample for a pure system without (annealed or quenched) disorder.[11] Actually, for any classical O(N) model, S is logarithmically divergent as $\lambda \rightarrow \infty$ (or as $K \rightarrow \infty$) as a result of the Goldstone mode(s). However, this does not entail true disorder, since it represents rigid rotations of all spins in the lattice as a whole, which only rotate the direction of **M**, but do not reduce its magnitude. The type of ground state which has been thought to be incompatible with long-range order is that which has dis-

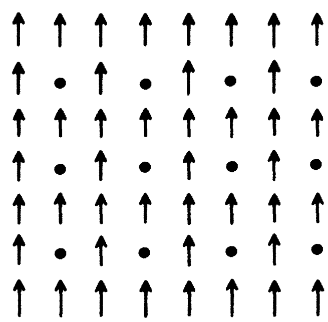

FIG. 5. A pictorial representation of a two-dimensional slice which contributes to nonzero ground-state entropy.

order truly distinguished from the Goldstone modes. A proof that after removing the zero-mode nondisordering contribution to the entropy, our system has finite ground-state entropy, is provided by the class of spin configurations in Fig. 5. Each spin marked with a heavy dot is free to rotate without yielding (except for a set of angles of measure zero) any nonzero v. Since there are $N_s/8$ of these spins, where N_s denotes the number of lattice sites, it follows that they make a finite contribution to the entropy (per site). Although such disorder does not remove the long-range order, it reduces the ground-state magnetization below unity.

Our work thus shows that vortex strings do indeed play a crucial role in the 3D O(2) model. The task of deriving the critical exponents in a way which takes these topological defects into acccount, as the KT theory did for (the nonalgebraic singularities in) the 2D O(2) model, remains an outstanding unsolved problem. Moreover, our model (2) exhibits a qualitatively new mechanism for ordering and the unusual behavior of long-range order in the presence of ground-state disorder.

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