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The phase diagram of a generalised *XY* model

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Abstract. A generalisation of the two-dimensional *XY* model is studied using Monte Carlo simulation. In this model, two-component, classical spins interact both ferromagnetically and nematically. Three phases occur as temperature and the two interaction strengths are varied: a high-temperature, disordered phase, and two low-temperature phases with algebraic correlations in, respectively, the ferromagnetic and nematic order parameters. The critical behaviour at the phase boundaries is examined: the high-temperature phase is entered via Kosterlitz–Thouless transitions, whilst the low-temperature phases are separated by an Ising transition.

1. Introduction

There has been recent interest (Korshunov 1985, 1986, Lee and Grinstein 1985, Sluckin and Ziman 1988) in the statistical mechanics of a class of generalised, two-dimensional *XY* models. In these models, classical two-component spins interact with both ferromagnetic and nematic coupling, so the potential energy for a pair of spins has two minima as a function of their relative angle. At one minimum the spins are parallel; at the other they are antiparallel. The simplest Hamiltonian of this kind is

$$H = -\sum_{\langle ij \rangle} [\Delta \cos(\theta_i - \theta_j) + (1 - \Delta) \cos 2(\theta_i - \theta_j)]. \tag{1}$$

In this equation θ_i, $0 \leq \theta_i < 2\pi$, indicates the spin orientation at site i; the summation is over nearest-neighbour pairs of sites on a square lattice; Δ, $0 \leq \Delta \leq 1$, is the ferromagnetic coupling; and $1 - \Delta$ is the nematic coupling.

It has been suggested that this model may represent superfluid ^{3}He films (Korshunov 1985) and liquid crystal films (Lee and Grinstein 1985). In addition, the model has theoretical appeal because of the exotic low-temperature excitations that it supports.

There are four kinds of excitation that are expected to be important: spin waves, integer vortices, domain walls and half-integer vortices. Spin waves and integer vortices are familiar from studies of the ferromagnetic *XY* model, $\Delta = 1$ (Kosterlitz and Thouless 1973, Kosterlitz 1974). Domain walls and half-integer vortices control behaviour near the nematic limit, $\Delta \ll 1$. A domain wall is a line (on the dual lattice) across which spins are antiparallel. It may either close on itself or end at a half-integer vortex: a point singularity around which spin directions rotate through an angle π on circumnavigation.

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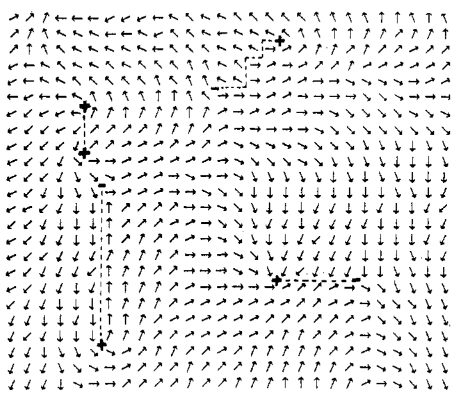

Figure 1. A configuration of the model generated by quenching from high temperature at $\Delta = 0.5$. Four domain walls are present, linking pairs of half-integer vortices.

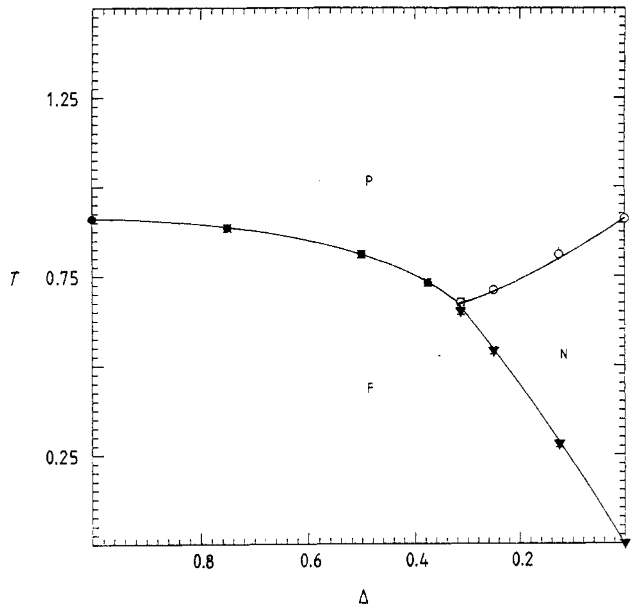

Figure 2. The calculated phase diagram for the model. The high-temperature disordered phase is denoted by P, the ferromagnetic phase by F and the nematic phase by N.

These excitations are illustrated in a configuration generated by quenching from high temperature (figure 1).

