Monte Carlo study of the planar spin model

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We have simulated the two-dimensional classical planar spin model using the Metropolis Monte Carlo technique. The loss of long-range order as a function of the size of the lattice was confirmed. The energy and specific heat were calculated for a square lattice of 900, 3600, and 10000 spins. A sharp specific-heat peak was found at $k_BT/J=1.02$ (J is the nearest-neighbor coupling), 15% above the transition temperature $k_BT_c/J=0.89$. T_c was determined by fitting the spin-spin correlation function and the susceptibility to the forms of the Kosterlitz-Thouless theory. The density of vortex pairs was computed and found to increase exponentially with inverse temperature. At T_c vortex pairs begin to unbind and also larger clusters of vortices appear and unbind as the temperature is increased. These larger clusters may be responsible for the specific-heat peak being sharper and closer to T_c than simple theories predict.

I. INTRODUCTION

The usual long-range order associated with low-temperature phases of three-dimensional systems is generally believed not to exist in two-dimensional (2-D) systems, with continuous symmetry, above absolute-zero temperature. In 2-D crystals Peierls[1] showed that the localization of particles on their lattice sites is destroyed by long-wavelength lattice waves. Similarly, using the spin-wave theory of Bloch[2] one finds that the spontaneous magnetization is destroyed by long-wavelength spin waves. In both cases the deviation from perfect order is given by a k-space integral which takes the form

$$\int \frac{d^dk}{k^2} ,$$

where the lower limit of the integral $\sim 1/L$ where L is the length of the system. In three dimensions the integral converges, but in two dimensions it diverges as $\ln L$ and the order is completely destroyed.

The above arguments use harmonic models. More general proofs using Bogoliubov inequalities have shown that under very general conditions long-range order is destroyed for 2-D crystals, magnets, superfluids, and superconductors.[3] Computer experiments on hard disks[4] and electrons[5] in two dimensions (both not covered by the above proofs) have also shown the loss of order as the size of the system is increased. Nevertheless these same simulations strongly suggest that a phase transition takes place. High-temperature series expansions[6] for 2-D spin systems also suggest that a phase transition exists. The natural question to ask is "What is the nature of the low-temperature phase, if the usual long-range order is absent?"

Kosterlitz and Thouless[7] (referred to hereafter as KT) dealt with these systems within a unified theoretical model. They contend that the 2-D low-temperature phase is characterized by a power-law decay in the pair-correlation function (as predicted by harmonic theory) modified by the presence of pairs of tightly bound topological defects of opposite "sign". At the transition temperature the pairs unbind to create a new phase where the correlations decay exponentially. In crystals the topological defects are dislocations, in magnets they are spin vortices, and in superfluid helium they are quantum vortices. The three-component spin model will not sustain vortices, because the singularity at the core of the vortex can be avoided by the core spins pointing outside the plane. Thus, in this case KT predict that there is no phase transition. The two-component spin model, called the planar spin model can support vortices and should therefore display a KT transition. Because the KT predictions for this model are the most well developed and because it is the easiest to simulate we have decided to use the planar model to test explicitly the predictions of the KT theory including a detailed examination of the behavior of the spin vortices.

While this work was in progress, two papers appeared on the Monte Carlo simulation of the planar model. McMillan[8] simulated a system of 1024 spins and looked at the specific heat and susceptibility. Miyashita *et al.*[9] simulated 225, 900, and 2500 spin systems to compare the size dependence of various quantities. We have duplicated McMillan's work on the specific heat and susceptibility for a 3600 spin system. Using the spin-spin correlation function and the susceptibility we were able to determine T_c by fitting the temperature dependence of these quantities to the KT theory. We have in addition carefully compared the specific-heat peak for the 3600 spin system with that of a 900 spin system. In addition to

duplicating other simulation work, which is important by itself to insure their reliability, we have gone beyond previous work by looking at some different aspects of the problem. We have confirmed the spin-wave theory predictions of the magnetization and the resulting loss of long-range order in the low-temperature phase. In addition we have calculated the equilibrium vortex density both above and below T_c, and showed that vortex pairs and larger clusters exist and do in fact begin to unbind at the transition temperature.

II. CALCULATIONAL PROCEDURE

The two-dimensional planar model is defined by the following reduced Hamiltonian:

$$\beta H = -\frac{1}{T} \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \ , \tag{1}$$

where T stands for $k_B T/J$, J is the coupling strength, θ_i is the angle made by spin i relative to some fixed axis in the plane, and the sum is taken over all nearest-neighbor pairs (each pair counted once). The spins are placed on a square lattice with periodic boundary conditions.

Simulations were performed using the traditional Metropolis Monte Carlo procedure.[10] The maximum change in angle per spin per step was adjusted every pass through the lattice to maintain an acceptance ratio of 0.5. A pass is defined as sequentially stepping through the lattice turning each spin once. In most cases the energy, susceptibility, and spin-spin correlation function were calculated every pass. Other quantities were computed less frequently.

Most of our work was performed on a 3600 spin lattice equilibrating, usually, for 1000 passes and averaging over another 2000 passes. The large equilibration time was used to minimize the correlations between runs taken at neighboring temperatures. The first run was taken at $T=2.0$ starting from a random configuration. The system is then cooled in steps varying between 0.20 away from T_c and 0.05 near T_c. Starting from $T=0.80$ we then heated the system back through the transition. A summary of the 3600 spin results is shown in Tables I and II.

