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LETTER TO THE EDITOR

Three-state square lattice Potts antiferromagnet

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Abstract. The three-state antiferromagnetic Potts model on a square lattice is investigated via phenomenological renormalisation group methods. In contrast to previous calculations, our results indicate that there exists neither an ordered phase nor a massless phase with algebraic decay of correlations. The sole critical point is at zero temperature, where an essential singularity is found.

The current interest in the antiferromagnetic q -state Potts model derives from the prediction of Berker and Kadanoff (1980) that for hypercubic systems with spatial dimensionality d exceeding a q -dependent critical value, a transition will take place into a low-temperature phase characterised by the algebraic decay of correlations (i.e. a massless phase). The most likely candidate for this behaviour in two dimensions is the three-state Potts model, to which we restrict ourselves henceforth. To be precise, we consider a square lattice with sites $r = (i, j)$. At each of these there is a spin $s_r = 0, 1, 2$. The reduced Hamiltonian (which includes a factor $-1/k_B T$) is given by

$$\mathcal{H} = \frac{J}{T} \sum_{(r,s)} \delta_{s_r s_s} + \frac{J'}{T} \sum_{(t,u)} \delta_{s_t s_u} \quad T \geq 0 \tag{1}$$

where (r, s) and (t, u) respectively run through the set of nearest- and next nearest-neighbour pairs of lattice sites. We consider the antiferromagnetic case $J < 0$ only. The next nearest-neighbour interaction J' , if non-zero, is taken positive. This ferromagnetic interaction reduces the infinite (log-extensive) ground-state degeneracy to a sixfold one: each of the two simple square sublattices may condense into one of three ferromagnetic $q = 3$ Potts ground states, the states of the sublattices being different. The ordered state is characterised by the two-component order parameter

$$M_1 + iM_2 = \left\langle \sum_{i,j} (-)^{i+j} \exp(2\pi i s_{i,j}/3) \right\rangle.$$

The symmetry of these six ground states determines the universality class of the model: the six-state clock model. In the latter, ferromagnetic, model a spin of unit length at each lattice site is given by an angle $n\pi/3$, $n = 0, 1, \dots, 5$. The symmetry transformations which leave the Hamiltonian invariant induce a group of transformations on the ground states. For the six-state clock model and the model defined by equation (1) the respective symmetry groups thus obtained are isomorphic.

First consider the case $J' = 0$. At zero temperature this $q = 3$ Potts model is equivalent to the 'square' ice model (Lieb and Wu 1972), which has a finite entropy

(Lieb 1967). The partition function of a generalisation of this model was calculated exactly by Baxter (1970). Denoting the number of sites in state i by n_i and associating an activity z_i with this state ($i = 0, 1, 2$), he calculated the partition function

$$Z = \sum g(n_0, n_1, n_2) z_0^{n_0} z_1^{n_1} z_2^{n_2}$$

where the summation is over all non-negative integers n_0, n_1 , and n_2 such that $n_0 + n_1 + n_2 = N$, the total number of lattice sites; $g(n_0, n_1, n_2)$ is the number of allowed configurations with given n_0, n_1 , and n_2 . Baxter found a continuous phase transition at $z_0 = z_1 = z_2 = 1$ with $\langle n_i \rangle = N/3$. For $z_0 > z_1 = z_2$ one expects a condensation into one of two states: $s_r = 0$ predominantly on either one of the two sublattices, which corresponds to $M_1 \neq 0, M_2 = 0$. For $z_0 < z_1 = z_2$, on the other hand, one expects $s_r = 1$ and $s_r = 2$ to condense on different sublattices, corresponding to $M_1 = 0, M_2 \neq 0$. Although the order parameters M_1 and M_2 are not known, the continuous transition at $z_0 = z_1 = z_2 = 1$ seems to imply that both vanish as $z_0 \rightarrow 1$, while the corresponding correlation functions decay algebraically as a function of distance. Thus, a massless phase, if present, would extend down to zero temperature.

