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LETTER TO THE EDITOR

Phase transition in a two-dimensional three-state Potts model with the addition of an infinite-range coupling

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Abstract. We study the two-dimensional three-state Potts model with nearest-neighbour and infinite-range interaction at different values of the two coupling constants. We analyse the intermediate region between the pure infinite-range interaction and the nearest-neighbour one. We find a first-order phase transition for all values of the coupling constants on the coexistence curve except for the pure nearest-neighbour interaction where Baxter's result holds. A Monte Carlo simulation which supports our theoretical expectation is expounded.

The action of the q-state Potts model (Wu 1982) on a cubic lattice is

$$A = K \sum_{(i,j)} \delta_{\sigma_i \sigma_j} \tag{1}$$

where σ_i ($\sigma_i = 1, \ldots, q$) is the spin on the ith lattice site and the sum runs over nearest-neighbour pairs.

The nature of the phase transition in three-dimensional lattices for $q = 3$ is controversial. Some authors find a second-order phase transition (using renormalisation group methods (Zaprudskii 1977) or high-temperature expansions (Enting and Domb 1975)), while numerical results indicate a first-order phase transition partially superposed with a second-order phase transition (Blöte and Swendsen 1979) or a pure first-order one (Knak Jensen and Mouritsen 1979). In Fucito and Parisi (1981) and Fucito and Vulpiani (1982) it is shown by renormalisation group methods and Monte Carlo simulations that the three-dimensional three-state Potts model is very unstable to perturbation and this may explain the different conclusions given in the literature.

The situation is well known in two dimensions for $q = 3$: the model described by the action (1) has a second-order phase transition (Baxter's (1973) analytical result).

On the other hand the model with only infinite-range interaction exhibits a first-order phase transition (Wu 1982).

The two-dimensional $q = 3$ model with the addition of another interaction (antiferromagnetic, multi-site, non-nearest-neighbour) describes many interesting problems, most of which are not yet solved. Recently the two-dimensional $q = 3$ Potts model with three bodies on a triangular lattice has been studied (Saito 1982) and the phase transition changes from second to first order when coupling constants are changed.

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We study a two-dimensional $q=3$ Potts model on a quadratic lattice of N sites with nearest-neighbour and infinite-range interaction described by the action

$$A[K,\lambda,N,\{\sigma\}]=K\sum_{(i,j)}\delta_{\sigma_i\sigma_j}+\frac{\lambda}{N}\sum_{i,j=1}^{N}\delta_{\sigma_i\sigma_j} \tag{2}$$

where the notations are the same as in (1).

This model in two dimensions and $q=2$ (i.e. a modified 2-Ising model) has been recently studied in Livi *et al* (1982); the authors claim that there is a critical line in the λ, K plane and the system exhibits only a second-order phase transition.

In two dimensions for $q=3$ there is a first-order phase transition at the point $\lambda=\lambda_c$, $K=0$ while $\lambda=0$, $K=K_c$ is a critical point. Our aim is to investigate the behaviour of the phase separation line between these two points.

Our result is that the transition is always first order at non-vanishing λ. Let us formulate an argument to justify this idea.

The infinite-range part in (2) may be transformed ($\delta_{\sigma_i\sigma_j}=\sum_{r=1}^{q}\delta_{\sigma_i r}\delta_{r\sigma_j}$) into

$$\frac{\lambda}{N}\sum_{i,j=1}^{N}\delta_{\sigma_i\sigma_j}=\frac{\lambda}{N}\sum_{r=1}^{q}\left(\sum_{i=1}^{N}\delta_{\sigma_i r}\right)^2 \tag{3}$$

and using the gaussian transformation

$$\exp A=\int\prod_{r=1}^{q}\mathrm{d}H_r\exp\left[K\sum_{(i,j)}\delta_{\sigma_i\sigma_j}+\sum_{r=1}^{q}\left(H_r\sum_{i=1}^{N}\delta_{\sigma_i r}\right)-\frac{N}{4\lambda}\sum_{r=1}^{q}H_r^2\right]. \tag{4}$$

We can identify the partition function from (4) as

$$\begin{aligned}Z[K,\lambda,N]&=\sum_{\{\sigma\}}\exp A[K,\lambda,N,\{\sigma\}]\\&=\int\prod_{r=1}^{q}\mathrm{d}H_r\exp\left[-NH^2/4\lambda+NF(K,\boldsymbol{H}/K)\right]\end{aligned} \tag{5}$$

where $F(K,\boldsymbol{H})$ is the free energy per site of the Potts model (1) with a magnetic field $\boldsymbol{H}=(H_1,\ldots,H_q)$ and $H^2=\sum_{r=1}^{q}H_r^2$. In the limit $N\to\infty$ we can perform a saddle point approximation which leads to

$$f(K,\lambda)=\min_{\boldsymbol{H}}\left[F(K,\boldsymbol{H}/K)-H^2/4\lambda\right]. \tag{6}$$

f is the free energy per site of the model (2). We can now expand $F(K,\boldsymbol{H})$ for small $\boldsymbol{H}$:

$$\begin{aligned}F(K,\boldsymbol{H})=&\sum_{n,m=1}^{q}a_{nm}(K)H_nH_m+\sum_{n,m,l=1}^{q}b_{nml}(K)H_nH_mH_l\\&+\sum_{n,m,l,p=1}^{q}c_{nmlp}(K)H_nH_mH_lH_p+O(H^5).\end{aligned} \tag{7}$$