We also performed more extensive runs near the specific-heat peak as well as runs on different sized systems. These results and error estimates of various quantities will be discussed in the relevant sections below.

TABLE I. Monte Carlo data cooling the 3600 spin system. Temperature listed in column 1, energy in column 2, standard deviation of the mean energy in column 3, correlation length in column 4, η from high-temperature form of spin-spin correlation function in column 5, η from low-temperature fit in column 6, susceptibility in column 7, and vortex-pair density in column 8. Last temperature listed, $T=1.15$, started from a completely random configuration.

T	Energy	σ_E	ξ	η	η	$\langle S^2 \rangle$	ν_{pair}/spin
2.00	−0.5470	0.0007				4	0.094
1.80	−0.6200	0.0007				5	0.092
1.60	−0.7149	0.0015				10	0.085
1.40	−0.8539	0.0010				15	0.065
1.30	−0.9411	0.0016	2.5	0.23		19	0.050
1.25	−0.9903	0.0025	3.0	0.25		46	0.044
1.20	−1.0479	0.0028	3.9	0.27		38	0.034
1.15	−1.1096	0.0020	4.9	0.26		123	0.028
1.10	−1.1741	0.0037	6.0	0.25		145	0.026
1.05	−1.2431	0.0017	11.8	0.28		280	0.016
1.00	−1.3188	0.0023	23.8	0.29		656	0.012
0.95	−1.3828	0.0027	29.2	0.25	0.319	1120	0.007
0.90	−1.4365	0.0014			0.261	1259	0.003
0.85	−1.4807	0.0013			0.238	1378	0.002
0.80	−1.5271	0.0009			0.245	1722	0.001
0.75	−1.5668	0.0006			0.170	1833	0.0
0.70	−1.6002	0.0004			0.162	1923	0.001
0.60	−1.6674	0.0003			0.130	2097	0.0
0.50	−1.7291	0.0005			0.101	2386	0.0
0.30	−1.8434	0.0003			0.062	2914	0.0
0.10	−1.9493	0.0001			0.0157	3333	0.0
1.15	−1.1029	0.0068	6.43	0.30		58	0.031

TABLE II. Monte Carlo data warming the 3600 spin system. Temperature listed in column 1, energy in column 2, standard deviation of the mean energy in column 3, correlation length in column 4, η from high-temperature form of spin-spin correlation function in column 5, η from low-temperature fit in column 6, susceptibility in column 7, and vortex-pair density in column 8. Last temperature listed, $T=1.15$, started from a completely ordered configuration.

T	Energy	σ_E	ξ	η	η	$\langle S^2\rangle$	v_{pair}/spin
0.85	−1.4855	0.0013			0.230	1484	0.003
0.90	−1.4383	0.0012			0.248	1305	0.005
0.95	−1.3850	0.0015	28.0	0.25	0.302	1163	0.007
1.00	−1.3237	0.0019	27.6	0.28		734	0.010
1.05	−1.2451	0.0020	6.4	0.19		174	0.026
1.10	−1.1714	0.0031	4.1	0.20		108	0.027
1.15	−1.1111	0.0032	6.7	0.31		61	0.032
1.20	−1.0447	0.0025	3.1	0.21		57	0.031
1.40	−0.8518	0.0016	1.9	0.22		14	0.057
2.00	−0.5485	0.0005	0.9	0.12		4	0.096
1.15	−1.1063	0.0070	5.0	0.26		64	0.032

III. LOSS OF LONG-RANGE ORDER

We have already mentioned above that the spin-wave theory predicts that the spontaneous magnetization, M, goes to zero in the thermodynamic limit. Instead of M, we will use the mean-square angular displacement, $\langle\theta_i^2\rangle$, to discuss the order in our system, because within the spin-wave approximation there is an exact expression for $\langle\theta_i^2\rangle$ and because it is analogous to the mean-square particle displacement used in discussing order in crystals. In any system $\langle\theta_i^2\rangle$ diverges if θ_i is measured relative to a fixed axis since a uniform rotation costs no energy. Thus, we define θ_i as the angle relative to the direction of the instantaneous total spin. This is analogous to subtracting out the change in the center of mass in a system of particles, to compute particle positions.

We will now review some results from simple spin-wave theory and show how they are confirmed by our Monte Carlo simulation. In addition to illustrating the nature of the low-temperature phase, this exercise will serve to define certain functions used later on in the paper.

