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LETTER TO THE EDITOR

Phase diagram of the $Z(5)$ model on a square lattice

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Abstract. A general five-state model, which contains the five-state Potts model and a solid-on-solid model as special cases, is studied. We find that the high-temperature paramagnetic and the low-temperature ordered phases are separated either by a line of first-order transitions or by an intermediate phase with algebraic decay of correlations. The phase diagram is proposed on the basis of general considerations and Monte-Carlo simulations.

Models of interacting spins on two-dimensional lattices have been the object of numerous recent theoretical investigations (for a recent review see, e.g., Barber 1980). Some of these models are of special interest to statistical mechanicians because of their rich and complex phase structure and interesting critical behaviour. Many models have physical realisation (Domany and Riedel 1978, Tosatti 1978, Bak 1979). Some others are of interest to field theorists (e.g. Kogut 1979).

In particular, the class of planar vector models has received considerable attention (Jose *et al* 1977, Cardy 1978, Kadanoff 1978, Wu 1979, Nishimori 1979, Horn *et al* 1979, Elitzur *et al* 1979, Einhorn *et al* 1980, Guth *et al* 1980). In these models one considers an angle θ_i associated with each site of a two-dimensional lattice, with the Hamiltonian

$$H\{\theta_i\} = +\sum_{\langle ij\rangle} V(\theta_i - \theta_j) - h_N \sum_i \cos N\theta_i \tag{1}$$

where $V(\theta)$ is a periodic even function,

$$V(\theta + 2\pi) = V(\theta) = V(-\theta), \tag{2}$$

such that the energy of a pair of nearest-neighbour spins $\langle ij\rangle$ is lowest when $\theta_i = \theta_j$:

$$V(0) < V(\theta \neq 0). \tag{3}$$

When $h_N = 0$, the model possesses a continuous symmetry, and exhibits the behaviour predicted by Kosterlitz and Thouless (1973) and Kosterlitz (1974). In the limit $h_N \to \infty$, the model reduces to one of discrete vectors, allowed to point to N discrete directions.

Most theoretical studies concentrated on the case of the Villain (1975) form for the interaction $V(\theta)$, i.e.

$$\exp(-V(\theta)) = \sum_l \exp[-\tfrac{1}{2}K(\theta - 2\pi l)^2]. \tag{4}$$

In the limit $h_N \to \infty$, one obtains the discrete N-state Villain model.

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Jose *et al* (1977) studied the relevance of N-fold anisotropy fields h_N near the Gaussian line of fixed points which governs the critical behaviour of the generalised isotropic Villian model they have introduced. They found that the relevance of such fields depends on the temperature (or K^{-1}) and on N, namely that the anisotropy field is relevant for temperatures $T < T_1(N)$. For $N < 4$ the critical temperature T_1 satisfies $T_1 > T_{KT}$, where T_{KT} is the temperature above which the Kosterlitz–Thouless phase becomes unstable. Therefore, they predict that the planar model, as defined by equations (1) and (4), with $N \geqslant 5$, *in the limit of small* h_N will have two transitions: from the paramagnetic to a Kosterlitz–Thouless (massless) phase, and at some lower temperature to a phase with conventional long-range order. Jose *et al* also considered the extremely anisotropic limit, that of the discrete N-state Villain model. In this limit they derived a duality relation, but no information concerning the phases and number of transitions.

Elitzur *et al* (1979), using duality and comparing correlations of the discrete model with those of the isotropic ($h_N = 0$) one by means of a Griffiths inequality, were able to show that for $N > N_c$ the discrete Villain model must also have two transitions. However, they did not give a rigorously derived value for N_c. According to their estimate, the discrete five-state Villain model should have two transitions. More recently, Einhorn *et al* (1980) proposed a physical mechanism that explains the occurrence of two transitions in terms of a wall interpenetration and vortex liberation transitions respectively. An alternative, presumably equivalent description is obtained using 'two Coulomb gases' (Kadanoff 1978). Einhorn *et al* also predict that the five-state model has three phases. One of the aims of the present communication is to further substantiate this prediction.

