From Continuous to First-Order Transition in a Simple XY Model

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(Received 31 January 1984)

An XY model of classical spins, on a two-dimensional square lattice, with nearest-neighbor interaction $V(\theta)=2J[1-(\cos^2\theta/2)^{p^2}]$ is studied by a Monte Carlo simulation that also monitors the vortex excitations. Both continuous and first-order transitions are found. In the latter the density of vortices sharply increases at the transition point. The transition turns first order, because the shape of V is such that vortex-antivortex pair formation is suppressed at low temperatures for $p \gtrsim 3$.

PACS numbers: 05.70.Fh, 05.50.+q, 64.60.Cn

Very recently, an interesting extension of the two-dimensional XY model for classical spins (of unit length) with ferromagnetic nearest-neighbor interaction has been introduced by Domany, Schick, and Swendsen.[1] In this model the potential is given by

$$V(\theta)=2J[1-(\cos^2\theta/2)^{p^2}], \quad J>0. \tag{1}$$

The orientation of the spins is given by angular variables θ_i and $\theta \equiv \theta_i-\theta_j$, where (i,j) is a pair of nearest-neighbor sites. For $p=1$, the potential reduces to that for the pure XY model. As p is raised, it has an increasingly narrow well of width $\sim \pi/p$ and for $\theta \gtrsim \pi/p$ it is essentially constant at $V(\pi)=2J$. Ordinary spin-wave behavior at low temperatures is ensured by the behavior of $V(\theta) \approx J\frac{1}{2}p^2\theta^2$ near the minimum.

In Ref. 1, this model was studied as a function of p. More specifically, it was shown, by means of Monte Carlo (MC) simulation, that for very large values of p a first-order, rather than a continuous, transition[2,3] takes place. Thus one has, indeed, a simple model in which one can study the change in the nature of the phase transition as a function of one parameter, whose variation affects the nearest-neighbor interaction in such a transparent manner. It was also argued in Ref. 1, that more than one type of excitation may play a role in changing the nature of the transition, as one would become relatively more important than the other by the alteration of the potential. However, as the underlying excitations were not studied, the arguments were not definitive.

In this Letter, both the transition and the underlying vortex excitations are studied by means of MC simulations for a wide range of p values. It appears that vortex excitations alone are sufficient to account for both the continuous and first-order transitions, but in a qualitatively different manner. Indeed, one might expect only vortices to be involved, since, for any p, the model only exhibits the same continuous symmetry as the pure XY model. The physical picture is very simple. For small p, the potential well in (1) is rather wide so that vortices and antivortices enter the system gradually as the temperture T is increased. At the Kosterlitz-Thouless point a continuous transition takes place through the dissociation of the vortex-antivortex pairs.[2] For large p, the potential well is narrow, so that there is an insufficient increase of vortex density at low T for the dissociation mchanism to operate; then, at some temperature, they can suddenly appear in great numbers and a first-order transition occurs. All this will be illustrated by the numerical results to be presented in the remainder.

Standard MC calculations[4] are performed, operating directly on the angular variables. This has the advantage that the vortices can be found explicitly by computing the vorticity of each elementary square of the lattice.[5,6] The following quantities are computed: (i) the average energy per site ϵ, (ii) the specific heat per site C (from the energy fluctuations), (iii) the total average density $n_{\rm av}$ of vortex-antivortex pairs, mainly on a lattice of 600 spins[7] with periodic boundary conditions, and (iv) the derivative Γ of the helicity modulus γ.[8] Γ is defined as

$$\Gamma \equiv \frac{1}{2}\frac{d}{d\beta}(\beta\gamma)=\Omega^{-2}[\epsilon_\Omega-\epsilon_p], \quad \beta=1/T, \tag{2}$$

where ϵ_Ω is the energy with twisted boundary conditions in, say, the x direction (twist per spin Ω) and periodic boundary conditions in the y direction, and ϵ_p is the energy with fully periodic boundary conditions. Antiperiodic boundary conditions, i.e., $\Omega=\pi/L$ (where L is the linear dimension of the lattice in x direction), will be used in the computation. As has been extensively investigated for the pure XY model,[6] Γ behaves very characteristically for a continuous phase transition, since it is directly