The spin-wave approximation consists of replacing the reduced Hamiltonian by[11]

$$\mathcal{H}_{\text{sw}}=\frac{1}{2T}\sum_{\langle i,j\rangle}(\theta_i-\theta_j)^2 =\frac{1}{2T}\sum_{\langle i,j\rangle}\theta_i G_{ij}^{-1}\theta_j \ , \tag{2}$$

where we allow θ_i to assume all values from $-\infty$ to $+\infty$ and where G_{ij} is the lattice Green function given by

$$G(\vec{n})=\frac{1}{N}\sum_{\vec{k}}{}'\frac{e^{i\vec{k}\cdot\vec{n}}}{4-2\cos(k_x)-2\cos(k_y)} \ , \tag{3}$$

where $\vec{n}$ is the displacement vector connecting sites i and j and all lengths are measured in units of one lattice spacing. All quantities of interest can be obtained as a function of $G(\vec{n})$. For example,

$$\langle\theta^2\rangle=TG(0) \ , \tag{4a}$$

$$\langle|M|\rangle=\langle\cos\theta\rangle\approx 1-\tfrac{1}{2}TG(0) \ , \tag{4b}$$

$$C(\vec{n})=\langle\vec{S}(\vec{n})\cdot\vec{S}(0)\rangle=e^{-T[G(0)-G(\vec{n})]} \ , \tag{4c}$$

$$\langle E\rangle=-2\langle\vec{S}(1)\cdot\vec{S}(0)\rangle=-2e^{-T[G(0)-G(1)]} \ , \tag{4d}$$

where $\langle|M|\rangle$ is the mean magnitude of the spontaneous magnetization, $C(\vec{n})$ is the spin-spin correlation function, and $\langle E\rangle$ is the energy per spin.

If one approximates $G(\vec{n})$ by an integral then one finds the following explicit results:

$$\langle\theta^2\rangle=\frac{T}{4\pi}(\ln N+\ln 2) \ , \tag{5a}$$

$$\langle|M|\rangle=1-\frac{T}{8\pi}(\ln N+\ln 2) \ , \tag{5b}$$

$$C(\vec{n})=\text{const}\times\frac{1}{n^{T/2\pi}}\ \text{for large } n \ , \tag{5c}$$

$$\langle E\rangle=-2+\tfrac{1}{2}T \ , \tag{5d}$$

$$\chi=\frac{1}{N}(\langle S_{\text{tot}}^2\rangle-\langle S_{\text{tot}}\rangle^2)=N^{1-T/4\pi} \ , \tag{5e}$$

$$\langle M^2\rangle=\frac{1}{N^2}\langle S_{\text{tot}}^2\rangle=N^{-T/4\pi} \ , \tag{5f}$$

where S_{tot} is the total spin, χ is the reduced susceptibility, and $\langle M^2\rangle$ is a quantity occasionally used as the order parameter in spin systems. The last equation shows that this quantity tends to zero in the thermo-

dynamic limit. Below T_c, χ does not diverge in 3-D systems because $\langle S_{\rm tot}\rangle$ is nonzero, but in the planar model $\langle S_{\rm tot}\rangle = 0$ and χ diverges for all temperatures below T_c.

All these results agree very well with our Monte Carlo results. The well-known $\ln N$ dependence of $\langle\theta^2\rangle$ is shown in Fig. 1 for $T=0.1$. This is the analog of the divergence of the mean-square displacement of a particle from its lattice site found in two-dimensional crystals. The slope and intercept of the line in Fig. 1 are $0.007\,86 \pm 0.000\,16$ and $0.006\,03 \pm 0.001\,04$ compared to the spin-wave prediction of 0.007 96 and 0.005 52, respectively.

The magnitude of the magnetization also decreases as $\ln N$ as described above. The susceptibility diverges as $N^{1-\eta/2}$ with $\eta = 0.0158 \pm 0.0003$ compared to spin-wave prediction of 0.0159. For this calculation we set $\langle S_{\rm tot}\rangle = 0$ because it would take too many passes for $S_{\rm tot}$ to average to zero.

The mean-square magnetization per spin, $\langle M^2\rangle$, goes to zero as the size of the lattice is increased since it is equal to $N^{-\eta/2}$.

The energy per spin agrees quite well with spin-wave theory at $T=0.1$, but already at $T=0.3$ corrections are necessary to explain the Monte Carlo results.

For $C(\vec{n})$ we fitted our data [for $\vec{n}=(nx,0)$] to $C(n)=e^{-\eta\tilde{G}(n)}$ where $\tilde{G}(n)=2\pi[G(0)-G(n)]$.

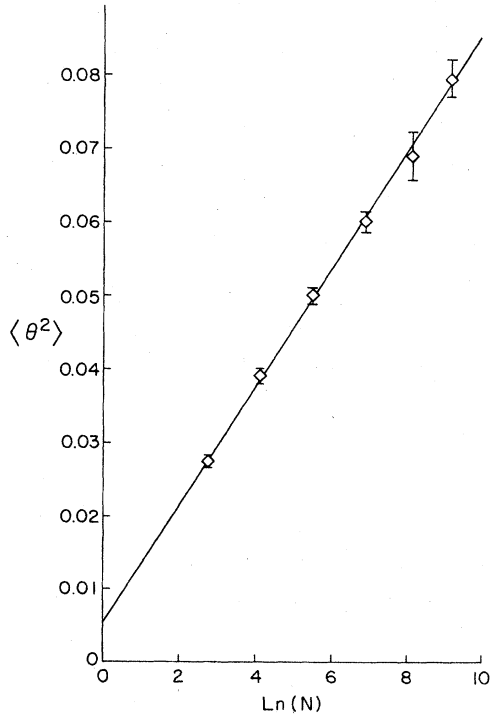

FIG. 1. $\langle\theta^2\rangle$ vs $\ln(N)$ at $T=0.1$. The straight line is the prediction of spin-wave theory.