It should be noted that the considerations of Elitzur *et al* utilise the Villain form of the interaction. One problem of interest that has not been studied extensively is the effect of the form of $V(\theta)$ on the phases and the nature of the transition. This problem is of particular interest, since the most general discrete model contains the N-state Potts model which is known to have a single transition from a paramagnetic phase to a phase with conventional long-range order. Moreover, this transition is known to be of first order for $N > 4$ (Baxter 1973). Thus the general discrete five-state model can be viewed as the simplest possible testing ground for situations where application of a symmetry-breaking field destroys a first-order transition, and changes the phase structure and critical properties of the system. While such situations were studied in some detail for three-dimensional systems and models (Bak *et al* 1976, Domany *et al* 1977, Kerszberg and Mukamel 1979, R Ditzian *et al* 1980, unpublished), not much is known about the manner in which first-order transitions become continuous in two-dimensional models.

To be explicit, we study the way the first-order transition of the five-state Potts model turns into two transitions with an intermediate Kosterlitz–Thouless phase as the interaction $V(\theta)$ is changed from the Potts to the Villain form. A convenient parametrisation of the most general five-state model with $V(\theta)$ of (2) and (3) can be defined as follows. Choose the normalisation $V(0) = 0$, and define

$$x_1 = \exp[-V(\tfrac{2}{5}\pi)/kT] \qquad x_2 = \exp[-V(\tfrac{4}{5}\pi)/kT] \tag{5}$$

with $0 < x_1, x_2 < 1$. This general five-state model was studied by Nishimori (1979), who used the Migdal–Kadanoff approximate renormalisation group method (Migdal 1975, Kadanoff 1976), and by Wu (1979). We believe that the phase diagrams predicted by both workers are incorrect. Our model reduces to the five-state Potts model on the line

$$x_1 = x_2 \tag{6}$$

and to the discrete five-state Villain model on the trajectory (parametrised by $0 < K < \infty$)

$$x_j = \sum_{l=-\infty}^{\infty} \exp[-\tfrac{1}{2}K(\tfrac{2}{5}\pi j - 2\pi l)^2]\Big(\sum \exp[-\tfrac{1}{2}K(2\pi l)^2]\Big)^{-1}. \tag{7}$$

Another line of special interest is the boundary of figure 1, i.e.

$$x_2 = 0. \tag{8}$$

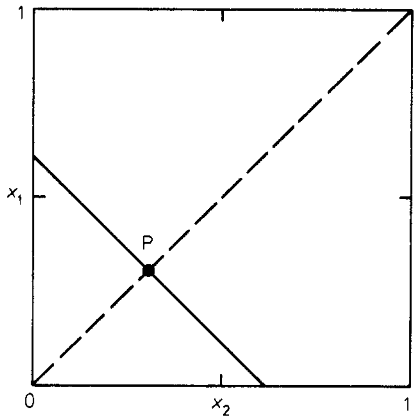

Figure 1. Parameter space of a general five-state mode. x_1 and x_2 are defined in equation (5). The line $x_1 = x_2$ corresponds to the five-state Potts model. The self-dual line (equation 10)) is also shown. On the lines $x_1 = 0$ and $x_2 = 0$ the five-state model is equivalent to an SOS model.

We shall show that on this line (and also on the line $x_1 = 0$) the discrete five-state model is completely equivalent to a solid-on-solid (SOS) type model, defined in terms of a non-compact local integer variable— $\infty < n_i < \infty$. This latter model, which was discussed by Emery and Swendsen (1977) as a limiting case of a family of SOS models, is believed to be in the universality class of the XY model.

