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First- and second-order phase transitions in the Potts model

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Abstract. The nature of the phase transition in the Potts model is studied when second neighbours or infinite range couplings are added. A new criterion, recently proposed, is applied.

Recently much attention has been devoted to the problem of recognising the order of phase transitions for lattice spin models (see for example Enting and Wu 1982, Fucito and Parisi 1981) as well as for lattice gauge theories. From the theoretical point of view, if the phase transition is second order, one expects to be able to describe the critical behaviour with field theoretical methods (Wilson and Kogut 1974).

A classical example is the q-state Potts model on a hypercubic d-dimensional lattice whose reduced Hamiltonian is

$$\mathcal{H} = \frac{K}{2} \sum_{\substack{i,j \\ |i-j|=1}} \delta_{\sigma_i,\sigma_j} \tag{1}$$

where the sum is over nearest-neighbour sites and the statistical variables $\sigma = 0, 1, \ldots, q-1$. It is well known that a 'critical' value of q exists, $q_c(d)$, depending on the space dimension d, where the phase transition changes order, becoming a first-order one. Exact results (Baxter 1973) give $q_c(2) = 4$ while $q_c(3) < 3$ has been obtained by Monte Carlo simulations (Blöte and Swendsen 1979) as well as approximate methods (Kogut and Sinclair 1981, Livi *et al* 1983). However, it is not understood very well what happens to the order of the phase transition if one adds other couplings to the Hamiltonian (1), for example

$$L \sum_{\substack{i,j \\ |i-j|=\sqrt{2}}} \delta_{\sigma_i,\sigma_j}, \tag{2}$$

$$\frac{\lambda}{N} \sum_{i,j} \delta_{\sigma_i,\sigma_j}, \tag{3}$$

where N is the number of sites of the lattice.

The coupling (2) is the simplest one, in addition to the coupling (1) which can appear if one starts to perform real space renormalisation group calculations on the Potts model. In this respect it would seem that the renormalisation group framework is suitable for discussing also the order of a phase transition when competing interactions are present. However, from the technical point of view it is already difficult to discuss the order of the transition for the model (1) in low dimension (Nienhuis *et al* 1979). It is well known that the mean field approximation to the model (1) always predicts a first-order phase transition when $q > 2$, i.e. $q_c = 2$. Thus it is impossible, in such an approximation, to understand how the order of the phase transition changes when couplings of the type (2) or (3) are considered. However, it is possible to take into account corrections to the mean field using Onsager's reaction field (Dekeyser *et al* 1983). With such an approximation one improves the value of $q_c(d)$ and obtains that q_c can depend on the other couplings. Monte Carlo simulations seem to be in agreement with this behaviour (Saito 1982, Fucito and Vulpiani 1982). This paper has a twofold purpose. The first one is to study the three-dimensional and three-state Potts model (1) when the coupling (2) is added; we discuss also the two-dimensional and three-state model (1) when the infinite range potential (3) is added. The second purpose is to extend the application of a new criterion for distinguishing between first- and second-order phase transitions (Livi *et al* 1983).

Let us start by recalling what is the criterion we want to apply for distinguishing the order of the phase transition in a spin model. Let us look at the free energy density in the mean field approximation for the model (1) (Mittag and Stephen 1974) as a function of the 'magnetisation', $m \equiv \langle (q\delta_{\sigma,0} - 1)/(q-1) \rangle$:

$$\Gamma(K, m) = \frac{1+(q-1)m}{q} \ln[1+(q-1)m] + \frac{q-1}{q}(1-m)\ln(1-m) - dK\frac{1+(q-1)m^2}{q}. \quad (4)$$

The spontaneous magnetisation of the system, in such an approximation, is given by the value of m for which (4) has a minimum. This gives the well known equation of state (we have chosen to break the symmetry along the 'axis' $\sigma = 0$)

$$m = \frac{\mathrm{Tr}_\sigma \exp(2dKm\delta_{\sigma,0})(q\delta_{\sigma,0}-1)}{(q-1)\,\mathrm{Tr}_\sigma \exp(2dKm\delta_{\sigma,0})} = \frac{e^{2dKm}-1}{e^{2dK}+q-1} \quad (5)$$

which can be obtained also by considering a single spin immersed in an effective 'magnetic field' $h = 2dKm$. All this can be generalised to include a class of approximations which will be called mean-field-like approximations. Let us consider a cluster $\mathscr{C}$ of spins inside which we treat exactly the interactions of the model (1) (or some modification of it); we call the Hamiltonian for such a cluster $H_{\mathscr{C}}(\sigma)$, while the interactions between internal spins and external ones are modified in the following way:

$$\delta_{\sigma_i,\sigma_j} \to b\delta_{\sigma_i,0}, \qquad i \in \mathscr{C}, j \notin \mathscr{C}, \quad (6)$$

where b is a sort of magnetisation. The Hamiltonian for this interaction will be called $b\tilde{H}_{\mathscr{C}}(\sigma)$.