Since we included small values of n we must use the discrete form of G. The spin-wave prediction is that $\eta_{\rm sw} = T/2\pi = 0.0159$ at $T=0.1$. This compares very well with the fitted value of 0.0157 ± 0.0005 where the fitted curve is within a few tenths of a percent of the Monte Carlo data. However, at $T=0.3$ this simple approximation breaks down with $\eta_{\rm sw}=0.048$ compared to computed results of $\eta=0.062$. One expects η to deviate from the spin-wave prediction when vortex pairs are present; however at this temperature no vortices were observed, thus the difference is probably due to higher-order corrections in spin-wave theory.

IV. CORRELATION FUNCTIONS

According to the KT theory the correlation length and the susceptibility diverge near T_c as e^{b/t^ν} where $t=(T-T_c)/T_c$ and KT suggest that b is around 1.5 and ν is 0.5. Thus, we use these functions to find T_c. We can obtain the correlation length from the spin-spin correlation function which above T_c is of the form[8]

$$C(n)=e^{-\eta\tilde{G}(n)}(e^{-n/\xi}+e^{-(L-n)/\xi}) \quad , \tag{6}$$

where ξ is the correlation length and L is the length of the lattice. The exponential decay is due to the unbinding of vortices in the KT theory. $\tilde{G}(n)$ has the periodicity of the lattice; thus to insure that $C(n)=C(n+L)$ we must add the second term in the bracket. Below T_c we assume $C(n)$ has the spin-wave form, $e^{-\eta\tilde{G}(n)}$, generalized so that η need not equal the spin-wave prediction $T/2\pi$, but is determined by fitting to the Monte Carlo data.

The results for η and ξ for all temperatures for the 3600 spin lattice are shown in Tables I and II. By comparing the two tables we see that η is reasonably well behaved, but the correlation length is difficult to pin down. The value for ξ can only be trusted when it is at most less than the largest distance in the horizontal direction which is 30 for a 60×60 lattice with periodic boundary conditions. For example at $T=0.95$ ξ is probably much larger than 30 and thus the values listed in Tables I and II should be incorrect. In addition at $T=0.95$ one finds that the low-temperature form for $C(n)$ fits the data as well as the high-temperature form.

To compare with KT theory we tried fitting the data from $T=1.0$ to 1.2 with the KT form $\xi=Ce^{b/t^\nu}$. We used values of b from 0 to 2.5 and ν from 0.45 to 0.75 and T_c from 0.74 to 0.99 to fit the average of the heating and cooling data. We then adjust C using a least-squares routine to get the best fit.

When we have a standard deviation between the fitted curve and the data of approximately 1.0, relative to correlation lengths between 3 and 30, the best fits fall between $T_c=0.89$, $\nu=0.70$, and $b=0.90$ and

$T_c = 0.93$, $\nu = 0.55$, and $b = 0.90$. KT predict $T_c = 1.35$, $\nu = 0.5$, and $b \sim 1.5$. A somewhat better prediction by Villain[12] gives $T_c = 0.85$. Shugard *et al.*,[13] using a simulation of the roughening model which maps onto the planar model, find $T_c = 0.90$. McMillan finds $T_c = 0.90 \pm 0.02$ in his simulation of a 1024 spin lattice. These results suggest that T_c almost certainly lies between $T = 0.85$ and $T = 0.95$. High-temperature series expansions predict that $\nu = 0.7 \pm 0.1$.[14]

The susceptibility, χ, defined as $\langle S_{\text{tot}}^2 \rangle$, also diverges as e^{b'/t^ν} according to KT theory. We treated our data for χ in the same way as the data for ξ. When we have a standard deviation less than 9.0, relative to χ values from 40 to 700, the best fits fall between $T_c = 0.89$, $\nu = 0.70$, and $b' = 1.10$ and $T_c = 0.92$, $\nu = 0.48$, and $b' = 1.70$. McMillan[9] found $T_c = 0.92$ for $\nu = 0.50$ and $T_c = 0.88$ for $\nu = 0.70$.

The fits for χ and ξ should give the same value for T_c and ν, thus the most consistent fit is $T_c = 0.89$ and $\nu = 0.70$ with the uncertainty pointing to slightly larger values of T_c and smaller values of ν. Figures 2 and 3 show the fitted curves and the average value of the heating and cooling data for χ and ξ.

Another prediction of KT theory is that $\eta = 0.25$ at T_c. The average of heating and cooling values of η at $T = 0.90$ is 0.254 and at $T = 0.85$ it is 0.243 which indicates that T_c lies between $T = 0.90$ and 0.85, consistent with our previous estimate of $T_c = 0.89$. This value for T_c is thus probably accurate to within a few percent.