Two symmetries of the model should be noted (Wu 1979). First, the partition function is invariant under interchanging x_1 and x_2; therefore the phase diagram is symmetric with respect to reflection about the Potts line. Second, a duality transformation (Wu and Wang 1976), given by

$$\begin{aligned} \tilde{x}_1 &= [1 + \tfrac{1}{2}(\sqrt{5} - 1)x_1 - \tfrac{1}{2}(\sqrt{5} + 1)x_2]/(1 + 2x_1 + 2x_2), \\ \tilde{x}_2 &= [1 - \tfrac{1}{2}(\sqrt{5} + 1)x_1 + \tfrac{1}{2}(\sqrt{5} - 1)x_2]/(1 + 2x_1 + 2x_2), \end{aligned} \tag{9}$$

leaves the partition function invariant (up to a simple multiplicative constant). This transformation has a line of self-dual points, given by

$$1 + 2x_1 + 2x_2 = \sqrt{5}. \tag{10}$$

We now turn to the line $x_2 = 0$. On this line, the relative angle between two nearest neighbours can take the values of 0 or $\pm\frac{2}{5}\pi$; the value $\pm\frac{4}{5}\pi$ is not allowed. Each configuration can be characterised by a set of integers $\{n_i\}$; $n_i = 1, 2, \ldots, 5$, that define the angle at site i as $\theta_i = \frac{2}{5}\pi n_i$. Alternatively, we can characterise each configuration by a set of arrows placed on the edges of the lattice according to the following convention. If i, j are two neighbouring sites, and $\theta_i = \theta_j$, no arrow is placed on the edge. If $\theta_i = \theta_j + \frac{2}{5}\pi$ an arrow pointing from j to i is put there; an oppositely directed arrow appears when $\theta_i = \theta_j - \frac{2}{5}\pi$. A unique arrow configuration corresponds to each $\{\theta_i\}$ configuration, and there are five $\{n_i\}$ configurations that yield the same arrow configuration. The allowed arrow configurations of a basic square (plaquette) are shown in figure 2. The partition function of the five-state model on the $x_2 = 0$ line is given by

$$Z(x_1, x_2 = 0) = 5 \sum_C x_1^{A(C)} \tag{11}$$

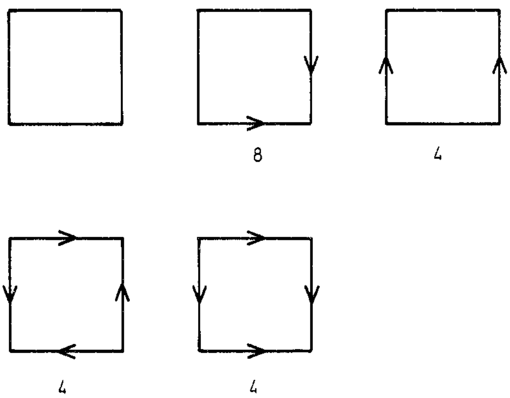

Figure 2. Allowed arrow configurations of a basic square for $Z(N \geq 5)$ models on the $x_2 = 0$ line.

where C is a configuration of arrows such that every plaquette is allowed, i.e. appears in figure 2, and $A(C)$ is the number of arrows in C. It is easy to see that for any discrete N-state planar model, with $N \geq 5$ and interaction that allows only relative angle $\pm 2\pi/N$ with Boltzmann weight x (and 0 with weight 1), the partition function has the same form as (11), and the allowed arrow configurations are the same as those of figure 2. Furthermore, consider a solid-on-solid model, defined in terms of integers $-\infty < n_i < \infty$ and nearest-neighbour interactions of the form (Emery and Swendsen 1977)

$$K|n_i - n_j|^p. \tag{12}$$

In the limit $p \to \infty$, only configurations with $|n_i - n_j| = 0, 1$ are allowed. Note that this model is by no means equivalent to the one solved by Van Beijeren (1977) or those studied by W J Shugard *et al* (1980, unpublished). This SOS model, defined in terms of a non-compact variable, has the same form for the partition function as equation (11). It is also easy to show that the following equality between correlation functions holds:

$$\langle \cos(\theta_i - \theta_k) \rangle_N = \left\langle \cos\left(\frac{2\pi n_i}{N} - \frac{2\pi n_k}{N}\right) \right\rangle_{\text{SOS}} \tag{13}$$

where on the left-hand side the average $\langle\ \rangle_N$ is evaluated for an N-state discrete model on the special line, and the right-hand side in the ensemble of the SOS model (12) in the $p \to \infty$ limit.