As the $b_{n,m,l}(K)$ are not vanishing at $q=3$, $F(K,\boldsymbol{H})$ has two minima with respect to $\boldsymbol{H}$ for $\boldsymbol{H}=\boldsymbol{H}^{(1)}$ and $\boldsymbol{H}=\boldsymbol{H}^{(2)}$ with $F(K,\boldsymbol{H}^{(1)})\gtrless F(K,\boldsymbol{H}^{(2)})$ for $K\gtrless K_c$. These two minima assume the same value only for $K=K_c$. For the sake of clearness figure 1 shows F against H where $H_r=H\alpha_r$ with α_r fixed. Therefore figure 2 gives the expected behaviour of the two minima of F as well as of $F(K,\boldsymbol{H}/K)-H^2/4\lambda$ with respect to K.

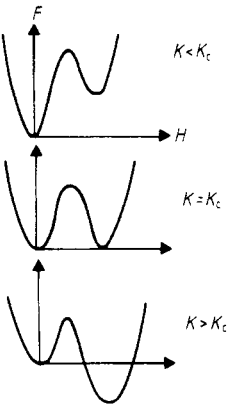

Figure 1. Free energy F against magnetic field H for model (1).

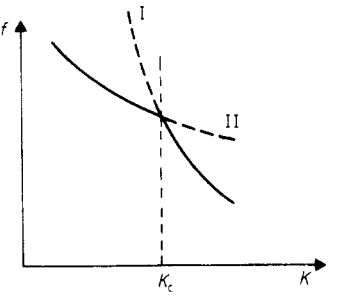

Figure 2. Free energy f against K for model (2). The curves I and II are drawn for the two different minima of $F(K, H/K) - H^2/4\lambda$ as a function of H.

We can infer from (6) that df/dK has a discontinuity at K_c. Only for a particular choice of the coefficients a, b, c, in (7) will the two curves f in figure 2 join smoothly to each other, yielding a continuous df/dK.

Then there is an indication of a first-order, discontinuous, transition. Since the coefficients in (7) are not exactly known, we have no rigorous proof for our conclusion but just a heuristic argument. We have therefore performed a Monte Carlo (MC) computation to check our idea. The most direct way to determine the order of the transition consists in numerically computing the internal energy $E(K)$. In this manner one can see if an energy gap does exist around K_c as well as if there is a hysteresis curve (1st-order transition). Such an approach is problematic since hysteresis effects are present up to 10^4 MC steps because of critical slowing down (e.g. see Binder 1981 and Saito 1982).

Nevertheless this method is useful to determine the K_c roughly, but it needs a very long computation time to check the order of the phase transition. We have therefore determined first the transition coupling $K = K_c$ for every λ performing our simulation on a 60×60 square lattice with periodic boundary condition.

We have gathered results for $\lambda = 0.1$, 0.2, 0.4, 0.8, 1.6. The coexistence line ending at the Baxter critical point is shown in figure 3.

We have then used the 'mixed phase' techniques as developed in Bhanot and Creutz (1980) and Fucito and Vulpiani (1982) with 2500 MC steps, to check the kind of transition. We prepared a system by adding a high-temperature configuration ($K < K_c$) and a low-temperature one ($K > K_c$).

Then we get MC computation on such a system at a fixed K near K_c and we plot the 'instantaneous' internal energy E against MC steps. Figure 4 shows the result for $\lambda = 0.2$ at four different values of K.

There is clear evidence for a gap of the internal energy at the transition. Similar results are obtained for the other values of λ. We conclude that there is good evidence for the transition to be first order up to $\lambda = 0$ (Baxter's point) according to our theoretical argument. Our result is in agreement with the result of Saito (1982) for the two-dimensional $q = 3$ Potts model on a triangular lattice, which seems to indicate that the three-state Potts model is unstable to perturbations.

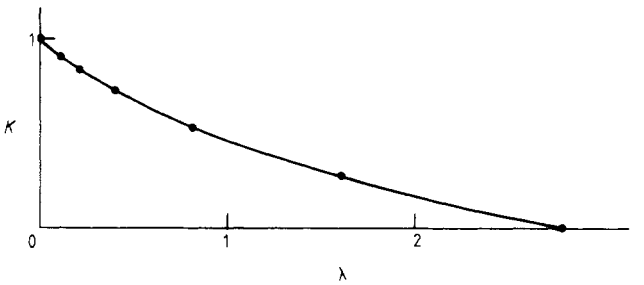

Figure 3. Coexistence line of the phase diagram in the plane λ, K.

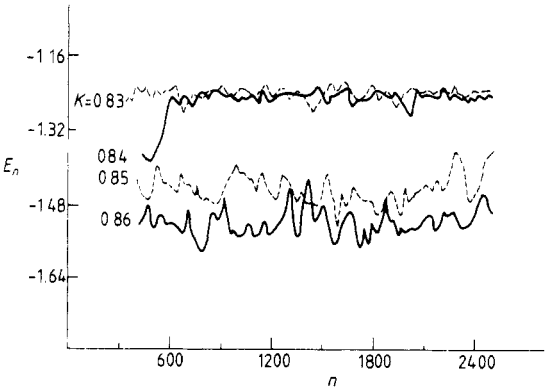

Figure 4. Mixed phase runs for $\lambda = 0.2$. Internal energy (units of K) against Monte Carlo steps at different K around K_c.

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