We can also compare the quality of the fit to the

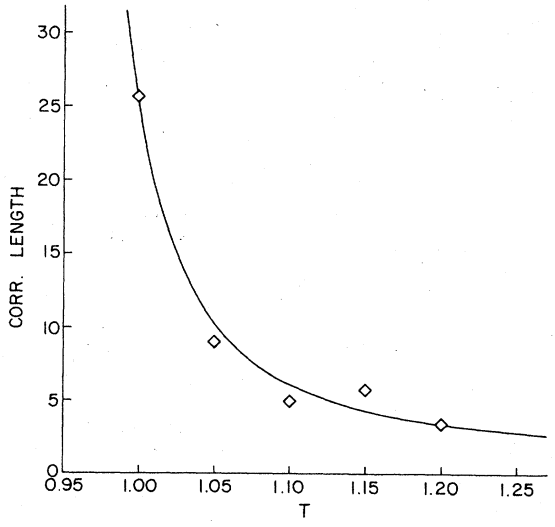

FIG. 2. Plot of correlation length vs temperature. Data points are the average values of heating and cooling runs. Solid curve is fit to KT theory with $T_c = 0.89$ and $\nu = 0.7$.

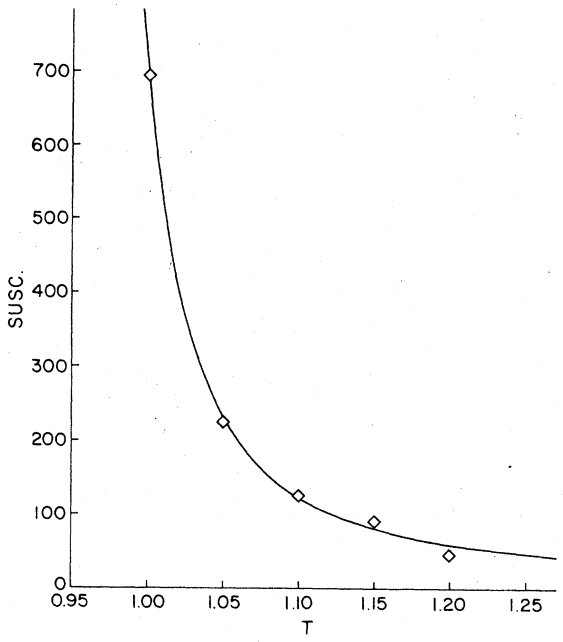

FIG. 3. Plot of susceptibility, $\langle S^2 \rangle$, vs temperature. Data points are the average of heating and cooling data. Solid curve is fit to KT theory with $T_c = 0.89$ and $\nu = 0.7$.

KT theory with that to a conventional power-law divergence of the susceptibility with critical exponent γ. McMillan used a Padé approximate to the high-temperature series expansion to find $\gamma = 2.3$ and $T_c = 1.0$. Rogiers *et al.*[15] find $\gamma = 2.50$ for the spin-$\frac{1}{2}$ x-y model. Fitting χ to a power law we find $\gamma = 1.4$, $T_c = 0.96$, and a standard deviation of 9.4, which is somewhat worse than that found for the fit to the KT theory. This does not rule out a power-law divergence since we may not be close enough to T_c to calculate γ accurately. Luther and Scalapino proposed a theory with a power-law divergence and predicted that $\eta = 0.35$ at T_c.[16] We found $\eta \approx 0.31$ at $T = 0.95$, which is close enough not to rule out their theory, but not nearly as close as our agreement with KT theory that $\eta = 0.25$. Finally, usually second-order phase transitions have anomalies in the specific heat at the same temperature as T_c. However, we find the specific-heat peak at $T = 1.02$, a temperature clearly above where the correlation length diverges.

We therefore conclude that although a conventional phase transition for the planar model cannot be ruled out, the predictions of the KT theory conform better to our Monte Carlo data.

Zittartz[17] has also presented a theory of the planar model. He predicts values of $\eta > 1$, which are clearly ruled out by our simulation.

V. SPECIFIC HEAT

The energy was computed every pass for 900, 3600, and 10 000 spin lattices. Results for all three systems are shown in Table III. The data for the 900 spin lattice were obtained by equilibrating for 500 to 1000 passes and averaging for 1000 to 6000 passes except for the points at $T=1.0$, 1.05, and 1.10 where we present data equilibrated for 4000 passes and averaged over 8000 passes. The equilibration number of passes was determined empirically so that the energy had clearly stopped drifting. The number of passes used to construct the averages was such that fluctuations in the energy were effectively averaged out. The three points near $T=1.05$ were run longer to accurately determine the location of the specific-heat peak. The 10 000 spin lattice was equilibrated for 100 passes and averaged over 400 passes.

As mentioned before the 3600 spin system was averaged over 2000 passes both heating and cooling. To determine the accuracy of the mean value of the energy at each temperature we break up the 2000 passes into ten block averages of 200 passes each. The standard deviation of the mean energy, listed in column 3 of Tables I and II, is the standard deviation of the ten blocks divided by $\sqrt{9}$. Generally when we used only half the blocks the standard deviation of the mean decreased by roughly $\sqrt{2}$ as it should if the blocks are indeed independent data points. The resulting data are all accurate to within 0.32% and the heating and cooling data are always within two standard deviations of each other. The 900 and 10 000 spin systems are accurate to within 1% and 2%, respectively.

TABLE III. Monte Carlo averages of energy for three different sized lattices. Averages for 3600 spin system include heating and cooling data, plus data at $T=1.0$ and 1.05 equilibrated for 1250 passes and averaged over 5000 passes.