The reasons for this equivalence between models with compact and non-compact variables is evident when one observes the allowed plaquette configurations of figure 2. On the special line $x_2 = 0$, the only allowed configurations are those in which *no basic square can have finite vorticity*. Therefore, on this line no allowed configurations will have a closed path along which the θ_i variable undergoes a full 2π rotation. Thus the fact that θ_i is a compact variable is never reflected in the energy of an allowed configuration.

A more formal proof of the equivalence of the two models can be given as follows. Choose an arbitrary integer variable function $f(k)$; the expression

$$Z = \sum_{m_\mu=-\infty}^{+\infty} \sum_{n=0}^{N-1} \prod_{\text{links}} f(\Delta_\mu n + Nm_\mu) \tag{14}$$

represents the statistical sum of the most general nearest-neighbour $Z(N)$ model.

Any integer-valued link variable m_μ can be written as

$$m_\mu = \Delta_\mu P + \epsilon_{\mu\nu} a^\nu \frac{1}{a\,.\,\Delta} M \tag{15}$$

where P and M are integers and a^ν is an arbitrary vector. The P variable can be used to extend the summation on n to infinity, i.e.

$$Z = \sum_{M=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \prod_{\text{links}} f\left(\Delta_\mu n + N\epsilon_{\mu\nu} a^\nu \frac{1}{a\,.\,\Delta} M\right). \tag{16}$$

Now if we choose for $f(k)$ the function

$$\bar{f}(k) = \begin{cases} 1 & k = 0 \\ x & k = \pm 1 \\ 0 & \text{otherwise} \end{cases} \tag{17}$$

we get a zero contribution to Z unless

$$-1 \leqslant \Delta_\mu n + N\epsilon_{\mu\nu} a^\nu \frac{1}{a\,.\,\Delta} M \leqslant +1. \tag{18}$$

Applying the $\epsilon^{\rho\mu}\Delta_\rho$ operation to the previous equation on a square lattice we obtain

$$-4 \leqslant NM \leqslant +4 \tag{19}$$

and therefore if $N \geqslant 5$, M, being an integer, must be zero. Obviously, since $M = \epsilon^{\mu\nu}\Delta_\nu m_\mu$, M plays the role of the vorticity. Therefore for the particular $\bar{f}(k)$ chosen

$$Z = \sum_{n=-\infty}^{\infty} \prod_{\text{links}} \bar{f}(\Delta_\mu n), \tag{20}$$

i.e. the SOS model.

The implications of this equivalence are quite important for the various discrete N-state planar models. The SOS model is dual to a continuous XY-type model, with the interaction

$$V(\theta) = \ln(1 + 2x \cos\theta). \tag{21}$$

Since in the SOS representation the model is well defined for any $x < 1$ we do not believe that any special problem arises for the values of x for which the argument of the log may be negative. Therefore if the SOS model does have a transition it will be in the Kosterlitz–Thouless universality class, and the system will have a 'massless' phase, with algebraic decay of correlations. This phase will occur when $x_1 > x_2$ is greater than some critical value, x_c. Therefore for $x_1 > x_c$ no correlation function of the SOS model can decay exponentially; in particular, the function $\langle\cos(\frac{2}{5}\pi n(0) - \frac{2}{5}\pi n(R))\rangle_{SOS} = \Gamma(R)$. This implies that for $x_1 > x_c$ the five-state model will also have (on the $x_2 = 0$ line) algebraic decay of correlations. The continuation of this segment of the $x_2 = 0$ line into the x_1–x_2 plane constitutes the intermediate Kosterlitz–Thouless phase predicted for $N > 5$ by Elitzur *et al.*

Similar considerations, when applied for the Ashkin–Teller (or $Z(4)$) model on a triangular lattice, also indicate the existence of a massless phase. Again this phase is expected to be present near the $x_2 = 0$ line where x_2 is the Boltzmann weight that corresponds to a relative angle of $\pm\pi$ between two neighbouring spins.