A different phase diagram was suggested by Cardy (1981) and by Grest and Banavar (1981): an ordered low-temperature phase separated by a massless phase from a high-temperature disordered phase. However, there are serious problems with both of these calculations. First, Cardy's analysis applies to an xy model in the presence of an infinitesimal staggered field. It is only for the infinite field that the Potts model is recovered. Second, the interpretation of the Monte Carlo data of Grest and Banavar due to the zero-temperature critical point is ambiguous and those authors are unable to draw any definite conclusions.

In view of these difficulties we have performed a phenomenological renormalisation calculation (Nightingale 1976, 1978). This method has been successfully applied to a variety of systems, using either a two-dimensional classical or a one-dimensional quantum mechanical formulation. In particular, this method has proven to be sufficiently powerful to detect the presence of a massless phase (Roomany and Wyld 1980, Hamer and Barber 1981).

The phenomenological renormalisation procedure may be summarised as follows. Using a transfer matrix technique, one calculates the inverse correlation length $\kappa(T, n)$ of an infinite strip with periodic boundary conditions of width n at temperature T . Given κ as a function of both T and n , the renormalised temperature $T_b = T_b(T)$, associated with a rescaling using Kadanoff blocks of size e^b , is implicitly defined by

$$\kappa(T, n) = e^{-b} \kappa(T_b, e^{-b} n). \quad (2)$$

So as to be able to compare the functions T_b obtained from systems of increasing sizes, it is convenient to define $\beta \equiv dT/db$, the generator of the infinitesimal transformation $T_{\delta b} = \beta \delta b$. From equation (2) it follows that

$$\beta(T) = \frac{1 + \partial \ln \kappa / \partial \ln n}{\partial \ln \kappa / \partial T} \quad (3)$$

From data of strips of sizes n_1 and n_2 one obtains the approximation

$$\beta(T) \approx \frac{1 + \ln(\kappa_1/\kappa_2)/\ln(n_1/n_2)}{(\kappa_1^T \kappa_2^T / \kappa_1 \kappa_2)^{1/2}} \quad (4)$$

where $\kappa_i = \kappa(T, n_i)$ and $\kappa_i^T = \partial \kappa(T, n_i) / \partial T$.

In our analysis we shall employ the following result (Roomany and Wyld 1980). If for T close to some critical value T_c , β displays powerlaw behaviour with an exponent $\tilde{\nu} + 1$, i.e.

$$\frac{dT}{db} = \beta(T) \approx \frac{1}{\tilde{\nu}A} (T - T_c)^{\tilde{\nu}+1} \quad T \geq T_c \quad (5)$$

then κ has an essential singularity

$$\kappa \sim \exp[-A(T - T_c)^{-\tilde{\nu}}]$$

as one sees immediately by integrating equation (5) and substituting the result in the scaling relation (2).

Calculating β for the pure Potts antiferromagnet ($J' = 0$) as described above we conclude that there is neither a massless nor an ordered phase. The only critical point is the Baxter point located at $T = 0$. Our conclusion is based on the similarity of the results of this calculation to those obtained from a similar calculation on the isotropic Ising antiferromagnet on a triangular lattice. In that model, $T = 0$ being the only critical point is an exact result: $\tilde{\nu} = 1$ (Stephenson 1970). Figure 2 is again a log-log plot of β against T . We find $\tilde{\nu} = 0.75$. In the Potts case we obtain $\tilde{\nu} = 1.3$.

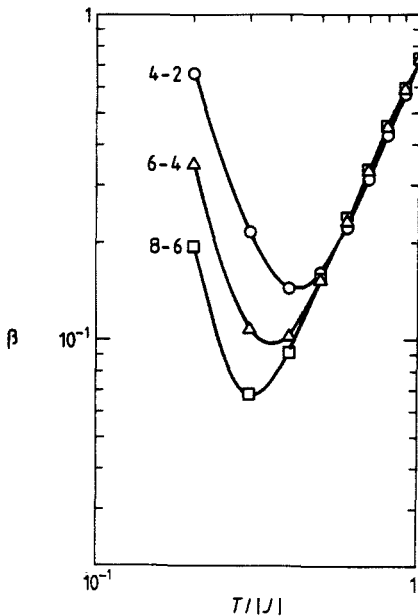


Figure 1. Log-log plot of the β function for the antiferromagnetic $q = 3$ Potts model, showing powerlaw behaviour as a function of T ; approximations are obtained from system sizes $n_1 = 4, 6, 8$ and $n_2 = 2, 4, 6$.