Temperature	900	3600	10 000
0.10		−1.9493	
0.30	−1.845	−1.8434	
0.50	−1.730	−1.7291	
0.60	−1.667	−1.6674	
0.70	−1.594	−1.6002	
0.75		−1.5668	
0.80	−1.524	−1.5271	−1.512
0.85	−1.484	−1.4831	−1.468
0.90	−1.438	−1.4379	−1.422
0.95	−1.386	−1.3839	−1.370
1.00	−1.3310	−1.3209	−1.302
1.05	−1.2537	−1.2447	−1.245
1.10	−1.1864	−1.1727	−1.178
1.15	−1.117	−1.1075	−1.116
1.20	−1.055	−1.0463	−1.060
1.25	−1.006	−0.9903	−0.998
1.30	−0.952	−0.9411	
1.40	−0.863	−0.8528	
1.60	−0.731	−0.7149	
1.80		−0.6200	
2.00	−0.580	−0.5477	

There are two ways of computing the specific heat, C_v, from a Monte Carlo simulation. The first is to calculate $\langle E^2\rangle - \langle E\rangle^2$ which is proportional to C_v. This method was tried, but the results near the specific-heat maximum differ greatly between heating and cooling and also are strongly dependent on how many passes are included in the computation. This is not surprising since this method relies on subtracting two large fluctuating quantities, and thus the resulting specific heat will depend strongly on what fluctuations are included. These fluctuations are strongest near the specific-heat peak making the computation difficult in this region.

The other method of obtaining C_v is to differentiate the energy with respect to temperature. As shown in Fig. 4 the energy curve is very smooth so that the value of C_v at T midway between two neighboring temperatures T_1 and T_2 is very close to $(E_1-E_2)/(T_1-T_2)$. To check whether we were biasing the shape of the curve we also tried fitting three points to a parabola and differentiating to find C_v at the middle point. The two methods give the same results well within the uncertainty of the data.

The specific-heat results are shown in Fig. 5. As can be seen both the 900 and 3600 spin systems have a sharp peak near $T_p=1.02$. McMillan[8] found a peak at 1.07 with 1024 spins. The results for the 10 000 spin system are unclear, but not inconsistent. Much longer running times would be necessary to get accurate C_v data for 10 000 spins. The height of the peak appears to be independent of lattice size.

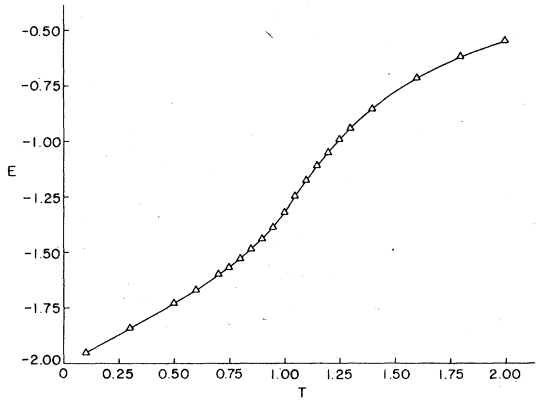

FIG. 4. Plot of energy per spin vs temperature for 3600 spin lattice. Solid curve is composed of straight lines between neighboring data points.

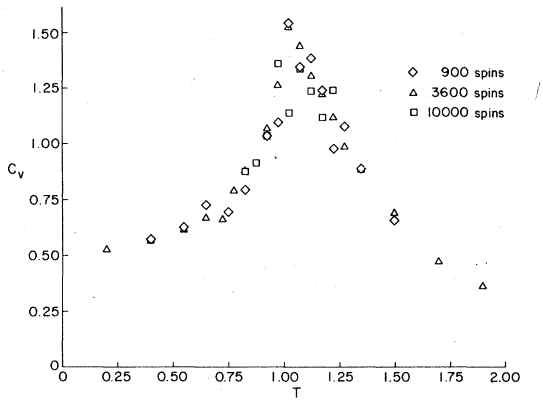

FIG. 5. Specific heat per spin vs temperature for 900, 3600, and 10000 spin systems.

Berker and Nelson[18] have calculated C_v for a system of vortices using a Debye-Hückle approach. They found a rounded peak about 38% above T_c, whereas our data show a sharp peak 15% about T_c. It is thus clear that their approach is too simplified to account for features present in our Monte Carlo simulation.

The specific heat has also been calculated using Migdal's decimation procedure.[19] Here T_c was found to be below the specific-heat peak, but again the peak was much flatter than we observe.

VI. VORTICITY

The central physical ideal of the KT theory is that the power-law decay of the spin-spin correlation function is modified by the presence of bound vortex pairs in the low-temperature phase and then at T_c the pairs unbind causing correlations to fall off exponentially in the high-temperature phase. To determine the vorticity within any region one merely travels around a closed loop and calculates the change in direction of the spins along the path. If there is a single vortex of unit strength within the loop, then the net change in spin direction will be 2π times an integer. We will call this integer the vorticity. On a square lattice the core of a vortex consists of four spins at the corners of a 1×1 square or plaquette. The only possible way for the vorticity to be greater than one is if the four spins have relative angles of π, $-\pi$, π, and $-\pi$ as one goes around the plaquette. This situation has a negligible probability of occurring, thus only vortices of unit strength need be considered.