Savit (1980) studied $Z(N)$ models on triangular lattices using another 'decompactification' method and reached the conclusion that for $N \geqslant 5$ three phases exist. Of course this does not contradict our expectation that already for $N = 4$ two transitions occur. The critical value x_c can be estimated by calculating the interface free energy, σ, associated with two domains magnetised along different directions, say $\theta_1 = 0$ and $\theta_2 = \frac{2}{5}\pi$. This free energy should vanish at the transition. Following Muller–Hartman and Zittartz (1977) we estimate σ by considering only wall configurations that do not have bubbles and overhangs. While this method yields the exact free energy for the Ising model, it may only be used for estimating σ associated with the model considered in this work. We find

$$\sigma = 2K + \ln\tanh K, \qquad K = -\tfrac{1}{2}\ln x_1, \tag{22}$$

which is the result found for the Ising model. Setting $\sigma = 0$ an estimate for the critical value x_c is obtained:

$$x_c = \sqrt{2} - 1. \tag{23}$$

The point $(x_c, 0)$ does not lie on the self-dual line and therefore one expects to find a phase transition at the point which is dual to $(x_c, 0)$. This result is in agreement with the phase diagram (figure 3) where one finds two lines of critical points. An upper bound for x_c can be estimated noting that the SOS model, having less freedom for its variable than the discrete Gaussian model, is probably more ordered. Therefore we expect the transition to a massless phase to occur at a lower temperature than in a Gaussian model. The physical interpretation of this transition in the language of Einhorn *et al* is simply a wall interpenetration. Since the vortices do not exist in this model they cannot interfere with the wall transition.

Consider now the vicinity of the Potts line, $x_1 = x_2$. At $x^* = (\sqrt{5} + 1)^{-1}$ the Potts model has a first-order transition, with a *finite* latent heat. When the Potts symmetry is slightly broken, the latent heat may decrease; however, it does not seem likely to vanish for an arbitrarily small deviation from the Potts line. Thus, contrary to the prediction of Wu (1979), we believe that the first-order nature of the transition persists for finite deviations from the Potts line.

These considerations imply the qualitative phase diagram of figure 3. We have indicated three possible ways in which the three transition lines (two limit the intermediate Kosterlitz–Thouless phase, and the third is the extension of the first-order Potts transition) can meet. Of the three possibilities, that of figure 3(a) seems to be the most plausible. The phase diagram of figure 3(b) implies the existence of a first-order

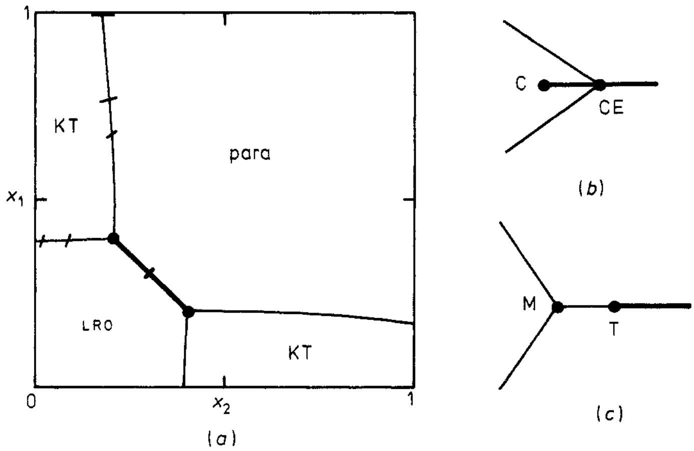

Figure 3. (*a*) Phase diagram of the $Z(5)$ model. There are three phases: disordered (para), massless (KT) and a phase with conventional long-range order (LRO). The transition from para to LRO is either first order or via an intermediate KT phase. (*b*) and (*c*) are other possible ways in which the line of first-order transitions connects to the KT phase boundary. See text for discussion.

