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LETTER TO THE EDITOR

q-state Potts models in d dimensions: Migdal–Kadanoff approximation

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Abstract. The first- and second-order phase transitions of the q-state Potts models are obtained in arbitrary dimension d. Critical and tricritical behaviours merge and annihilate at $q_c(d)$, clearing the way to first-order transitions at $q > q_c(d)$ by the condensation of effective vacancies. The value of $q_c(d)$ decreases with increasing d, from diverging as $\exp[2/(d-1)]$ at $d \to 1^+$, to $q_c(2) = 3.81$ (cf exact value of 4), to lower values at $d > 2$. For given d, a changeover in critical behaviour occurs at $q_1(d)$, as the critical fixed points merge from the Potts-lattice-gas region to the undiluted Potts limit. It is suggested that the power law singularities of the percolation problem ($q \to 1^+$) have logarithmic corrections.

Potts (1952) models are composed of an array of local degrees of freedom, each of which can be in one of q states. The energy is determined only by whether neighbouring degrees of freedom are in the same state or not. As such, the q-state Potts models are a generalisation of the Ising model ($q = 2$). These models achieved recognition because several pieces of exact information were derived for their non-trivial phase transition in two dimensions. Baxter (1973) showed that the transition is second order for $q \leq q_c = 4$, and first order for $q > q_c$. The discovery of experimental realisations increased the interest in $q > 2$ Potts models. Examples are adsorbed systems in two dimensions (Alexander 1975, Domany *et al* 1977), and materials undergoing displacive transitions (Aharony *et al* 1977), cubic magnets (Barbara *et al* 1978), multi-component fluid mixtures (Das and Griffiths 1979), and intercalated materials (Bak and Domany 1979) in three dimensions. Further, in any dimension, formal extension to $q = 1$ yields the percolation problem (Fortuin and Kasteleyn 1969).

In two dimensions, calculations using the position-space renormalisation-group method linked experimental phase diagrams and microscopic descriptions of overlayers (Schick *et al* 1977, Berker *et al* 1978, Ostlund and Berker 1979). Even for given $q \leq q_c$, the second-order phase transition can be turned into first-order beyond a tricritical point, by the introduction of annealed vacancies into the system, which, when present in sufficient numbers, undergo a condensation (Berker *et al* 1978). This situation is actually realised in unsaturated overlayers. The renormalisation-group study of the changeover at $q_c = 4$ from second-order to first-order transitions revealed an analogous mechanism (Nienhuis *et al* 1979). The $q > q_c$ Potts models, with no actual vacancies, have local regions of complete disorder which are entropically favoured, their large multiplicity being due to the large q value. Such regions act as effective vacancies, and their condensation causes the first-order transition. Further, by the unified study of both effective and actual vacancies, a previous conjecture (den Nijs 1979) for the exact

values of the thermal exponents at the $q \leq q_c$ critical points was extended to the tricritical points (Nienhuis *et al* 1979). New conjectures followed, for the magnetic exponents (Nienhuis *et al* 1980b, Pearson 1980) and the equation of state (Nauenberg and Scalapino 1980, Cardy *et al* 1980).

The previous position-space renormalisation-group calculations in dimension $d = 2$ used, initially, the cell-cluster approximation (Nienhuis *et al* 1979) and, more quantitatively, the variational approximation (Nienhuis *et al* 1980a, Burkhardt 1980). We develop here a particular form of the Migdal–Kadanoff (Migdal 1975, Kadanoff 1976) approximation which is less sophisticated, but more flexible. Independently, Nauenberg and Scalapino (1980) mention that they have carried out a similar renormalisation transformation. (The present calculation can alternatively be viewed as the exact solution of a family of hierarchical Potts models (Berker and Ostlund 1979).) This reveals that the picture of critical, tricritical and first-order transitions in Potts models is qualitatively applicable to arbitrary $d \neq 2$ as well. This is not surprising, in view of the physical generality of the vacancy condensation mechanism. The changeover value q_c decreases with increasing d, in agreement with other recent renormalisation-group calculations, namely ε-expansion at $d = 4$ (Aharony and Pytte 1980) and variational at discrete values of d close to 2 (Nienhuis *et al* 1980c, Riedel 1980). The Migdal–Kadanoff transformation should be quantitatively most reliable in the limit $d \to 1^+$. Most notably, it is found that q_c increases as $\exp[2/(d-1)]$ as d approaches one (Berker *et al* 1980). We have discussed results in this limit separately. On the other hand, $d = 2$ results are surprisingly quantitative (figure 1*a*). Furthermore, the treatment raises and addresses qualitatively new phenomena in arbitrary d (figure 2).