The vorticity of a single vortex can be positive or negative. The vorticity within a region is the sum of the vortex strengths of those vortices contained in the region. Thus, if there are equal numbers of positive and negative vortices the net vorticity is zero. The interaction potential between vortices goes as $q_i q_j \ln r_{ij}$ where q_i is the vorticity of the ith vortex and r_{ij} is the separation between the two vortices. Thus, the vortices are analogous to parallel infinite charged wires. This analogy is very useful in discussing vortices and will be exploited below.

Vortices have been seen in previous Monte Carlo simulations.[9,20] However, they were generated by taking a random starting configuration and then running the simulation at very low temperatures. In this way metastable vortices were produced, but these have nothing directly to do with the phase transition. In our simulations we also started with a random configuration, but our first run was at $T = 2.0$, a temperature far above T_c. We then cooled down slowly through the transition and then heated back up through T_c. The vortices generated by our simulations therefore represent equilibrium phenomena.

To determine the vorticity within a curve of length L we computed the change in angle from one spin to the next, being sure to define the angle difference between neighboring spins to lie within $-\pi$ and π. To compute the vortex-pair density we calculate the number of vortices in the system by computing the vorticity around every square in the lattice with side length equal to one lattice spacing, counting the number of positive and negative vortices. The vortex-pair density, v, is defined as the sum of the positive (or negative) vortices divided by the area of the lattice. In this way we can also check to see if the total vorticity is zero as it must be with periodic boundary conditions, and is necessary from energetic arguments.

The vortex-pair density was calculated for the last configuration after 3000 passes at each temperature. The results are shown in the last column of Tables I and II.

To determine how the vorticity changes from pass to pass we calculated v at the end of every 200 passes for $T = 1.15$ starting from a completely ordered configuration as well as a completely random configuration. The vortex-pair density was virtually identical for each at the end of 3000 passes, and fluctuated around the average value by about 10% over the last 2000 passes. Generally, except at temperatures where there are very few vortices present, the difference between heating and cooling values is less than 20%.

Another indication that we are looking at an equilibrium sample of vortices is that at low temperatures $v \sim e^{-2\mu/T}$ where 2μ is the energy necessary to create a vortex pair. A plot of $\ln v$ vs $1/T$ is shown in Fig. 6. As can be seen for low temperatures $\ln v$ is proportional to $1/T$ with the slope being -9.4 ± 0.3 which is close to the value estimated by KT of $2\mu = 10.2$.[7] Near the specific-heat maximum the curve levels off indicating a much smaller chemical potential as it becomes easier to generate more vor-

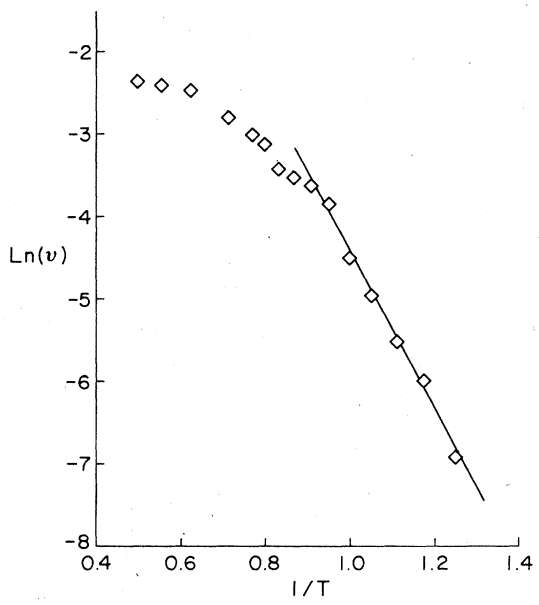

FIG. 6. Log of vortex-pair density vs $1/T$ for 3600 spin lattice. Straight line is least-squares fit to low-temperature data.

tices when many vortices are already present disordering the spins.

To understand what the vortices are doing at the transition we have displayed in Fig. 7 the position of positive and negative vortices for each temperature computed between $T=0.80$ and 1.05. This temperature range includes T_c and the specific-heat maximum. The KT theory predicts that well below T_c all vortices will be tightly bound in pairs with the mean separation between members of a pair, d, being around one lattice spacing and very much smaller than r, the mean separation of one pair from another. As T_c is approached d increases and r decreases as more vortex pairs appear. At T_c the first pairs unbind, that is there exists some pairs with d of the same order as r. Just above T_c a few percent of the pairs will unbind and far above T_c essentially all the vortices will be unbound.

From Fig. 7 we see that the KT picture is close to correct. However, there are some important modifications needed. Up to $T=0.80$ all the vortex pairs are tightly bound in pairs as shown in Fig. 7(a). The first pair with d greater than a lattice spacing appears at $T=0.85$. Also, note that a cluster of four vortices also appears at this temperature. At $T=0.90$ the