A phase diagram has been proposed (figure 2) for the model in the Δ–T plane (where T is temperature), mainly from considering behaviour near the boundaries $T = 0$, $\Delta = 0$ and $\Delta = 1$ (Korshunov 1985, Lee and Grinstein 1985). To characterise the phases, two correlation functions are important. The first

$$G_1(r) = \langle \cos(\theta_0 - \theta_r) \rangle$$

is sensitive only to ferromagnetic order, in which spins have a common direction. The second

$$G_2(r) = \langle \cos[2(\theta_0 - \theta_r)] \rangle$$

is sensitive both to ferromagnetic order and to nematic order, in which spins have a common axis but no unique direction. In the high-temperature phase both correlation functions are expected to decay exponentially with separation, r. Algebraic order is expected in both quantities in the low-temperature ferromagnetic phase:

$$G_1(r) \sim r^{-\eta_1} \qquad G_2(r) \sim r^{-\eta_2}$$

whilst in the low-temperature nematic phase $G_1(r)$ should decay exponentially and $G_2(r)$ algebraically.

The reasons for anticipating this phase diagram are as follows. Close to the ferromagnetic line $(1 - \Delta \ll 1)$, one has essentially the conventional XY model, analysed by Kosterlitz and Thouless (1973), and Kosterlitz (1974). At low temperatures, spin waves destroy the long-range order of the ground state, leaving power-law decay of correlations. The high-temperature phase is entered via a transition at which integer vortex–anti-vortex pairs unbind. On the purely nematic line, a modified version of this picture applies. Since, with $\Delta = 0$, the energy of a configuration depends on spin directions only modulo π, $G_1(r)$ is necessarily zero for $r \neq 0$. By the same argument, half-integer vortices are possible. One therefore expects a half-integer vortex-unbinding transition at which the decay of $G_2(r)$ changes from power-law to exponential. Finally, the transition between the two low-temperature phases is best understood in the low-temperature, nematic corner of the phase diagram: T and Δ small. This transition is driven by domain walls, which have an energy per unit length roughly proportional to Δ. By analogy with the Ising model, the wall free energy is expected to decrease with increasing temperature. At a critical temperature of order Δ (still supposing $\Delta \ll 1$), the wall free energy vanishes, domain walls proliferate and the system passes from the ferromagnetic to the nematic phase. This transition is of particular interest since neither of the phases it separates have long-range order, yet it is expected to belong to the two-dimensional Ising universality class.

The aim of the present work is to test these ideas by Monte Carlo simulation of the model given as (1). We are able to identify the three transitions described, and also the multicritical point at which the three phases meet. These calculations complement an earlier numerical study by Sluckin and Ziman (1988), who mapped the two-dimensional statistical mechanical model onto a one-dimensional quantum spin chain.

2. Calculation and results

The Metropolis algorithm was used to calculate specific heat and the correlation functions, $G_1(r)$ and $G_2(r)$, for the model defined by (1). Systems of sizes from 4^2 to 64^2 spins were studied. Initial work (figures 3–5) used 8×10^3 Monte Carlo steps per spin, at each of 330 points in the Δ–T plane; subsequent calculations (figures 6–10) used 8×10^5 Monte Carlo steps per spin at selected values of Δ.

The algorithm was implemented on a processor array consisting of 17 INMOS T-414 Transputers. Details of the computational techniques have been described elsewhere (Askew *et al* 1986, 1988).

Broad confirmation of the proposed phase diagram is provided by the measured specific heat and inverse susceptibilities. The susceptibilities are integrals of the two correlations functions

$$\chi_{1,2} = \sum_r G_{1,2}(r).$$

Algebraic decay, $G(r) \sim |r|^{-\eta}$, of a correlation function in a low-temperature phase

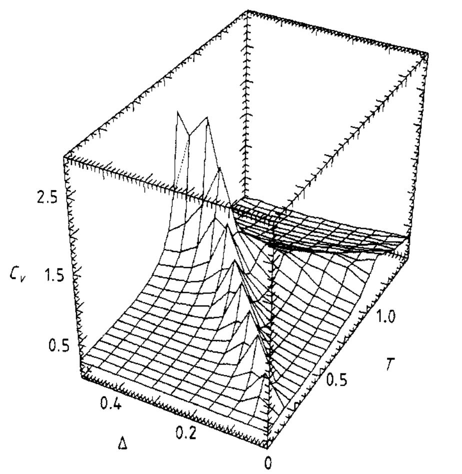

Figure 3. The specific heat of the model in the Δ–T plane.