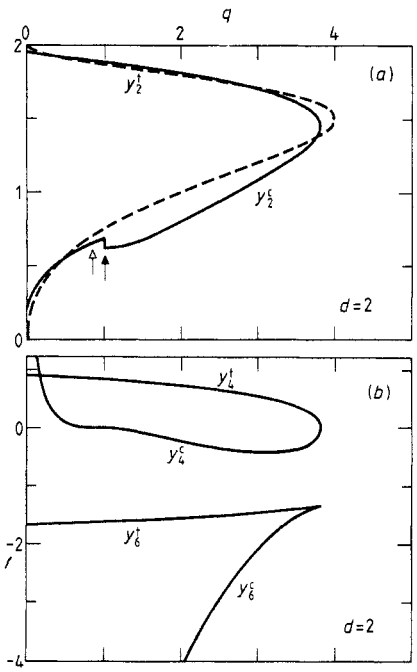

Figure 1. The critical (c) and tricritical (t) thermal eigenvalues of the $d = 2$ Potts models, as obtained with the Migdal–Kadanoff approximation. The special points q_0 and q_1 are indicated by the open and filled arrows. In broken curves, the conjectured exact values (den Nijs 1979, Nienhuis *et al* 1979) for y_2 are shown. The scaling field of $y_4^c (q < q_1)$ is e^{-G}.