In this way the equation of state in an external field h is

$$m_{\mathscr{C}}(K, h, b) = (1/N_{\mathscr{C}}) \ln Z_{\mathscr{C}}(K, h, b), \quad (7a)$$

$$Z_{\mathscr{C}}(K, h, b) = \mathrm{Tr}_\sigma \exp\Big(H_{\mathscr{C}}(\sigma) + b\tilde{H}_{\mathscr{C}}(\sigma) + h \sum_{i \in \mathscr{C}} (q\delta_{\sigma_i,0} - 1)/(q-1) \Big), \quad (7b)$$

where $N_{\mathscr{C}}$ is the number of sites of the cluster $\mathscr{C}$.

For a cluster of a single point, $H_{\mathscr{C}} = 0$ and $\tilde{H}_{\mathscr{C}} = 2dK\delta_{\sigma,0}$, while for a cluster of a couple of nearest-neighbour sites, $H_{\mathscr{C}} = K\sigma_{\sigma,\sigma'}$ and $\tilde{H}_{\mathscr{C}} = (2d-1)K(\delta_{\sigma,0}+\delta_{\sigma',0})$. The generalisation to the model (1) including terms of the type (2) or (3) is obvious. The mean field approximation consists in setting $b = m$ in equations (7). However, this does not give a rapid improvement in the estimate of the transition temperatures. It is well known that it is possible to obtain very good estimates of the transition temperatures using consistency equations à la Bethe (Domb 1960). The generalised Bethe approximation is obtained by considering two different clusters $\mathscr{C}$ and $\mathscr{C}'$ and requiring that the b field in (7a) is given by imposing that the magnetisation does not depend on the cluster we used, i.e.

$$m = m_{\mathscr{C}}(K, h, b) = m_{\mathscr{C}'}(K, h, b). \tag{8}$$

(In general K will represent a set of couplings.) The m-dependent free energy density can be obtained from (8) as follows: eliminating b as a function of K, h and m, one gets an equation for h

$$h = f(K, m) \equiv (\partial/\partial m)\Gamma(K, m) \tag{9}$$

where $\Gamma(K, m)$ is the Legendre transform with respect to h of the free energy density $F(K, h)$,

$$\Gamma(K, m) = F(K, h) + hm. \tag{10}$$

Thus the integration of (9) with respect to m gives us Γ apart from a constant. These observations allow the use of (9) for $h = 0$ to determine the transition temperature, in this approximation. The value of K, K_{II}, at which the linear term in m vanishes, determines the inverse temperature at which a second-order phase transition occurs. If we are dealing with a first-order phase transition we can appeal to the Maxwell construction to evaluate the inverse temperature K_I.

Figure 1 shows the typical behaviour of the free energy density as a function of m, $\Gamma(K, m)$, for the model (1) with $q > 2$ (if more than one coupling is present, only

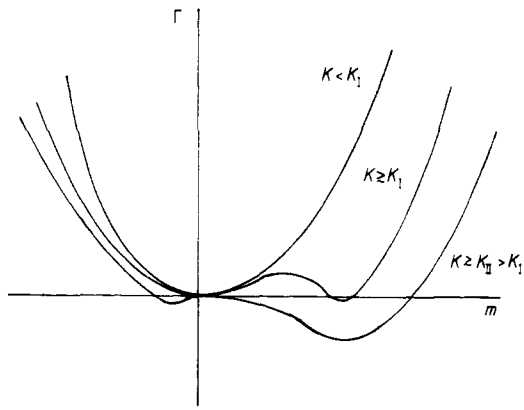

Figure 1. Qualitative shape of the free energy Γ against the magnetisation m for a mean-field-like approximation for the Potts model for $q > 2$.

one of them is allowed to change). For $K < K_I$ the absolute minimum in the interval $(-(q-1)^{-1}, 1)$ is at $m = 0$. For $K_I < K < K_{II}$, $m = 0$ is a relative minimum while the absolute minimum is at $m \neq 0$. At $K = K_{II} > K_I$ the relative minimum at the origin moves continuously into the $m < 0$ region, the origin becomes a maximum. However, this second-order phase transition is present in an 'unstable' way. Indeed, from the point of view of the stability of the free energy, the true transition would be of first order. Furthermore, if one tries to improve the mean field approximation by considering greater and greater clusters of sites, one realises that the behaviour that we have just described is still present. Thus, if we do trust the principle of minimisation of mean-field-like free energies, then we must give up describing first- and second-order phase transitions in the mean field framework: this is true, at least, for Potts model and lattice gauge theories. We are instead going to consider both first- and second-order phase transitions, which are present in every mean-field-like approximation, on the same footing. The way of distinguishing the true nature of the phase transition is the content of the conjecture we propose.