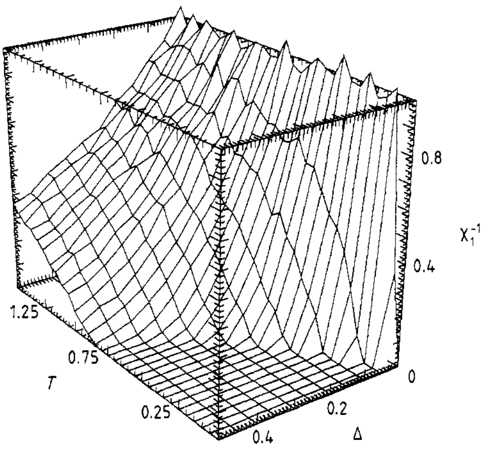

Figure 4. The inverse ferromagnetic susceptibility, χ_1^{-1}.

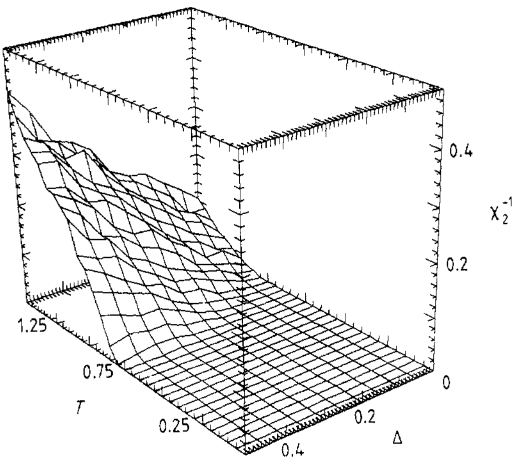

Figure 5. The inverse nematic susceptibility, χ_2^{-1}.

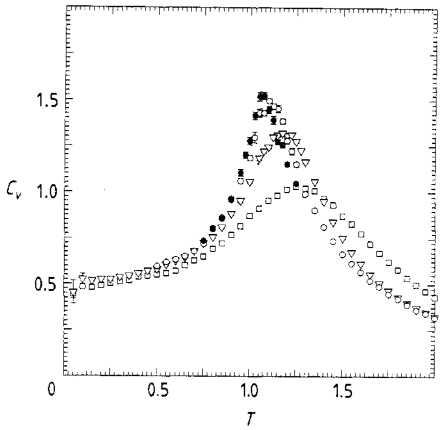

Figure 6. The specific heat at $\Delta = 1$ (pure ferromagnetic XY model). The broad maximum is associated with vortex unbinding. The symbols □, ▽, ○ and ● denote system sizes of 4^2, 8^2, 16^2 and 32^2 respectively.

implies that the associated susceptibility diverges with (linear) system size, L, as $\chi \sim L^{2-\eta}$.

The specific heat (figure 3) has a sharp ridge along the anticipated locus of the Ising transition between the ferromagnetic and nematic low-temperature phases, which is consistent with a logarithmic divergence (as for the two-dimensional Ising model), cut off by finite system size. A second ridge in the specific heat, broader, lower and at higher temperatures, is associated with vortex unbinding; its maximum is expected to lie above the Kosterlitz–Thouless transition temperature (Kosterlitz 1974). The phases can be identified by the behaviours of the inverse susceptibilities, χ_1^{-1} and χ_2^{-1}. Both fall to zero

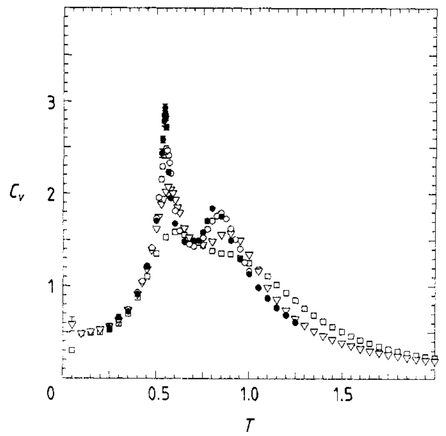

Figure 7. The specific heat at $\Delta = 0.25$. The sharp, lower-temperature peak is associated with an Ising transition, and the broad, higher-temperature maximum with vortex unbinding. Symbols indicate system sizes as in figure 6.

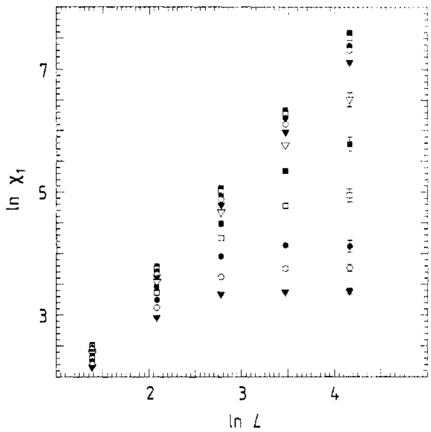

Figure 8. A double-logarithmic plot of ferromagnetic susceptibility against system size for $\Delta = 1$: $\ln \chi_1$ versus $\ln L$. The symbols ■, □, ●, ○, . . ., ▼ indicate temperatures $T = 0.75, 0.80, \ldots, 1.25$ respectively.