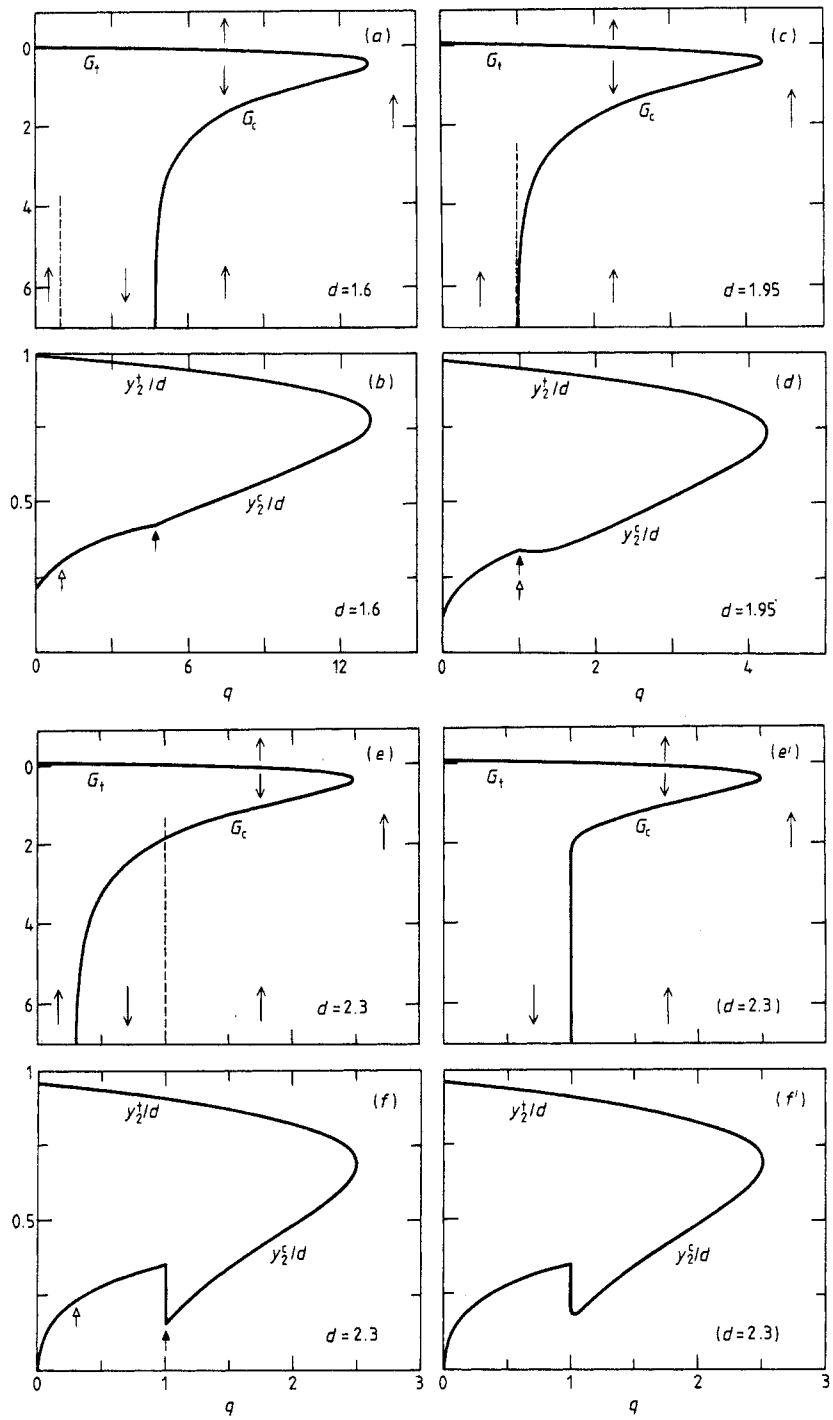

Figure 2. (a, c, e): Fixed-point locations G^* of the critical (c) and tricritical (t) branches. The projections of the $q = 1$ fixed lines are shown with broken lines. Arrows indicate the renormalisation-group flows. (b, d, f): The corresponding leading thermal eigenvalues. The special points q_0 and q_1 are indicated by the open and filled arrows. (e', f'): Our hypothesis for the true $d > d_0$ behaviour, based on the modification of (e, f).

The renormalisation-group mechanism for the changeover at q_c is based on the fact that the pure Potts model, which does not manifestly contain vacancies, is not retained under rescaling (Nienhuis *et al* 1979). A single rescaling yields a renormalised system with manifest vacancies. Accordingly, the renormalisation-group study is within the context of the Potts-lattice-gas model†,

$$-\mathcal{H}/k_B T = J \sum_{\langle ij \rangle} t_i t_j (\delta_{s_i s_j} - 1) - \frac{F}{2} \sum_{\langle ij \rangle} (t_i - t_j)^2 + G \sum_i t_i, \tag{1}$$

which was originally introduced to study ordering in the presence of actual vacancies (Berker *et al* 1978), in adsorbed submonolayers. At each site i of a hypercubic lattice, the Potts variable $s_i = a, b, c, \ldots$ can take one of q values, and $\delta_{s_i s_j} = 1$ (0) for $s_i = s_j$ ($s_i \neq s_j$). The lattice-gas variable $t_i = 0$ (1) means that site i is vacant (occupied). The sums $\langle ij \rangle$ are over all pairs of nearest-neighbour sites. The limit $G \to \infty$ removes all vacancies from the system.

The Migdal–Kadanoff renormalisation is effected here by choosing a superlattice composed of hypercubes of side twice the original lattice constant. All couplings not along hypercube edges are deleted and those along the edges are strengthened. The latter step is the "bond-moving" approximation. The transformation is completed by summing over all degrees of freedom not at hypercube corners. The first two terms in the Hamiltonian (1) are the couplings subjected to bond-moving. This separation of the Hamiltonian ensures that the effect of the bond-moving approximation vanishes in both the weak- and strong-coupling limits (Emery and Swendsen 1977). We found this scheme to be crucial for obtaining the changeover phenomenon of Potts models. (This type of separation also showed (Berker and Nelson 1979) that the Villain model becomes unstable to vacancies exactly at the XY separatrix point, suggesting the equivalence of effective vacancies and vortices in the $d = 2XY$ model.) The resulting recursion relations are rather simple:

$$\begin{aligned}
&J' = \ln(R_3/R_4), \qquad F' = \ln(R_1 R_3/R_2^2), \qquad G' = G - d \ln(R_1 \tilde{f}/R_3), \\
&R_1 = 1 + q\tilde{f}^{-1} g, \qquad R_2 = 1 + [1 + (q-1)\tilde{x}^{-1}] g, \\
&R_3 = 1 + [1 + (q-1)\tilde{x}^{-2}] \tilde{f} g, \qquad R_4 = 1[2\tilde{x}^{-1} + (q-2)\tilde{x}^{-2}] \tilde{f} g,
\end{aligned} \tag{2}$$

where ($\tilde{J} = \ln \tilde{x}$, $\tilde{F} = \ln f$, $G = \ln g$) and (J', F', G') are respectively the bond-moved and renormalisation interactions. At this point, the condition (Nienhuis and Nauenberg 1975)

$$G' = b^d G \tag{3}$$

(where b is the length-rescale factor) of the first-order fixed point ($G^* = 0$; J^*, $F^* = \infty$) will not be obeyed, because the bond-moving approximation eliminates sites by completely decoupling them from the infinite lattice. This is cured by shrinking the lattice during the bond-moving described above, so that the density of sites is conserved on the infinite lattice. This is akin to the systematic correction introduced in the position-space renormalisation-group study of localisation (Lee 1979). The effect here is to fix the length-rescale factor as

$$b = (1 + d)^{1/d}. \tag{4}$$

† An alternative, but presumably equivalent, procedure maps the $d = 2$ Potts models to $d = 1$ quantum models, and follows by renormalisation (Sólyom and Pfeuty 1980).