Now we come to the reasons which will justify our conjecture. It is known (Brydges *et al* 1982, Sokal 1982) that for a certain class of spin models the mean field critical coupling K_c^{MF} is a rigorous lower bound to the true critical coupling K_c. What we can observe is that this holds for all the mean-field-like approximations for the two-dimensional q-state Potts model in a square, honeycomb and triangular lattice for which the exact solutions are known and $q_c = 4$ (Baxter *et al* 1978). That is to say, for all the mean-field-like estimates of K_I and K_{II}

$$q < q_c \qquad \text{implies} \qquad K_I < K_{II} < K_c. \tag{11}$$

This cannot be a surprise, but what is a surprise is that at a certain value of $q = \bar{q} > q_c$, depending on the mean field approximation used, K_{II} is an overestimate of the exact value of K_{trans} at which the transition takes place, while K_I still remains below K_{trans} and approaches it from below better and better as the approximation improves. Thus we are led to the following conjecture for lattice spin models:

(a) if there exists *at least* a mean-field-like approximation (see below) for which it happens that $K_{II} > K_{trans}$, then the true transition is first order;

(b) if this does not happen, i.e. $K_{II} < K_{trans}$ for every mean-field-like approximation, then the true transition is second order.

In the case of the Potts model, Livi *et al* (1983) obtain the exact q_c's for the above-mentioned two-dimensional lattices and an estimate of $q_c(d)$ for all d.

The following remarks regard the way in which one proceeds in practice: (i) if one has at disposal exact results for K_{trans} (as for example for the two-dimensional Potts model or four-dimensional $\mathbb{Z}_2$ gauge theory using duality arguments) or very good estimates for K_{trans}, coming from Monte Carlo experiments or series expansion methods, then one uses a few mean-field-like approximations together with the conjecture. It is obvious that, having at disposal only a finite number of approximations, we can surely say if the transition is first order, applying conjecture (a). Notwithstanding the conjecture (b) does not seem efficient, from the practical point of view, it allows one to get good results even if one has at disposal a few approximate values of K_{II}. (ii) When we have not at disposal the results mentioned in (i) we take as a good estimate of K_{trans} the value of a good mean-field-like approximation and we compare it with a K_{II} coming from a worse mean field approximation (Livi *et al* 1983).

Now we come to the applications. The first model, which is important from the physical point of view, is described by the reduced Hamiltonian

$$\mathcal{H} = \frac{K}{2} \sum_{\substack{i,j \\ |i-j|=1}} \delta_{\sigma_i,\sigma_j} + \frac{L}{2} \sum_{\substack{i,j \\ |i-j|=\sqrt{2}}} \delta_{\sigma_i,\sigma_j}. \tag{12}$$

We consider the three-dimensional, three-states case. If $L = 0$ the transition is a very weak first-order phase transition (Blöte and Swendsen 1979, Swendsen *et al* 1982). What do we expect when $L \neq 0$? Intuitively if $L > 0$ we expect that the transition would remain of the first order because the number of neighbouring spins is increasing, which would be equivalent to an effective nearest-neighbour Potts model in a higher dimensionality. Conversely, if $L < 0$ the same argument tells us that the transition could become of second order. Monte Carlo simulations (Fucito and Vulpiani 1982) seem to confirm this behaviour.

Now we want to obtain the same quantitative estimate of the value of L at which the phase transition becomes of the second order, using our conjecture. We considered the clusters with one site ($\mathscr{C}_1$), two nearest-neighbour sites ($\mathscr{C}_2$) and a cubic cluster ($\mathscr{C}_3$). In table 1 we report some values of the transition couplings at different values of L. $K_{II}^{(12)}$, $K_{II}^{(13)}$ and $K_{I}^{(13)}$ are the values of the transition couplings obtained using (8) with the clusters $\mathscr{C}_1$, $\mathscr{C}_2$ and $\mathscr{C}_1$, $\mathscr{C}_3$ respectively ($K_{II}^{(23)}$ is practically the same as $K_{II}^{(12)}$). The intersection of the transition lines $K_{II}^{(12)}(L)$ and $K_{I}^{(13)}(L)$ occurs at $L = -0.16$, $K = 0.94$ and according to our conjecture it is an estimate of the value of L at which the transition changes order: second order for $L < -0.16$, otherwise it is first order. This result is in agreement with Monte Carlo simulations (Fucito and Vulpiani 1982) which predict a change of order in the phase transition in the region $-0.2366 < L < 0$. Monte Carlo data suggest that the curve $K_{\text{trans}}(L)$ is well approximated by a straight line whose intersections with $K_{II}^{(12)}(L)$ and $K_{II}^{(13)}(L)$ are ($L = -0.027, K = 0.62$) and ($L = -0.055, K = 0.70$) respectively. However, these two last estimates are not very accurate due to the lack of numerical results, even if they are qualitatively in agreement with the previous result. It is worthwhile to remark that in this framework, using a simple technique, one is able to distinguish the order of the phase transition when standard techniques are very difficult to apply. Now let us consider the model (1) when the perturbation (3) is added. The interest for such a model is only for testing if our technique works properly and, due to the peculiarity of the perturbation (3), it is also less physical than the model we investigated above. Furthermore, it is known (Capel *et al* 1979) from general arguments that an infinite range perturbation of the type (3) makes unstable the character of the phase transition at $\lambda = 0$. In the case we are considering, i.e. $d = 2$ and $q = 3$, for $\lambda = 0$ the phase