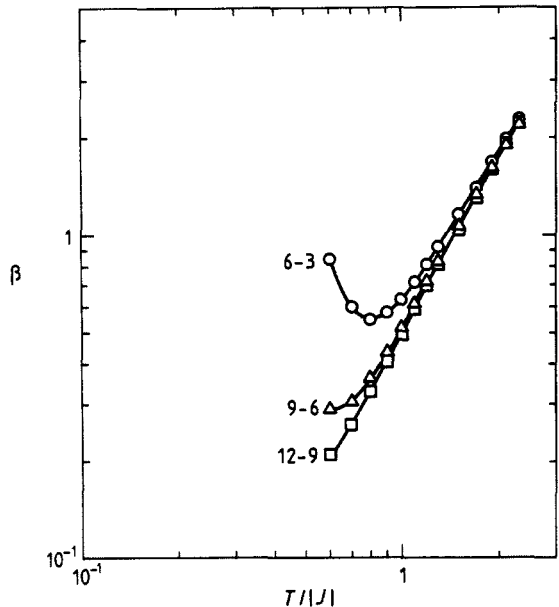


Figure 2. Plot qualitatively similar to figure 1 for the antiferromagnetic triangular Ising model obtained from system sizes $n_1 = 6, 9, 12$ and $n_2 = 3, 6, 9$.

The β function shown in figure 1 was calculated using a symmetric transfer matrix; the triangular lattice was obtained from a square one by adding next nearest-neighbour bonds along diagonals alternating from row to row in the infinite direction of the periodic strip.

We have also considered the effects of a next nearest-neighbour ferromagnetic interaction J' . Our results for $\beta(T)$ are shown in figure 3 for four values of $J'/|J|$. As β vanishes at $T = 0$, the temperature derivatives are negative there, which implies the existence of a phase with long-range order at low temperatures. The nature of the transition to this phase is unclear from the data. However, it is believed that the six-state clock model (which contains the $q = 6$ Potts model as a special case) orders either via a first-order transition or via a massless phase (Baxter 1973, Elitzur *et al* 1979). The signature of the former is a divergent slope at $T = T_c$ of $\beta(T)$ (Blöte *et al* 1981), which is inconsistent with our data. The signature of the latter is a finite region over which $\beta(T) = 0$, which is not inconsistent with it. Much more clearly indicated is the linear dependence of the transition region on J' , which reinforces our conclusion that the three-state Potts model with nearest-neighbour interactions has but one transition: at zero temperature.

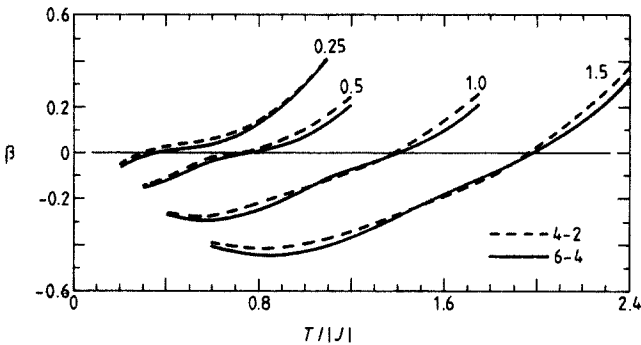


Figure 3. The β function for the antiferromagnetic $q = 3$ Potts model with ferromagnetic next nearest-neighbour couplings for $J'/|J| = 0.25, 0.5, 1.0, 1.5$. System sizes: $n_1 = 6, 4$ and $n_2 = 4, 2$.

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