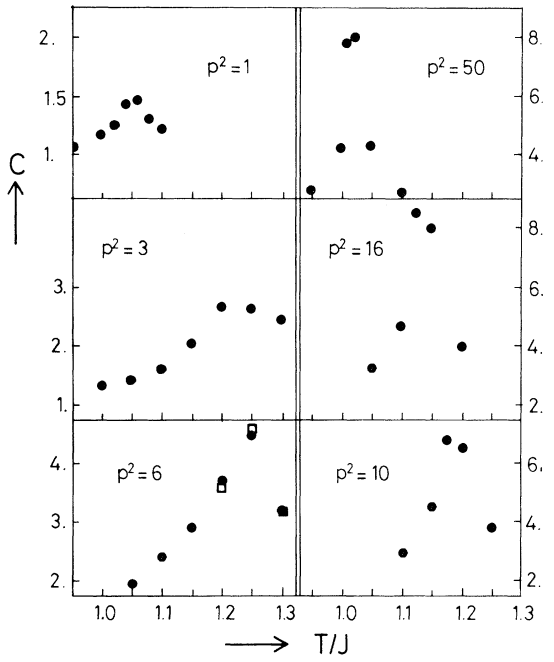

FIG. 1. The specific heat peak at various p values on a 20×30 lattice. Open squares on a 30×30 lattice. The pure XY-model results are on a different scale.

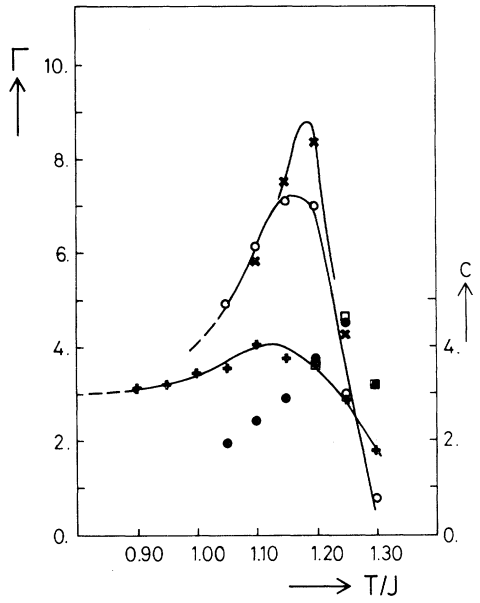

FIG. 2. Γ (left scale) at $p^2=6$ on a 10×10 (crosses), 20×30 (open circles), and 30×30 (tilted crosses) lattice. C (left scale) on a 20×30 lattice (full circles), and 30×30 lattice (open squares) at $p^2=6$. Curves are drawn to guide the eye.

related to the exponent η that governs the algebraic decay of the correlation function through $\beta\gamma=(2\pi\eta)^{-1}$. A continuous phase transition in the present model can thus be inferred from the behavior of Γ which, for $p\neq1$, is expected to be much the same as for the pure XY model.

In Fig. 1 the specific heat in the region of the peak is exhibited for various values of p, including $p=1$.[6] For $p^2=1,3,6$ a shift to higher T is observed and the peak becomes narrower as p increases. The average energy varies smoothly in this region and C saturates at a value C_{max} that increases with p (compare data on 900 spins at $p^2=6$). The results for Γ and C at $p^2=6$ are displayed in Fig. 2. This is typically a continuous transition: Γ has ex-

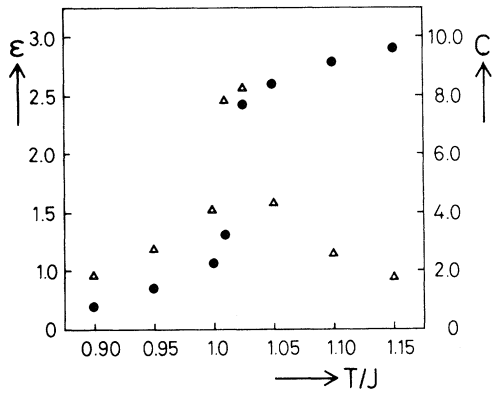

FIG. 3. ε (left scale) and C (right scale) at $p^2=50$. Energy data (full circles), specific-heat data (open triangles).