(for large L) in the ferromagnetic phase; χ_1^{-1} is non-zero and χ_2^{-1} is zero in the nematic phase, and both are non-zero in the high-temperature phase. Figures 4 and 5 illustrate this.

A more detailed study of the specific heat has been made at two values of Δ: $\Delta = 1$, the ferromagnetic XY model; and $\Delta = 0.25$, for which all three phases can be reached by varying temperature. The similarity between the specific heat maximum associated with vortex unbinding at $\Delta = 1$ (figure 6) and the corresponding (higher-temperature) maximum at $\Delta = 0.25$ (figure 7) is striking. The lower-temperature specific heat peak at $\Delta = 0.25$, marking the Ising transition, has an amplitude that increases progressively with system size. One expects from scaling ideas (Ferdinand and Fisher 1969) that the peak height should be logarithmic in system size, and the increase in peak height with each doubling of system size is indeed roughly constant.

Algebraic decay of correlations in the low-temperature phases has been demonstrated by a finite-size scaling analysis of susceptibilities, also at $\Delta = 1$ and $\Delta = 0.25$. In the low-temperature phase of the purely ferromagnetic XY model ($\Delta = 1$), one expects $\ln\chi_1$ to vary linearly with $\ln L$, with slope $2 - \eta$. In the high-temperature phase, $\ln \chi_1$ has a limiting value for large L. This behaviour is demonstrated in figure 8. Furthermore, since $\eta = \frac{1}{4}$ at the Kosterlitz–Thouless transition (Kosterlitz 1974), the critical point can be identified as the temperature at which $\ln \chi_1$ versus $\ln L$ has slope $\frac{7}{4}$. Values of $\eta_1(T)$ derived in this way are shown in figure 9, from which we estimate $T_c = 0.93$. The result is in reasonable agreement with a recent, very extensive study of the purely ferromagnetic XY model (Gupta *et al* 1988), which gave $T_c = 0.898 \pm 0.002$. Similar algebraic decay of nematic correlations at $\Delta = 0.25$ is illustrated in figure 10.

3. Conclusions

The statistical mechanics of this generalised XY model was analysed by Korshunov (1985) and Lee and Grinstein (1985), mainly by considering the low-energy excitations.

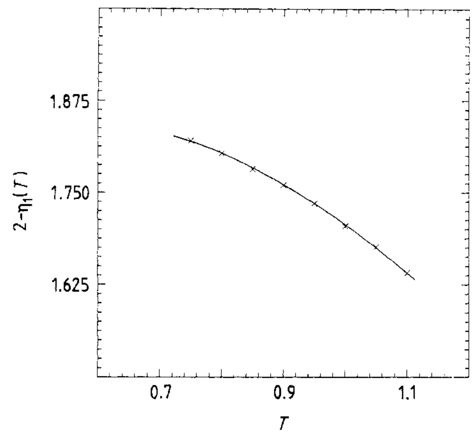

Figure 9. Values of $2 - \eta_1(T)$ versus temperature for $\Delta = 1$, derived from figure 8.

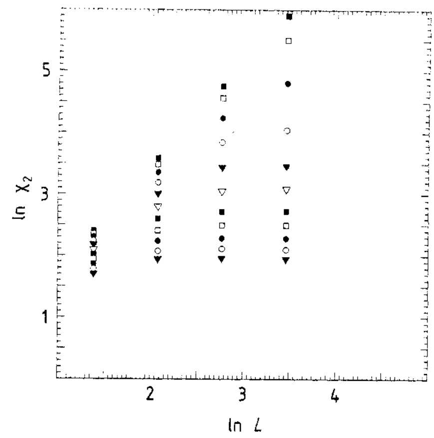

Figure 10. A double-logarithmic plot of nematic susceptibility against system size for $\Delta = 0.25$: ln χ_2 versus ln L. The symbols ■, □, ●, ○, . . . , ▼ indicate temperatures $T = 0.50, 0.55, 0.60, \ldots, 1.00$ respectively.

Such an approach is necessarily exact only in the low-temperature limit. The results of Monte Carlo simulation described in the present paper support their earlier conclusions and confirm the power of their approach. Finite-size scaling analysis of susceptibilities demonstrates the existence of two low-temperature phases with power-law correlations. The behaviour of the specific heat supports the idea that the transition between these low-temperature phases is in the two-dimensional Ising universality class, and that the high-temperature phase is reached via vortex-unbinding transitions.

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