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LETTER TO THE EDITOR

The two-dimensional *XY* model in random hexagonal anisotropy

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Abstract. The two-dimensional *XY* model in the presence of random hexagonal anisotropy has been investigated by Monte Carlo simulation. The results indicate the existence of two continuous transitions as the temperature is reduced. Each of the phases is characterised by algebraic decay of the pair correlation functions.

The static properties of the pure two-dimensional *XY* model are now believed to be well understood from the work of Kosterlitz and Thouless (1973, 1974). At low temperatures this system exhibits quasiferromagnetism, that is zero magnetisation accompanied by algebraic decay of spin–spin correlation functions. At the Kosterlitz–Thouless transition temperature T_{KT} vortices that are tightly bound in dipole pairs at low temperature become free and the system becomes paramagnetic. This picture of the critical properties is supported by the Monte Carlo simulation of Tobochnic and Chester (1979).

Here the effect of random symmetry breaking anisotropy on the above picture of the critical properties is investigated. The Hamiltonian for such a system is given by

$$-\left(J\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j)+h\sum_i\cos(p\theta_i+\varphi_i)\right) \tag{1}$$

where θ_i are site variables confined to a square lattice, the first summation is over nearest neighbours and φ_i are independent random variables uniformly distributed between 0 and 2π.

The utility of the second term in Hamiltonian (1) is as a model for the effect of substrate randomness on layers of absorbed atoms.

Hamiltonian (1) has been investigated using renormalisation group techniques by Houghton *et al* (1981), Cardy and Ostlung (1982) and Villain and Fernandez (1984). Cardy and Ostlung used the replica trick and the methods of Jose *et al* (1977) to derive a full set of renormalisation group equations that included fully the effect of vortices. They predicted that the Kosterlitz–Thouless phase would be stable against the random anisotropy for a range of temperature bounded away from zero and given by

$$4\pi J/p^2 < T < \pi J/2.$$

Both inequalities can be satisfied if $p > \sqrt{8}$. This result is supported by the real-space decimation calculation of Villain and Fernandez. However their calculation excludes vortices.

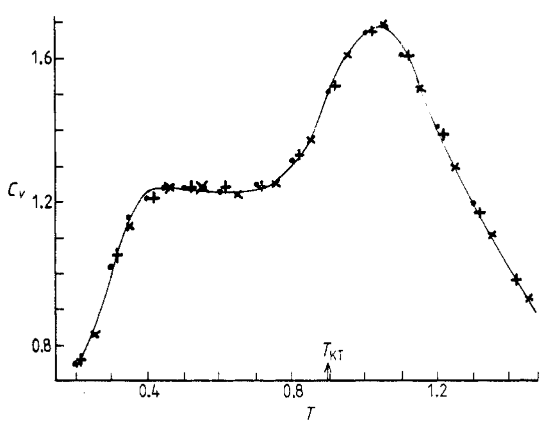

Figure 1. Specific heat C_v against temperature, ($\bullet = 32^2, + = 64^2, \times = 128^2$). The curve is a guide to the eye only.

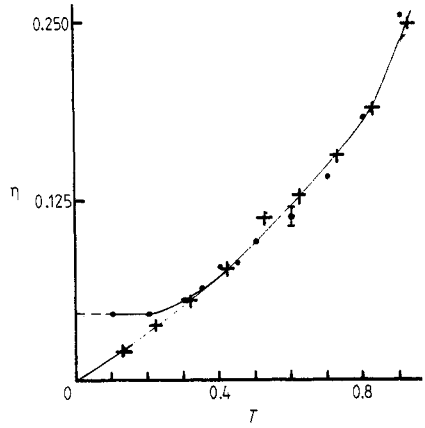

Figure 2. Results for η obtained from fitting equation (3) to Monte Carlo data. Data obtained for system size of 64^2. $\times$ denote pure system and $\bullet$ anisotropic system. The curve is a guide to the eye only.

At low temperatures the Cardy and Ostlung equation predicts a re-entrant paramagnetic state. Further they suggest that the transition at the low-temperature phase boundary may be first order.