transition terminating at a critical point within the Kosterlitz–Thouless phase. Such a transition could correspond to a discontinuity of the amplitude of the local vector field. Gibbs phase-rule-type arguments show that the phase diagram (*c*) is not likely to be realised. The Landau Hamiltonian associated with the para–LRO transition has the form

$$H = u_2 S^2 + u_4 S^4 + u_5 S^5 \cos 5\theta + O(S^6) \tag{24}$$

where (S, θ) defines the two-component order parameter of this transition. At the tricritical point T one has to satisfy three equations $u_2 = u_4 = u_5 = 0$. However, since the coefficients u_i are functions of only two variables, x_1 and x_2, the three equations are not likely to be satisfied. In other words the codimension (Griffiths 1975) of the tricritical point T is 3, and therefore it is not expected to appear in a two-dimensional parameter space.

In order to substantiate the arguments presented above, we have performed numerical Monte-Carlo simulations of relatively small systems. In order to trace a trajectory in the x_1–x_2 plane, we choose a point a, b and define a temperature trajectory by

$$x_1 = a^{1/T}, \qquad x_2 = b^{1/T}. \tag{25}$$

First we divided the self-dual line between the Potts transition point x^* and the boundary $x_2 = 0$ into segments, bounded by the points

$$[a_i, b_i] = [x^* + \tfrac{1}{10}(i-1)x^*, x^* - \tfrac{1}{10}(i-1)x^*], \tag{26}$$

and performed temperature sweeps near each of these points. The specific heat per spin, obtained by calculating the average energy fluctuation, is plotted in figure 4. Since in the thermodynamic limit the five-state Potts model has a first-order transition, a δ-function singularity in the specific heat is approached as the size of the system increases. Comparison of the specific heat per spin measured on the self-dual line for

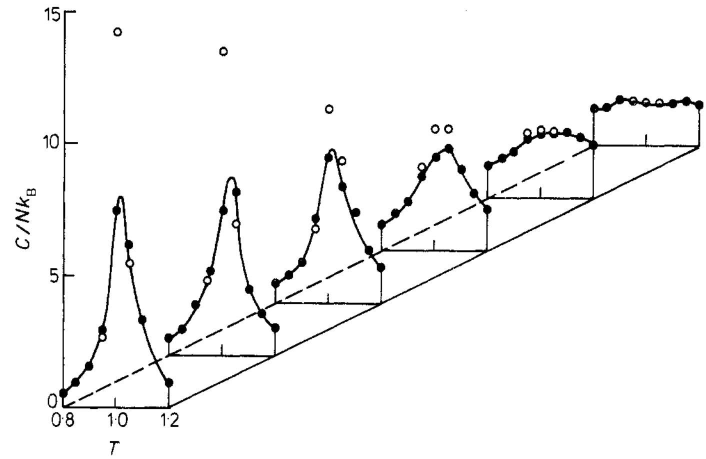

Figure 4. Specific heat per spin for temperature trajectories (equation (25)) across the self-dual line. The various curves correspond to the models defined by equations (25) and (26) for $i = 0, \ldots, 5$. The full curves correspond to a system of 10×10 spins, the open circles to 20×20.

systems of increasing size (up to 20×20) indicates that the magnitude does not saturate with size for the first three or four systems on figure 4. Thus we predict that the transition remains of first order along the segment of the self-dual line that extends from the Potts transition point to about $(x_1, x_2) \simeq (0{\cdot}4, 0{\cdot}2)$. Beyond this point, the specific heat saturates with size on the self-dual line, which means a non-divergent specific heat in the thermodynamic limit. In this regime the specific heat clearly exhibits two peaks at temperatures that correspond to points on the low/high-temperature side of the self-dual line. A temperature sweep that corresponds to the trajectory with

$$a = 0{\cdot}5335, \qquad b = 0{\cdot}0845 \tag{27}$$

is shown in figure 5. The point (27) is the self-dual point of the five-state discrete Villain model. The magnitude of these peaks is markedly smaller than those of the model near the Potts lines and a fast saturation with size is observed. The specific heat of the *XY* model was predicted to exhibit a finite rounded peak at some temperature T_p above the Kosterlitz–Thouless transition temperature. Numerical situations (Tobochnick and Chester 1979) indicate a sharp peak, about 15% above T_{KT}.