The bond-strengthening along the edges is done as

$$\tilde{J} = b^{d-1}J \qquad \text{and} \qquad \tilde{F} = b^{d-1}F, \tag{5}$$

so that the other conditions (Klein *et al* 1976)

$$J' = b^{d-1}J \qquad \text{and} \qquad F' = b^{d-1}F \tag{6}$$

of the first-order fixed point are obeyed. This way of fixing b does not affect the topology of our renormalisation flows.

As in the previous $d = 2$ treatments (Nienhuis *et al* 1979), this renormalisation-group transformation produces a line of critical fixed points, parametrised by $q \leqslant q_c$ and governing the second-order phase transitions, and similarly a line of tricritical fixed points. These critical and tricritical fixed points smoothly merge and annihilate at q_c, clearing the way to a first-order fixed line. The critical and tricritical thermal exponents for $d = 2$ are shown in figure 1. Agreement is satisfactory between this *approximate* calculation of the leading exponent y_2 and the values which are believed to be exact (den Nijs 1979, Nienhuis *et al* 1979). The changeover value $q_c = 3.81$ is obtained, to be compared with the exact value of 4 (Baxter 1973). All exponents exhibit a qualitative resemblance to their $d = 1^+$ behaviour (Berker *et al* 1980). The low-q structure of the critical branch is explained below.

Figure 2 shows the fixed-point locations G^* and the leading exponents y_2 for $d = 1.6$, 1.95, and 2.3. Viewing critical behaviour as a function of q, two other special points are found, such that $0 < q_0 \leqslant q_1 < q_c$. At q_1, the critical behaviour has a non-analyticity. The mechanism behind this is that the critical fixed points, which are stable within the phase boundary surface, occur in the diluted (undiluted) Potts region for $q > q_1$ ($q < q_1$). Below q_0, the non-trivial fixed point of the undiluted Potts limit becomes unstable to the sink ($G^* < \infty$, $J^* = F^* = 0$) of the diluted, disordered phase. We have exhibited, for $q < q_0$, the exponents of this unstable fixed point of the undiluted limit. At $d_0 \simeq 1.95$, $q_0 = q_1 = 1$, the d dependences of q_0 and q_1 are interchanged. For $d < d_0$, $q_0 = 1$ and $1 < q_1 < q_c$. With decreasing d, q_1 increases. As $d \to 1^+$, q_1 diverges as $\exp[\ln 4/(d-1)]$, but the qualitative picture is unchanged since q_c diverges faster as $\exp[2/(d-1)]$. For $d > d_0$, $0 < q_0 < 1$ and $q_1 = 1$. With increasing d, q_0 decreases toward zero. In this approximation, $q_c(d_0) = 4.2$. The distinct existences of undiluted and diluted fixed points were previously noted in variational renormalisation-group calculations (Nienhuis *et al* 1980a, Burkhardt 1980), but their merger and role interchange were not detected.

The occurrence of effective vacancies is favoured for large q and d, as reflected in the $q_c(d)$ phenomenon. Conversely, it is reasonable that the undiluted Potts model is stable at low q and d. On the other hand, we shall argue that the discontinuity in figure 2(f) is a figment of the approximation. At $q = 1$, the lattice-gas component (F, G) of the system recurs independently (Klein *et al* 1978) of the Potts component (J). The tricritical branch intersects the critical fixed point of this $q = 1$ lattice-gas component, $G^* = 0$, $F^* \neq 0$. The present linear transformation gives two lines of fixed points at $q = 1$, $F^* = 0$, $G^* \geq G_c(d)$, $J^* = J^*_{1,2}(G^*)$. As seen in figure 2(e), the critical branch intersects one of the latter fixed lines at finite G^* as $q \to 1^+$, and stability within the phase boundary surface globally shifts to $G^* = \infty$ as $q = 1$ is crossed. However, a nonlinear transformation would have given at $q = 1$, instead of the two fixed lines, two fixed points at $F^* = 0$, $G^* = \infty$ (Nelson and Fisher 1975). Based on this, a reasonable guess for the true $d > d_0$ behaviour is shown in figures 2(e', f'), with the critical branch rapidly but smoothly merging at $q_1 = 1$ from the diluted region to the undiluted limit. Either figure

2(*e*), or figure 2(*e'*) for $d > d_0$, as well as figures 2(*a*, *c*) for $d \leq d_0$, come with a marginal eigenvalue $y_4(q \to 1^+) = 0$, implying, within the context of this approximation, logarithmic corrections to the power law singularities of the percolation problem.

Finally, another shortcoming of the transformation is that, strictly interpreted, the undiluted limit has a non-trivial fixed point even for $q > q_1$, be it unstable to the diluted region. This is because the Migdal–Kadanoff transformation is operationally a decimation, and can only differentially project a many-site property such as effective vacancy occurrence.

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