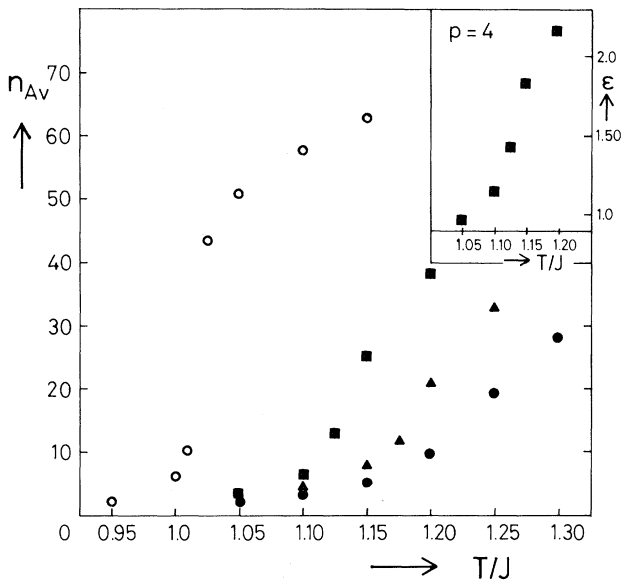

FIG. 4. n_{av} (left scale) on a 20×30 lattice, for $p^2=6$ (full circles), $p^2=10$ (full triangles), $p^2=16$ (full squares), and $p^2=50$ (open circles). ε at $p^2=16$ (inset and right scale).

actly the same features as in the pure XY model (the spin-wave limit is $\frac{1}{2}p^2$), viz. as L increases an even sharper peak occurs, consistent with a sharp jump in γ for the infinite system. The transition temperature is associated with the location, T_{KT}, of the maximum of Γ. Notice that the specific-heat maximum is still located *above* T_{KT}. In the pure XY model C_{max} lies approximately 10% above T_{KT}.[6] However, at $p^2=6$, the relative difference appears to be less than 5%.[7]

The results for $p^2=50$, also studied in Ref. 1, are shown in Fig. 3. In this case the transition is clearly first order: there is a near discontinuity in ϵ, and a large, sharp peak in C *at* the transition point $T\sim 1.01$, in complete agreement with the results of Ref. 1.[9] However, the behavior of the vortices now gives us more information about the mechanism of the transition. The vortex-antivortex pair density exhibits a sharp jump at the transition point, while for continuous transitions, at low p, it increases only gradually with temperature (Fig. 4). A dramatic illustration of the transition is obtained by displaying a typical configuration of vortices just below and above the transition point (Fig. 5).