Here preliminary results from a Monte Carlo simulation of Hamiltonian (1) are presented for the case of hexagonal anisotropy ($P = 6$) and the case $J = h = 1$. Comparison is made with the predictions of renormalisation group calculations. A checkerboard algorithm was used suitable for implementation on a DAP which is a highly parallel machine. The simulation was run for times ranging from 12000 to 200000 Monte Carlo steps per spin without any significant drift in the results reported here; the time stability of the results is thus judged to be good.

The specific heat was calculated by numerical differentiation of the energy. The results are shown in figure 1. The arrow indicates T_{KT} taken from Tobochnic and Chester. Three sizes of system shown are 32^2, 64^2 and 128^2. At a first-order transition the specific heat C_v scales as (Fisher and Berker 1982)

$$C_v \simeq l^2$$

where l is the linear dimension of the system. No such divergent behaviour is visible on figure 1, the only singularity being a kink at about $T = 0.4$. At and near this temperature a search has been made for bimodal behaviour of the energy fluctuation. Such behaviour is characteristic of a first-order transition. No bimodal behaviour was detected using a bin size of 0.008. This result together with figure 1 gives no support for the low-temperature transition being first order. Clearly the existence of a very weak first-order transition cannot be excluded; however, the results here are more consistent with the interpretation that there is only a weak singularity at about $T = 0.4$.

To determine the nature of the phases the spin pair correlation function has been calculated. This is given by

$$C(n) = \langle \cos(\theta_i - \theta_j) \rangle \qquad n = |i = j|$$

where $\langle \quad \rangle$ denotes thermal averaging and i and j are constrained to lie in the same row.

In the Kosterlitz–Thouless phase the pair correlation function decays asymptotically as

$$C(n) \simeq 1/n^{\eta} \tag{2}$$

Because of the finiteness of the lattice the approach of Tobochnik and Chester has been followed and data fitted to the finite lattice form of (2) given by

$$C(n) = \mathrm{e}^{-\eta G(n)}$$
$$G(n) = \frac{2\pi}{l^2} \sum_k \frac{1 - \mathrm{e}^{\mathrm{i}k_x n}}{4 - 2\cos k_x - 2\cos k_y}. \tag{3}$$

Fits were also attempted to the higher-temperature form of $C(n)$ given by

$$C(n) = \mathrm{e}^{-\eta G(n)} (\mathrm{e}^{-n/\varepsilon} + \mathrm{e}^{-(l-n)/\varepsilon}) \tag{4}$$

where ε is the correlation length, and also to simple exponential decay.

Below T_{KT} it was not possible to fit the data to (4) or to simple exponential decay. This was true for all temperatures below T_{KT} extending down to zero. In this temperature range ε became of the order of the size of the system and grew with increasing system size. This would seem to exclude the possibility that the lower phase transition is re-entrant into the paramagnetic state.

Figure 2 shows the results for η from a fit of $C(n)$ to form (3). Results for both the pure and the anisotropic system are shown together. For a range of temperature extending down to below $T = 0.4$, the values of η obtained for both models agree within numerical uncertainty. This is consistent with the prediction of Cardy and Ostlung that the anisotropy is irrelevant for a range of temperature bounded away from zero. Below $T = 0.4$ the values of η are clearly seen to diverge.

These results for $C(n)$ do not support the theory that the low-temperature phase is paramagnetic. Indeed the system appears to be quasiferromagnetic down to $T = 0$, with η becoming renormalised at low temperatures. Some support for this interpretation appears in the work of Villain and Fernandez. Their results for η in what they call the two-parameter approximation and given by their equations (4.12) and (4.13) show that η is renormalised at low temperature and the system remains quasiferromagnetic.

Thus Monte Carlo simulation has produced partial agreement with the results of Cardy and Ostlung. However, simulation has not produced any evidence for the low-temperature transition being first order or the low-temperature phase being paramagnetic. The effect of varying p and h as well as the time-dependent properties remain to be investigated and will be reported subsequently.

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