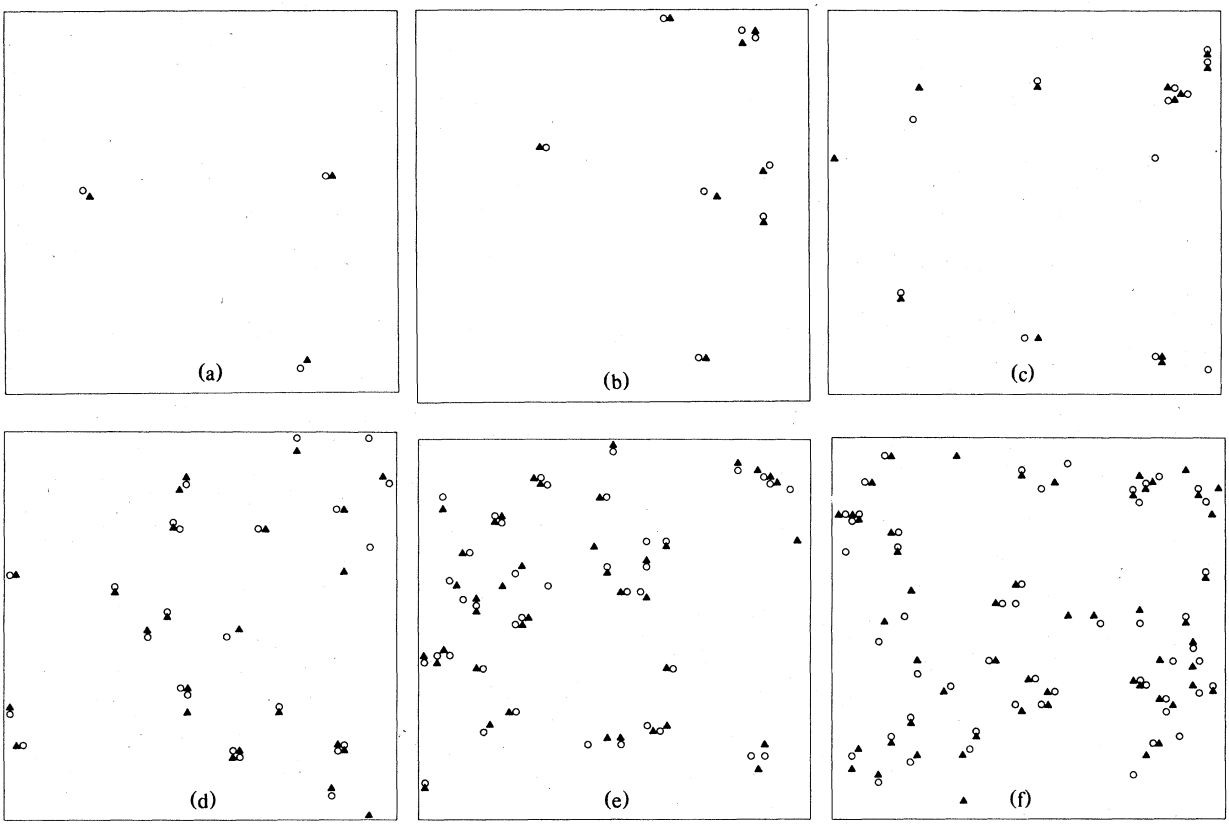

FIG. 7. Position of vortices for 3600 spin system for typical configurations. ○, positive vortices. ▲, negative vortices. (a) $T=0.80$, (b) $T=0.85$, (c) $T=0.90$, (d) $T=0.95$, (e) $T=1.00$, and (f) $T=1.05$.

first pair with $d \sim r$ appears. This is a satisfying confirmation of the KT picture since we have found $T_c = 0.89$. Also, note that a four vortex cluster splits up into a three vortex cluster and a single vortex. Just as the binding of large molecules is often less than that of smaller molecules we would expect that the large vortex clusters would unbind first. By $T = 0.95$ a significant fraction of the vortices belong to clusters with more than two vortices. For example, at $T = 0.95$, 39% of the vortices are in such larger clusters, as shown in Fig. 7(d). Indeed we see here an example of two vortex clusters of three vortices each unbound from each other, as well as a single vortex pulling away from a cluster of three other vortices. By $T = 1.0$ more complicated clusters appear and by $T = 1.05$, the identification of distinct clusters becomes difficult because of the large vortex density.

How would we expect these larger clusters to affect macroscopic quantities? We might expect T_c and possibly η at T_c to be slightly modified, but up to T_c almost all the vortices appear in bound pairs not larger clusters, thus the critical properties may not change very much. Above T_c, however, the effects may be dramatic with the correlation function falling off faster and the specific heat may rise faster. The larger clusters may be responsible for ν in $\chi \sim e^{b/t^{\nu}}$ being closer to 0.7 than 0.5 predicted by KT. Also, since unbinding would proceed faster with clusters, the specific-heat peak would be closer to T_c and sharper than simple theories predict, as we indeed observe.

VII. SUMMARY

In conclusion we have shown that the Monte Carlo simulation of the planar model can reproduce well-known low-temperature behavior and provide us with new information concerning the nature of the phase transition. We have seen the usual $\ln N$ loss of long-range order characteristic of two-dimensional systems with continuous symmetry. Our fits of correlation functions are consistent with the Kosterlitz-Thouless picture indicating a critical temperature around 0.89. We have found a sharp specific-heat peak at a temperature equal to 1.02. The shape and position of the peak relative to T_c indicate that simple analytic methods used so far are insufficient. Above T_c large vortex clusters unbind more easily than vortex pairs causing the specific-heat peak to be sharper and closer to T_c than previously calculated.

ACKNOWLEDGMENT

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