If the physical picture is correct, that the transition changes its nature basically because vortex-antivortex pair formation is inhibited by the shape of V, the value of p where this happens can be roughly estimated *a priori*.. If the maximum value of the relative nearest-neighbor orientation $\theta \lesssim \pi/2$, vortex-antivortex pairs cannot be formed at low T, since they are obtained as a change of θ by $\pm 2\pi$, upon summation of its value on the four bonds of a nearest-neighbor square of the lattice. Therefore the transition might still be continuous at $p\sim 2$, but it would be first order at $p\sim 4$ (see Fig. 6, top). The simulations at $p^2=10$ and 16 show specific-heat peaks qualitatively similar to the case $p^2=50$ (Fig. 1). In addition, at $p^2=16$ a clear break occurs in both n_{av} and ϵ (Fig. 4) at $T\sim 1.12$, which is also the location of the peak in C. The same features are hard to observe at $p^2=10$, so a comparison is made between the distribution of ϵ values for $p^2=6$ and 10 at $T=1.20$, a value close to the transition point in either case (Fig. 6, bottom). This clearly indicates that the transition is first order at $p^2=10$. The data are therefore completely consistent with the physical picture described above, placing the point where the transition changes its nature not far from $p=3$. The fact that the transition temperature for continuous transitions (which follows the peak in C but does not coincide with C_{max}) increases with p can also be understood intuitively. Vortex-antivortex pair formation is suppressed but, as long as p is not too large, enough pairs still have entered the system for the dissociation mechanism to operate at a higher temperature than in the pure XY model. In conclusion, then, this model exhibits both continuous and first-order transitions. Whichever occurs depends on the shape of the potential: If the well is too narrow to accommodate vortices in the low-T phase the transition is first order. Vortices appear to be solely responsible for the transition in either case.

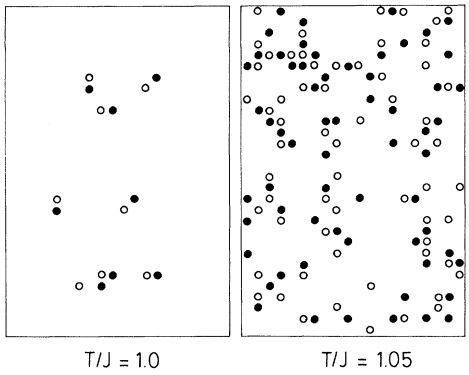

FIG. 5. Typical configuration of vortex-antivortex pairs (full and open circles, respectively) at $T=1$ and $T=1.05$ (taken after 10^4 MC steps per spin equilibration) on a 20×30 lattice.

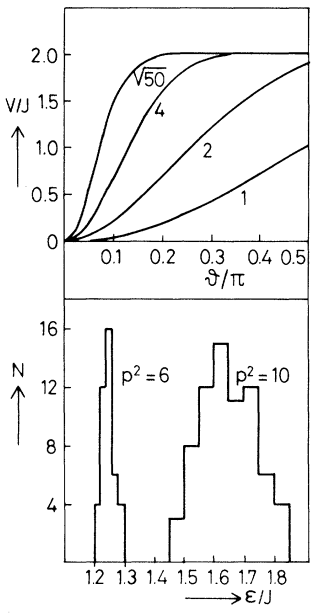

FIG. 6. The potential V as a function of θ for $p^2=1,4,16,50$. The part $\frac{1}{2}<\theta/\pi<1$ is not shown (top). The distribution of ϵ values at $T=1.20$. N is the number of occurrences of block averages of 2×10^3 spins each (bottom).

It is a pleasure to thank Dr. H. Knops for drawing my attention to Ref. 1.

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[2]J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).

[3]J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).

[4]Equilibration monitored and typically taken to be 6×10^3–10^4 MC steps per spin. Between 4×10^4–8×10^4 MC steps per spin are taken for averaging.

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[7]Comparison of Γ and C on a 30×30 lattice is made in Fig. 1. Finite-size effects on large lattices are studied for the first-order transition in Ref. 1 and for the continuous transition in the pure XY model in Ref. 6. These effects are small and unimportant for the conclusions drawn here. In particular, the location of T_{KT} and C_{max} changes only about 1% going from 4×10^2 to 10^3 spins and no further shift is detected upon increasing the number of spins to 6×10^3 (see Ref. 6).

[8]M. E. Fisher, M. N. Barber, and D. Jasnow, Phys. Rev. A **8**, 1111 (1973).

[9]The helicity modulus is not studied systematically for first-order transitions, but, indeed, its behavior is very different. At $p^2=50$ and 600 spins, we find a very sharp peak at the transition point: $\Gamma\simeq10$ at $T=0.98$, $\Gamma\simeq40$ at $T=1.0$ and $T=1.01$, while it is almost identically zero already for $T\gtrsim1.03$.