In order to verify that in the intermediate phase the correlation length is infinite, we calculated the susceptibility per spin, defined as

$$\chi = \frac{1}{N}\left(\left\langle\left(\sum_i \cos\theta_i\right)^2\right\rangle - \left\langle\sum_i \cos\theta_i\right\rangle^2\right); \tag{28}$$

χ is expected to diverge when ξ, the correlation length, diverges. Again, for finite systems this divergence is reflected in increasing values of χ as the size of the system increases. Indeed, we found that χ increases with size for a range of temperatures for various trajectories defined by equation (25). Since our susceptibility results were more stable (with smaller statistical error) on the high-temperature side, we used the lack of saturation of χ on the high-temperature side to estimate the appropriate boundary of

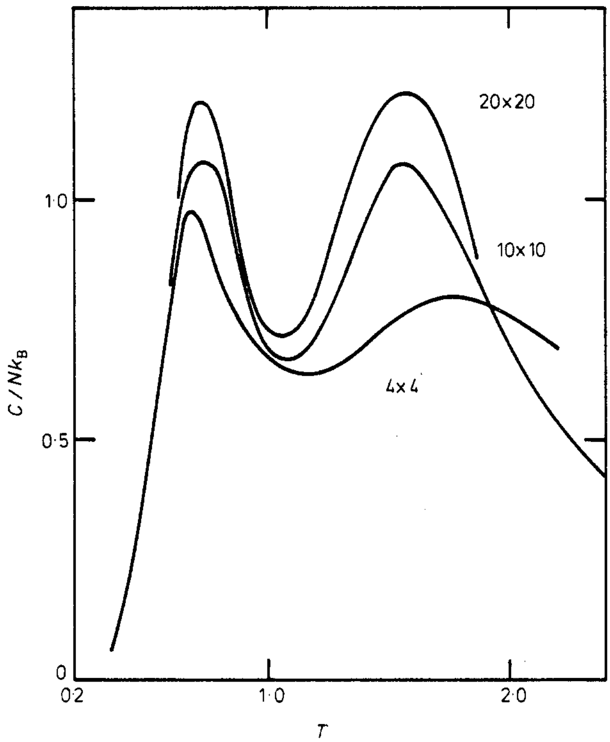

Figure 5. Specific heat per spin for a model defined by equations (25) and (27). The scale in this figure is different from that used in figure 4.

the intermediate Kosterlitz–Thouless phase, and determined the low-temperature boundary using duality (equation (9)).

The resulting phase diagram for the five-state model is shown in figure 3(*a*). We have also studied the size dependence of χ at some points inside the KT phase, and indeed found no indication of saturation with size, in accordance with the picture of algebraic decay of correlations in the entire intermediate phase.

In summary, we presented arguments concerning the nature of the phase diagram of a general planar five-state model. We argued that such a model will have either a single, first-order transition, or two transitions with an intermediate KT phase. Monte-Carlo simulation substantiated this picture, and yielded a qualitative estimate of the phase diagram. It is hoped that studies based on other methods, such as position-space renormalisation group (Mizrachi and Domany, unpublished) and series expansions, will further strengthen the qualitative aspects of the phase diagram, as well as sharpen the quantitative aspects of our numerical study.

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Note added. Recently, Cardy (1980) considered the phase diagram of discrete planar models in two dimensions. His phase diagram for $Z(S)$ is similar to the one presented in this Letter.

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