Table 1. Some values of the transition lines obtained in the mean-field-like approximations for the Potts model: K is the NN coupling, L is the NNN coupling. Monte Carlo results are reported in brackets.

L	K_{12}^{II}	K_{13}^{I}	K_{13}^{II}	
0	0.560	0.534	0.564	(0.550)
−0.100	0.792	0.781	0.806	
−0.180	0.981	0.984	1.00	
−0.237	1.117	1.128	1.145	(1.183)

transition is of second order and it is of first order as soon as $\lambda > 0$. More details and a more general discussion can be found in Capel *et al* (1979). Now let us apply our conjecture to this model. In this case we have at our disposal MC results (Fucito *et al* 1983) which predict that the transition line $K_{\text{trans}}(\lambda)$ starts at $\lambda = 0$, $K = \ln(1+3) = 1.005$ with a slope -0.95 ± 0.2 (we shall see that these data are sufficient). We used the cluster $\mathscr{C}_1$ of a single site, $\mathscr{C}_2$ of two nearest-neighbour sites and $\mathscr{C}_3$ of four sites around an elementary plaquette. For $\lambda \sim 0$ we easily obtain $K_{\text{II}}^{(12)}(\lambda) = 0.916 - 0.327 + O(\lambda^2)$ and $K_{\text{II}}^{(13)} = 0.932 - 0.354 + O(\lambda^2)$. Then, while the estimates of K_{trans} $(\lambda = 0)$ are rather good $(\sim 8\%)$, the slopes of the lines K_{II} near $\lambda = 0$ are well below the value of the slope given by MC simulation. If the trend of the K_{II} lines remains the same as we improve the approximation so that K_{II} $(\lambda = 0)$ goes toward the exact result, we obtain that the intersection of these lines with the exact one occurs exactly at $\lambda = 0$. It is obvious that if $K_{\text{II}}(\lambda = 0) \leqslant K_{\text{trans}}$ $(\lambda = 0)$ for any mean-field-like approximation, due to the fact that for $\lambda = 0$ the transition is of second order, we shall always obtain an intersection between $K_{\text{trans}}(\lambda)$ and $K_{\text{II}}(\lambda)$ at a certain $\bar{\lambda}$. We chose this model to test our conjecture just because we wanted to see if the convergence, $\bar{\lambda} \to 0$, is sufficiently rapid as the approximation improves.

Using the clusters $\mathscr{C}_1$, $\mathscr{C}_2$ and $\mathscr{C}_1$, $\mathscr{C}_3$ we get $\bar{\lambda} = 0.17$ and $\bar{\lambda} = 0.14$ respectively, which are indeed rather small. To test the above argument, which suggests that $\bar{\lambda} \to 0$ as the approximation improves, we have combined the three clusters to obtain a further generalisation of the mean-field-like approximation (Domb 1960). The result is $K_{\text{II}}^{(123)}(\lambda) = 0.974 - 0.414\lambda$ which intersects the $K_{\text{trans}}(\lambda)$ at $\lambda = 0.058$ and is quite a good value, suggesting that effectively $\bar{\lambda} \to 0$ as the approximation improves. By the way, we notice the rather good estimates of K_{trans} $(\lambda = 0)$. Furthermore, we have verified that the $K_{\text{II}}(\lambda)$ lines always remain above $K_{\text{trans}}(\lambda)$ after having intersected it.

In conclusion, we have considered some applications of a criterion for distinguishing between continuous and discontinuous transitions in spin models. First, we analysed the order of the phase transition in the three-dimensional and three-state Potts model when a second-neighbour interaction is added. The results have shown clearly that the new coupling can change the order of the phase transition.

The other model we considered, which is less interesting from the physical point of view, was the two-dimensional and three-state Potts model where, now, the new coupling is an infinitely long range and infinitely weak potential. The results were in good agreement with the analysis by Capel *et al* (1979).

These applications confirm that the proposed conjecture is a powerful tool for predicting the order of a phase transition in a given spin model.

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